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Eugenio Pozzoli

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SORBONNE UNIVERSITÉ

ED 386

Laboratoire Jacques Louis Lions, equipe Inria CAGE

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Résumé

La presente these étudie certains problèmes de contrôlabilité, de confinement et de transmission de l'équation de Schrödinger pour certains choix de variétés Riemanniennes. Nous présentons un test de contrôlabilité pour l'équation de Schrödinger bilinéaire à spectre discret qui permet de conclure la contrôlabilité approchée du système en vérifiant la contrôlabilité en dimension finie d'une famille infinie de projections et une condition spectrale faible du système en dimension infinie. Ce test peut être appliqué en particulier à l'étude du problème de la contrôlabilité de l'évolution quantique sur les variétés Riemanniennes, et il est particulièrement adapté aux systèmes à haut degré de symétrie (et donc à de sévères dégénérescences spectrales). Nous spécialisons la technique à l'équation de Schrödinger sur la variété physiquement pertinent SO(3) : de cette façon, nous fournissons une classification des symétries et des propriétés de contrôlabilité de la dynamique rotationnelle quantique des molécules. Le corps rigide symétrique ou asymétrique subit l'interaction entre son moment dipolaire et trois champs électriques orthogonaux comme contrôles, et le problème de contrôlabilité est résolu en termes de moments d'inertie et de configuration dipolaire. Grâce à la structure géométrique qui sous-tend la technique de contrôle, nous obtenons en fait des résultats plus généraux tels que la contrôlabilité approchée de la matrice de densité et la contrôlabilité approchée dans des topologies plus fines.

Notre approche spectrale et algébrique permet également d'identifier les fréquences et les polarisations nécessaires pour contrôler le système : sur la base de ces informations, nous simulons numériquement la dynamique rotationnelle de molécules chirales asymétriques de dimension finie.

En outre, nous nous concentrons sur les propriétés de confinement et de transmission quantiques pour l'équation de Schrödinger sur des variétés presque riemanniens généralisés de dimension deux. Ces structures sont des généralisations naturelles du cylindre de Grushin, et leurs Laplaciens associés contiennent des termes singuliers divergents. Le problème de l'auto-adjonction est d'abord analysé pour le Laplacien de courbure $-\Delta + cK$ sur des variétés presque Riemanniennes en 2D : ici, Δ et K désignent respectivement l'opérateur de Laplace-Beltrami et la courbure Gaussienne de la surface, $c \geq 0$ est une constante, et un tel opérateur est typiquement issu des procédures de quantification géométrique sur les variétés Riemanniennes. Si $c = 0$, le Laplacien Δ est connu pour être essentiellement auto-adjoint : un tel phénomène sur les variétés presque Riemanniennes est généralement appelé confinement quantique, car il implique qu'une particule quantique ne peut pas traverser les singularités de la structure, même si les particules classiques le peuvent. Nous prouvons qu'il n'y a pas de confinement quantique pour l'opérateur Laplacien de courbure, en montrant différentes propriétés des opérateurs de fermeture et adjoint.

Nous considérons ensuite l'opérateur de Laplace-Beltrami Δ_α associé à la structure α-Grushin, pour $\alpha \in [0, 1)$. Cette structure est une variété presque Riemannien généralisé à deux dimensions qui interpole entre le cylindre euclidien et le cylindre de Grushin. Nous classons les extensions locales auto-adjointes de Δ_α, en utilisant la théorie des extensions de Kreĭn-Višik-Birman pour les opérateurs symétriques semi-bornés. Les réalisations auto-adjointes sont caractérisées en termes de différentes conditions aux bords à imposer à la singularité de la structure. Grâce à notre analyse, nous obtenons également la régularité de Sobolev des conditions aux bords locales permises pour les évolutions de Schrödinger bien posées sur la surface anticonique α-Grushin.

Mots clés: Équation de Schrödinger, contrôle quantique, systèmes de contrôle bilinéaires, confinement quantique, approximations de Galerkin, dynamique rotationnelle, molécule symétrique, molécule asymétrique, molécule chirale, équation du corps rigide d'Euler, transfert sélectif d'énantiomères, variété presque Riemanniennes, plan de Grushin, procédures de quantification géométriques, auto-adjonction du Laplacien, opérateurs de Bessel, théorie des extensions auto-adjointes de Kreĭn-Višik-Birman.

Abstract

In this thesis we study some problems of controllability, confinement, and transmission for the Schrödinger equation for some choices of Riemannian manifolds. We present a controllability test for the bilinear discrete spectrum Schrödinger equation that allows to conclude the approximate controllability of the system by checking the controllability of overlapping finite-dimensional projections and a weak spectral condition of the infinite-dimensional system. This test can be applied in particular to study the controllability problem for the quantum evolution on Riemannian manifolds, and it is particularly suited for systems with high degree of symmetry (and hence, severe spectral degeneracies). We specialize the technique to the Schrödinger equation on the physically relevant manifold SO(3): in this way we furnish a classification of the symmetries and the controllability properties of the quantum rotational dynamics of molecules. The symmetric or asymmetric rigid body is experiencing the interaction between its electric dipole moment and three orthogonal electric fields as controls, and the controllability problem is solved in terms of the inertia moments and the dipole configuration. As a byproduct of the geometric structure behind the control technique, we actually obtain stronger results such as approximate controllability of the density matrix and approximate controllability in finer topologies.

Our spectral and Lie algebraic approach also allows the identification of frequencies and polarizations needed to control the system: based on this insight, we numerically simulate the rotational dynamics of finite-dimensional asymmetric chiral molecules.

Further, we concentrate on the properties of quantum confinement and transmission for the Schrödinger equation on two-dimensional generalized almost-Riemannian manifolds. These structures are natural generalizations of the Grushin cylinder, and their associated Laplacians contain diverging singular terms. The problem of self-adjointeness is firstly analyzed for the curvature Laplacian $-\Delta + cK$ on 2D almost-Riemannian manifolds: here Δ and K denote respectively the Laplace-Beltrami operator and the Gaussian curvature of the surface, $c \geq 0$ is a constant, and such an operator typically arises from coordinate-free quantization procedures on Riemannian manifolds. If $c = 0$, the Laplacian Δ is known to be essentially self-adjoint: such a phenomenon on almost-Riemannian manifolds is usually called quantum confinement, as it implies that a quantum particle cannot cross the singularities of the structure, even though classical particles do. We prove that there is no quantum confinement for the curvature Laplacian operator, by showing different properties of the closure and adjoint operators.

We then consider the Laplace-Beltrami operator Δ_α associated with the α-Grushin structure, for $\alpha \in [0, 1)$. This structure is a two-dimensional generalized almost-Riemannian manifold which interpolates between the Euclidean and the Grushin cylinder. We classify the local self-adjoint extensions of Δ_α, using the Kreĭn-Višik-Birman extension theory for semi-bounded symmetric operators. The self-adjoint realizations are characterized in terms of different local boundary conditions to be imposed at the singularity of the structure. As a byproduct of our analysis, we also obtain the Sobolev-regularity of the allowed local boundary conditions for well-posed Schrödinger evolutions on the α-Grushin anti-conic surface.

Keywords: Schrödinger equation, quantum control, bilinear control systems, quantum confinement, Galerkin approximations, rotational dynamics, symmetric-top molecule, asymmetric-top molecule, chiral molecule, Euler rigid body equation, enantiomer-selective population transfer, almost-Riemannian manifolds, Grushin plane, coordinate-free quantization procedures, self-adjointness of the Laplacian, inverse square potential, Kreĭn-Višik-Birman self-adjoint extension theory

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Chapter 1

Introduction

1.1 Controlled and free quantum evolution on Riemannian manifolds

1.1.1 Outline of the subject

Given a quantum particle subject to the (possible time dependent) Schrödinger equation, in this thesis we consider the following type of problems:

- is there a positive probability of finding it at any point of the space?
- by varying the time evolution of the potential via a fine number of parameters, is it possible to drive its wave function from any initial state arbitrarily close to any final state?

The first question can be attacked by trying to prove that the Schrödinger operator is essentially self-adjoint in a subset of the space. The second question is a classical question of controllability. Let us be more precise: the quantum evolution on a Riemannian manifold M with associated Riemannian volume ω is described through its *wave function* ψ, which is an element of the Hilbert space $L^2(M,\omega)$ of norm one. When a system is experiencing a (possibly time-dependent) potential, the evolution in $L^2(M,\omega)$ of the wave function is governed by the Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}\psi(p,t) = H\psi(p,t) + W(p,t)\psi(p,t)\,, \tag{1.1.1}$$

where $H = H_0 + V$ is an operator which stands for the quantization of the kinetic H_0 plus potential V energies, and $W : M \times \mathbb{R} \to \mathbb{R}$ is a potential of interaction with an external field. The usual choice for H_0 is given by $H_0 = -\Delta$, where Δ is the Laplace-Beltrami operator of the Riemannian manifold M. Other choices of H_0 present in the literature, coming from geometric quantizations, are given by $H_0 = -\Delta + cK$, where $c > 0$ is a positive real constant determined by the quantization procedure, and $K : M \to \mathbb{R}$ is the scalar curvature of the Riemannian manifold M (see, e.g., [13]). The operator $H + W$ is in general unbounded, symmetric and defined on the domain $C_0^\infty(M)$ of the smooth functions compactly supported on M. A first natural problem is given by the existence and uniqueness of solutions of the Schrödinger equation (1.1.1). If the potential of interaction W is time-independent, we denote by $\mathcal{D}(\overline{H+W})$ the completion of $C_0^\infty(M)$ w.r.t. the norm induced by $H + W$. The self-adjointness problem for the operator $H + W$ consists in establishing whether the space of functions $f \in L^2(M,\omega)$ such that $(H + W)f \in L^2(M,\omega)$, in the weak sense, coincides with $\mathcal{D}(\overline{H+W})$. As a consequence of a celebrated theorem by Stone [104], it turns out that the symmetry of the operator $H + W$ is not sufficient for a well-posed quantum evolution, since the latter property is equivalent to the essential self-adjointness of $H + W$: there exists a unique solution $\psi(\cdot) \in C^1(\mathbb{R}, L^2(M,\omega))$ to (1.1.1) with $\psi(t) \in \mathcal{D}(\overline{H+W})$ $\forall t \in \mathbb{R}$ if and only if the operator $H + W$ is self-adjoint. Moreover, the solution is implemented via a strongly continuous one-parameter unitary group, given by $\psi(t) = e^{-\mathrm{i}t(H+W)}\psi(0)$.

When the Riemannian manifold M is complete as a metric space, that is, is geodesicaly complete, a theorem by Gaffney states that Δ is essentially self-adjoint [61]. The same property holds for $-\Delta + cK$ if K is bounded; in particular, it holds when M is compact. So, thanks to Stone's and Gaffney's theorems, the free (i.e., in the absence of potentials) quantum evolution on a compact manifold without boundary is well-defined, w.r.t. $H_0 = -\Delta$ and also $H_0 = -\Delta + cK$. The same holds in the presence of bounded potentials.

In this thesis we are also interested in a complementary case, that is, when the manifold M is not complete (and the curvature K is not bounded). Let us figure out a simple one-dimensional example, motivated by singular

operators which we shall encounter later on, to show which different phenomena may occur in this case: consider a quantum particle moving on a punctured line $\mathbb{R} \setminus \{0\}$, and imagine that an inverse square potential $\frac{c}{x^2}$ is applied to the system, with amplitude $c \in \mathbb{R}$. The wave function for this system evolves on the sphere of $L^2(\mathbb{R})$ according to the equation

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = -\frac{\partial^2}{\partial x^2}\psi(x,t) + \frac{c}{x^2}\psi(x,t)\,, \quad \psi(\cdot,0) = \psi_0(\cdot) \in C_0^\infty(\mathbb{R} \setminus \{0\}).$$

We may want to know if there is a positive probability of finding the particle in any point of the space. In particular, if the initial state ψ_0 for this system is supported on one half-line, say $\mathbb{R}^+$, will the wave function spread also on the other half-line $\mathbb{R}^-$ during the evolution? The punctured line is a non-complete manifold, so in the absence of potential we may expect the quantum particle to cross the origin, with a dynamical transmission between $\mathbb{R}^+$ and $\mathbb{R}^-$. On the other hand, the singular behaviour of the inverse square potential at the origin may create a barrier which alters the dynamics. An answer to such a question is furnished by the study of the self-adjointness of the Schrödinger operator $H + W = -\frac{\partial^2}{\partial x^2} + \frac{c}{x^2}$ defined on the half-line with the domain $C_0^\infty(\mathbb{R}^+)$: by regarding the two linearly independent solutions of the stationary Schrödinger equation $-\psi''(x) + \frac{c}{x^2}\psi(x) = 0$ on $\mathbb{R}^+$, a celebrated theory of Weyl called *limit point-limit circle method* [112] implies that such an operator is essentially self-adjoint if and only if $c \geq 3/4$. As a consequence, when $c \geq 3/4$, the Schrödinger evolution is well-defined on $L^2(\mathbb{R}^+)$, and the wave function $\psi(t) = e^{-\mathrm{i}t\overline{(H+W)}}\psi_0$ is supported on $\mathbb{R}^+$ for all $t \in \mathbb{R}$, if $\mathrm{supp}\psi_0 \subset \mathbb{R}^+$. In particular, two wave functions ψ_+ and ψ_- respectively supported on $\mathbb{R}^+$ and $\mathbb{R}^-$ cannot be joined by a trajectory of the systems, and the quantum particle is confined in each half-line. On the other hand, a small variation of the amplitude c may destroy the self-adjointness, implying the possibility for the wave function to spread out the half-line, and also the necessity of some boundary condition at $x = 0$ to describe the interaction between the wave function and the singular potential.

Throughout the thesis we assume that the operators of interaction with the quantum system has the following affine form

$$W(p,t) = u_1(t)B_1(p) + \cdots + u_\ell(t)B_\ell(p)$$

where the B_i are control operators and the functions u_i are piecewise constant control laws. The controllability problem for the Schrödinger equation on a Riemannian manifold consists in establishing whether, for every pair of states ψ_0 and ψ_1 in the sphere of $L^2(M,\omega)$, there exists a choice of piecewise constant control laws $u_1,\dots,u_\ell$ and a time $T \geq 0$ such that the solution to the Schrödinger equation (1.1.1) with initial condition $\psi(0) = \psi_0$ satisfies $\psi(T) = \psi_1$. Such a problem has a negative answer if the control operators B_i are bounded [14, 107], so one has to look for weaker notions of controllability, such as approximate controllability.

Let us describe how such a problem can be analyzed: for simplicity, we consider now a compact manifold M without internal potential, that is $V = 0$. The controllability problem for (1.1.1) can be studied through its finite-dimensional spectral approximations: the compactness of M guarantees that H_0 is essentially self-adjoint, and also that the spectrum $\{\lambda_i\}_{i\in\mathbb{N}} \subset \mathbb{R}$ of H_0 is real discrete with the eigenfunctions $\{\phi_i\}_{i\in\mathbb{N}}$ of H_0 forming an orthogonal Hilbert basis of $L^2(M,\omega)$. Following the paper [27], for any $n \in \mathbb{N}$ one can then project the Schrödinger equation onto the $\mathrm{span}\{\phi_1,\dots,\phi_n\} \cong \mathbb{C}^n$ and study the controllability of the finite-dimensional quantum system

$$\mathrm{i}\frac{d}{dt}\psi(t) = H_0^{(n)}\psi(t) + \sum_{i=1}^{\ell} u_i(t)B_i^{(n)}\psi(t)\,, \quad \psi(t) \in \mathrm{span}\{\phi_1,\dots,\phi_n\}, \tag{1.1.2}$$

where $H_0^{(n)} = \mathrm{diag}(\lambda_1,\dots,\lambda_n)$ and $B_i^{(n)} = (\langle\phi_j, B_i\phi_k\rangle)_{j,k=1}^n$. This can be done in several ways, for example using the Lie-algebraic structure of the equation: (1.1.2) defines a left-invariant control system on the Lie group $U(n)$ for the propagator $U(t)^{(n)} := e^{-\mathrm{i}t(H_0^{(n)}+\sum_{i=1}^{\ell} u_i(t)B_i^{(n)})}$, that is controllable if and only if $\mathrm{Lie}\{\mathrm{i}H_0^{(n)}, \mathrm{i}B_1^{(n)},\dots,\mathrm{i}B_\ell^{(n)}\} = \mathfrak{u}(n)$ [75], where $\mathfrak{u}$ denotes the Lie algebra of $U(n)$. The question is then how to pass from the finite-dimensional to the infinite-dimensional equation. The first assumption needed is the essential self-adjointness of $H_0 + \sum_{i=1}^{\ell} u_iB_i$ on $\mathrm{span}\{\phi_i \mid i \in \mathbb{N}\}$. Then, a condition that guarantees the controllability of (1.1.2) and the (approximate) controllability of (1.1.1) can be given in terms of a non-resonant spectral graph constructed as follows (we recall that the controllability of (1.1.2) for every $n \in \mathbb{N}$ does not imply, in general, the controllability of (1.1.1): see section 3.1.2, example 3, for details). Let us suppose for the sake of simplicity that $\ell = 1$. Define Ξ as the subset of $\mathbb{N}^2$ given by all (k_1,k_2) such that $\langle\phi_{k_1}, B_1\phi_{k_2}\rangle \neq 0$. Assume that for every $(j,k) \in \Xi$ such that $j \neq k$, we have $\lambda_j \neq \lambda_k$ (meaning that degenerate states are not coupled by B_1). If there exists a subset S of Ξ such that the graph whose vertices are the elements of $\mathbb{N}$ and whose edges are the elements of S is connected, and moreover for every $(j_1,j_2) \in S$ and every $(k_1,k_2) \in \Xi$ different from (j_1,j_2) and (j_2,j_1),

$$|\lambda_{j_1} - \lambda_{j_2}| \neq |\lambda_{k_1} - \lambda_{k_2}|, \tag{1.1.3}$$

then the infinite-dimensional system (1.1.1) is approximately controllable. If such a graph exists, we say that the system admits a *non-resonant chain of connectedness*. Notice that, in particular, the existence of a non-resonant chain of connectedness can also be applied to check the controllability of the finite-dimensional approximations as in (1.1.2). Summarizing, the compactness of M (that implies the self-adjointness of H_0 and its discrete spectral decomposition) and the self-adjointness of $H_0 + \sum_{i=1}^{\ell} u_i B_i$ permit to conclude the (approximate) controllability of an infinite-dimensional system, if the following properties hold: (i) the controllability of a family of finite-dimensional systems as in (1.1.2), and (ii) a non-resonant condition (1.1.3) on the spectral gaps of H_0 used for the control.

If the manifold M is not compact, the spectrum of H_0 will not be discrete, but analogous controllability properties hold in the presence of a non-zero potential V, when it is such that the spectrum of $H_0 + V$ is discrete.

1.1.2 Outline of the main contributions of this thesis

In this thesis we follow the approach outlined for the controlled quantum evolution on compact Riemannian manifolds: we present a new spectral Lie-algebraic control condition, which generalizes the non-resonant chain of connectedness technique, and which is deeply related to the *Lie-Galerkin tracking condition* introduced in [28]. We apply it to the Schrödinger equation on the compact Lie group of rotation $M = \mathrm{SO}(3)$. This manifold naturally describes the rotational dynamics of symmetric and asymmetric rigid bodies, so that we refer to this problem as the controllability of the quantum rotational dynamics of symmetric and asymmetric molecules. In this way, we are able to classify the symmetries (i.e., the conserved quantities) and the reachable sets of quantum rotating molecules. We moreover numerically simulate some of our controllability results on rotational dynamics in experimentally relevant finite-dimensional subspaces of chiral asymmetric molecules. Problems of confinement and transmission for free quantum evolutions on singular Riemannian surfaces are then considered. We present a non-self-adjointness result for the curvature Laplacian $H_0 = -\Delta + cK$ on two-dimensional almost-Riemannian manifolds of step 2 (see Section 5.2 for a definition of these structures). We then study the self-adjoint extensions of the Laplace-Beltrami operator $H_0 = -\Delta$ on a collection of α-Grushin surfaces: we characterize four families of local self-adjoint extensions which describe allowed transmissions between the two-halves of the α-cylinder, or in other words boundary conditions that make the free quantum evolutions (1.1.1) well-defined on such singular Riemannian structures.

1.2 A controllability test for the discrete spectrum Schrödinger equation

1.2.1 State-of-the-art

The controllability criteria we discuss in this thesis concern the general framework of the bilinear multi-input Schrödinger equation on an infinite-dimensional Hilbert space $\mathcal{H}$

$$\mathrm{i}\frac{d\psi(t)}{dt} = (H + \sum_{j=1}^{\ell} u_j(t)B_j)\psi(t), \quad \psi(t) \in \mathcal{H}, \tag{1.2.1}$$

with piecewise constant control laws $(u_1, \dots, u_\ell)$ taking values in $U \subset \mathbb{R}^\ell$, being U a neighbourhood of the origin. The main spectral assumptions we need are the following: (i) the operators $H, B_1, \dots, B_\ell$ are self-adjoint; (ii) the operator H has discrete spectrum $\{\lambda_i\}_{i\in\mathbb{N}}$ (with associated eigenfunctions $\{\phi_i\}_{i\in\mathbb{N}}$); (iii) the operator $(H+\sum_{j=1}^{\ell} u_j B_j)$ is essentially self-adjoint on the set of finite linear combinations of eigenfunction of H, given by $\mathrm{span}\{\phi_i \mid i \in \mathbb{N}\}$, for all $u \in U$. Applications to cases of particular interests are, e.g. : (i) $\mathcal{H} = L^2(\Omega)$, where Ω is $\mathbb{R}^d$ or a bounded domain of $\mathbb{R}^d$ and $H = -\Delta + V$ has discrete spectrum, where Δ is the Laplacian (with e.g. Dirichlet boundary condition if Ω is a bounded domain); (ii) $\mathcal{H} = L^2(M, \omega)$, where M is a compact Riemannian manifold, ω is the Riemannian volume, and $H = -\Delta$ is minus the Laplace-Beltrami operator of M; (iii) $\mathcal{H} = L^2(M, \omega)$, where M is possibly not compact and $H = -\Delta + V$ has discrete spectrum; (iv) systems for which H has discrete spectrum and cannot be written as a sum of a Laplacian and a potential (for example, the so called Eberly Law model [81, 25]).

We say that a couple $(j, k) \in \mathbb{N}^2$ is a non-degenerate transition for (H, B_l) if $|\lambda_j - \lambda_k| = |\lambda_m - \lambda_n|$ implies $\{j, k\} = \{m, n\}$ or $\{j, k\} \cap \{m, n\} = \emptyset$ or $\langle \phi_m, B_l\phi_n\rangle = 0$. One of the main ideas behind the controllability criterium of the non-resonant chain of connectedness is the periodic excitation of a given spectral gap of the system: if $\sigma = |\lambda_j - \lambda_k| > 0$ is a spectral gap corresponding to a non-degenerate transition (j, k) for (H, B_l), coupled by B_l (i.e., $\langle \phi_j, B_l\phi_k\rangle \neq 0$), then a control law of the form $u_l(t) = \cos(\sigma t)/K$ induces a transfer of population from the state ϕ_j to the state ϕ_k. This idea, also called by physicists the *rotating wave approximation*, is based on averaging techniques applied to bilinear quantum systems (see, e.g., [41]). Following the paper [28], we thus define for any

$\sigma > 0$, the decoupled control Hamiltonians $\mathcal{E}_\sigma(B_l)$ as

$$\langle \phi_j, \mathcal{E}_\sigma(B_l)\phi_k \rangle = \begin{cases} \langle \phi_j, B_l \phi_k \rangle, & \text{if } |\lambda_j - \lambda_k| = \sigma \\ 0, & \text{otherwise,} \end{cases}$$

and denoting by $\Sigma_n := \{|\lambda_j - \lambda_k|,\ j,k = 1,\dots,n\}$, one can generalize the non-resonant chain of connectedness technique for finite-dimensional quantum systems of the form (1.1.2) as follows: if there exist $\sigma_1,\dots,\sigma_m \in \Sigma_n$ such that

$$\mathrm{Lie}\{\mathrm{i}H^{(n)}, \mathcal{E}_{\sigma_i}(\mathrm{i}B_l^{(n)}) \mid i = 1,\dots,m,\ l = 1,\dots,\ell\} = \mathfrak{u}(n),$$

then (1.1.2) is controllable. Further, to obtain the control of the original infinite-dimensional system, in [28] the authors added a non-resonant condition: one defines Ξ_n as the set of $(\sigma, l) \in \Sigma_n \times \{1,\dots,\ell\}$ such that, for every $N > n$,

$$\mathcal{E}_\sigma(\mathrm{i}B_i^{(N)}) = \left[\begin{array}{c|c} \mathcal{E}_\sigma(\mathrm{i}B_i^{(n)}) & 0 \\ \hline 0 & * \end{array}\right],$$

and hence Ξ_n is the set of frequencies which preserve the finite-dimensional truncations of the original system. Notice that in Ξ_n degenerate transitions are allowed, but only inside $\mathrm{span}\{\phi_1,\dots,\phi_n\}$. Then, if for every n_0 there exists $n \geq n_0$ such that

$$\mathrm{Lie}\{\mathrm{i}H^{(n)}, \mathcal{E}_\sigma(\mathrm{i}B_l^{(n)}), (\sigma, l) \in \Xi_n\} = \mathfrak{u}(n),$$

the Schrödinger evolution (1.2.1) is approximately controllable. The main advantage of this controllability criteria, called the *Lie-Galerkin tracking condition*, is that it allows the drift operator H to have a very degenerate spectrum, as for example in [28] it was applied to prove the approximate controllability of the Schrödinger equation on S^2.

1.2.2 A new controllability test

In this thesis we present a variation of the controllability criterium described above: the idea is to check the controllability of the approximations on a sequence of overlapping subspaces, instead of a sequence of increasing subspaces. This is inspired by symmetry considerations: if there exists an operator $J \neq H$ such that $[H, J] = 0$, it is convenient to project the evolution on the eigenspaces of J. We present here a simplified and more intuitive version, and a more general version in Section 3.1.3 which does not assume the existence of such a commuting operator J.

Let us assume that there exists a self-adjoint (possibly unbounded) operator J, with domain $\mathcal{D}(J)$, such that

- $\mathrm{span}\{\phi_k \mid k \in \mathbb{N}\} \subset \mathcal{D}(J)$,
- J has discrete spectrum and infinitely many distinct eigenvalues (possibly degenerate),
- $J(\mathrm{span}\{\phi_k \mid k \in \mathbb{N}\}) \subset \mathcal{D}(H)$ and J commutes with H on $\mathrm{span}\{\phi_k \mid k \in \mathbb{N}\}$.

Then, there exists an Hilbert basis, which we denote by $\mathcal{B}$, made by eigenvectors of H and J at the same time, that is, if $\phi_k^j \in \mathcal{B}$, then $H\phi_k^j = \lambda_k^j \phi_k^j$ and $J\phi_k^j = \mu^j \phi_k^j$. Denote by m_j the multiplicity of the eigenvalue μ^j, then we can label the basis $\mathcal{B}$ as $(\phi_k^j \mid j \in \mathbb{N}, k = 1, ..., m_j)$.

Consider $\mathcal{H}_j := \mathrm{span}\{\phi_k^j \mid k = 1, ..., m_j\}$, $j \in \mathbb{N}$, which are the eigenspaces of the operator J, and let us denote by

$$\Sigma_{j,j+1} = \{|\lambda_{k'}^{l'} - \lambda_k^l| \mid l, l' \in \{j, j+1\},\ k' = 0, ..., m_{l'},\ k = 0, ..., m_l\}$$

the spectral gaps in the subspace $\mathcal{H}_j \oplus \mathcal{H}_{j+1}$. Moreover, for every $j \in \mathbb{N}$, define the orthogonal projections

$$\begin{aligned} \Pi_{j,j+1} : \mathcal{H} \ni \quad \psi \quad &\mapsto \sum_{\substack{l=j,j+1,\\ k=1,\dots,m_l}} \langle \phi_k^l, \psi \rangle \phi_k^l \in \mathcal{H}, \\ \Pi_{0,j+1} : \mathcal{H} \ni \quad \psi \quad &\mapsto \sum_{\substack{l=0,\dots,j+1,\\ k=1,\dots,m_l}} \langle \phi_k^l, \psi \rangle \phi_k^l \in \mathcal{H}, \end{aligned} \tag{1.2.2}$$

and we define $B_i^{(j,j+1)} := \Pi_{j,j+1} B_i \Pi_{j,j+1}$, and $B_i^{(j+1)} := \Pi_{0,j+1} B_i \Pi_{0,j+1}$, for every $i = 1, ..., l$.

Denote by $\mathfrak{u}(j, j+1)$ the Lie algebra associated with the Lie group of the unitary operators on the space $\mathcal{H}_j \oplus \mathcal{H}_{j+1}$, that is, $\mathfrak{u}(j, j+1) := \mathfrak{u}(m_j + m_{j+1})$. We define

$$\Xi^0_{j,j+1} = \{(\sigma, i) \in \Sigma_{j,j+1} \times \{1, ..., l\} \mid \mathcal{E}_\sigma(\mathrm{i}B_i^{(h)}) = \left[\begin{array}{c|c|c} 0 & 0 & 0 \\ \hline 0 & \mathcal{E}_\sigma(\mathrm{i}B_i^{(j,j+1)}) & 0 \\ \hline 0 & 0 & 0 \end{array}\right] \text{ for every } h > j \},$$

and

$$\Xi^1_{j,j+1} = \{(\sigma, i) \in \Sigma_{j,j+1} \times \{1, ..., l\} \mid \mathcal{E}_\sigma(\mathrm{i}B_i^{(h)}) = \left[\begin{array}{c|c|c} * & 0 & * \\ \hline 0 & \mathcal{E}_\sigma(\mathrm{i}B_i^{(j,j+1)}) & 0 \\ \hline * & 0 & * \end{array}\right] \text{ for every } h > j \},$$

where $\mathcal{E}_\sigma(\mathrm{i}B_i^{(j,j+1)})$ is in the block $j, j+1$. A transition associated with spectral gaps in $\Xi^1_{j,j+1}$ may be resonant to a transitions between two state that are both inside or outside $\mathcal{H}_j \oplus \mathcal{H}_{j+1}$, while a transition associated with spectral gaps in $\Xi^0_{j,j+1}$ may only be resonant to a transition between two state that are both inside $\mathcal{H}_j \oplus \mathcal{H}_{j+1}$. In both sets $\Xi^s_{j,j+1}$, $s = 0, 1$, degenerate transitions are allowed, but only inside $\mathcal{H}_j \oplus \mathcal{H}_{j+1}$.

Let

$$\nu^s_{j,j+1} := \{H^{(j,j+1)}, \mathcal{E}_\sigma(\mathrm{i}B_i^{(j,j+1)}) \mid (\sigma, i) \in \Xi^s_{j,j+1}, \sigma > 0\}, \quad s = 0, 1.$$

Notice that $\nu^0_{j,j+1} \subset \nu^1_{j,j+1} \subset \mathfrak{u}(j, j+1)$. We denote by $\mathrm{Lie}(\nu^s_j)$ the Lie subalgebra of $\mathfrak{u}(n_j)$ generated by the matrices in ν^s_j, $s = 0, 1$, and define $\mathcal{T}_j$ as the minimal ideal of $\mathrm{Lie}(\nu^1_j)$ containing ν^0_j. Then we have the following result:

Theorem 1.2.1. *If $\mathcal{T}_j = \mathfrak{u}(n_j)$ for every $j \in \mathbb{N}$, then* (1.2.1) *is approximately controllable.*

A proof of a more general version of the above controllability test is given in Theorem 3.1.21.

1.3 The controlled Schrödinger equation on SO(3)

In Chapter 3 we apply the controllability test stated in Theorem 1.2.1 to classify the symmetries and the controllability properties of quantum rotational dynamics. We present a study of the Schrödinger equation associated with a rotating rigid body, also named a rotating top, that is a symmetric or asymmetric molecule rotating around its center of mass. The Schrödinger equation is infinite-dimensional, and the approximate controllability is obtained through its finite-dimensional approximations together with weak spectral conditions. The rigid top is experiencing the interaction of three orthogonal electric fields as controls, so that the dynamics is described via the following bilinear multi-input controlled Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}\psi(R, t) = \frac{1}{2}\left(\frac{P_1^2}{I_1} + \frac{P_2^2}{I_2} + \frac{P_3^2}{I_3}\right)\psi(R, t) - \sum_{j=1}^{3} u_j(t)\langle R\delta, e_j\rangle\psi(R, t), \quad \psi(\cdot, t) \in L^2(\mathrm{SO}(3)), \tag{1.3.1}$$

where $\frac{1}{2}\left(\frac{P_1^2}{I_1} + \frac{P_2^2}{I_2} + \frac{P_3^2}{I_3}\right)$ is the rotational Hamiltonian, I_1, I_2, I_3 are the moments of inertia of the molecule, P_1, P_2, P_3 are the angular momentum operators (their differential action is given in (1.3.10)), self-adjoint w.r.t. the Haar measure of SO(3), and $-\langle R\delta, e_i\rangle$ is the interaction Hamiltonian between the electric dipole moment δ of the molecule and the direction e_i of the electric field, $i = 1, 2, 3$ (its action as bounded multiplicative operator is given in (1.3.6)). The Hamiltonian that generates the evolution is also called Stark effect Hamiltonian, and the control law $u = (u_1, u_2, u_3) \in U$ is smooth or piecewise constant and represents an electric field polarized in the three orthogonal direction e_1, e_2, e_3, where $U \subset \mathbb{R}^3$ is a neighbourhood of the origin. Finally, $R \in \mathrm{SO}(3)$ is the matrix which describes the orientation of the molecule in the space.

Rigid molecules are subject to the classification of rigid rotors in terms of their inertia moments $I_1 \leq I_2 \leq I_3$: one distinghuishes asymmetric-tops ($I_1 < I_2 < I_3$), prolate symmetric-tops ($I_1 < I_2 = I_3$), oblate symmetric-tops ($I_1 = I_2 < I_3$), spherical-tops ($I_1 = I_2 = I_3$), and linear-tops ($I_1 = 0$, $I_2 = I_3$).

Rotations can in general couple to vibrations in the so-called ro-vibrational states. In our mathematical analysis, however, we shall restrict ourselves to the rotational states of the molecule, neglecting the vibrations. This approximation is in general well-justified on a physical level, being the rotational and vibrational transitions experienced at different scales. For further details on this subject called in literature the *distortable rotor*, we refer to [68, Chapter 8].

The capability of controlling molecular rotations can be very important in quantum physics and chemistry because of the variety of its applications, starting from well-established ones such as microwave molecular spectroscopy [45], rotational state-selective excitation of chiral molecules [51, 52], and going further to applications

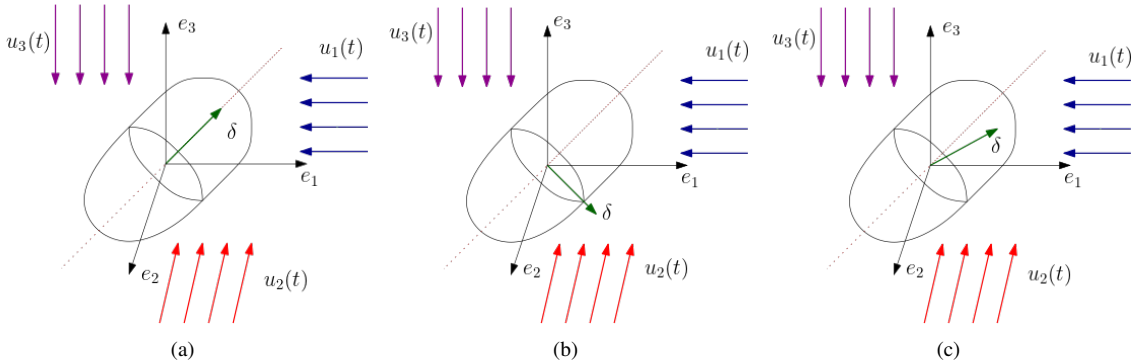


Figure 1.1: Three orthogonal electric fields to control the ellipsoid of inertia of a symmetric rigid molecule with: (a) dipole δ parallel to the symmetry axis; (b) dipole δ orthogonal to the symmetry axis; (c) dipole δ neither parallel nor orthogonal to the symmetry axis. The dipole configurations (a) and (b) correspond to non-controllable quantum systems, due to the presence of different symmetries, after Theorems 3.2.1 and 3.2.11. The dipole configuration (c) is (approximately) controllable, after Theorem 3.2.5.

in quantum information [115, 9]. The general problem on whether molecular rotation is controllable goes back to the early days of quantum control; for example, in the paper [72] crucial ideas were presented and in particular a first prove of the wave-function approximate controllability for a rotating linear-top was proposed. For a general overview on the controllability problem in molecular rotational dynamics we refer also to the review [77], where the controllability problem for the Schrödinger evolution on SO(3) was presented as an open problem, which is solved in this thesis (under non-resonant assumptions on the inertia moments).

1.3.1 State-of-the-art: the controlled Schrödinger equation on S^1 and S^2

Due to its discrete quantization, molecular dynamics perfectly fits the mathematical quantum control theory which has been established until now. In fact, the control of the Schrödinger equation has attracted substantial mathematical interest in the last 15 years (see [11, 16, 29, 67, 76, 93, 17] and references therein). The partial differential equation (1.3.1) is an example of closed quantum system modelled through a bilinear infinite-dimensional multi-input Schrödinger equation of the form (1.2.1). The controllability of (1.2.1) is a well-established topic when the Hilbert space $\mathcal{H}$ is finite-dimensional, thanks to general controllability methods for left-invariant control systems on compact Lie groups (see [74, 75, 54, 65]). When $\mathcal{H}$ is infinite-dimensional and the control operators $B_1, \dots, B_\ell$ are bounded (as in (1.3.1), where $\mathcal{H} = L^2(\mathrm{SO}(3))$ and the control operators are trigonometric polynomials of the Euler's angles, cf. (1.3.6)), it is known that (1.2.1) is not exactly controllable [15, 107]. Hence it is natural to look for weaker controllability properties such as approximate controllability.

Given two vectors ψ_0, ψ_1 in $\mathcal{H}$ of norm one, we say that ψ_1 is approximately reachable from ψ_0 if for any $\epsilon > 0$, there exist a control law u (in a class of admissible functions) and a time $T \geq 0$ such that the solution to the system (1.2.1) with initial condition $\psi(0) = \psi_0$ satisfies $\|\psi(T) - \psi_1\| < \epsilon$. Then (1.2.1) is said to be approximately controllable if, for any ψ in $\mathcal{H}$ of norm one, all unit vectors are approximately reachable from ψ.

Approximate controllability and exact controllability are known to be equivalent conditions for finite-dimensional bilinear quantum systems [29], and more in general for any finite-dimensional bilinear systems as it is proved in the very recent paper [39]. However, this is not the case for infinite-dimensional systems.

Approximate controllability results of (1.2.1) have been obtained with different techniques: adiabatic control [3, 36], Lyapunov methods [87, 92, 93] and Lie-algebraic methods [24, 25, 27, 41, 42, 28, 40, 76].

In particular, the problem of controlling the rotational dynamics of a planar molecule by means of two orthogonal electric fields has been analyzed in [27], where approximate controllability has been proved using a suitable non-resonance property of the spectrum of the rotational Hamiltonian. In [28] the approximate controllability of a linear-top controlled by three orthogonal electric fields has been established. There, a sufficient condition for controllability, called the Lie-Galerkin tracking condition, has been introduced in an abstract framework and applied to the linear-top system; such a condition is based on the controllability of the finite-dimensional approximations combined with weak spectral conditions which permits to treat severe degenerate and resonant spectra. Let us recall these two models already studied in the literature.

- **Planar molecule** The system of a planar bipolar molecule interacting with two orthogonal controls is

modelled by the following bilinear controlled Schrödinger equation on the circle S^1:

$$\text{(1.3.2)} \qquad \mathrm{i}\frac{\partial}{\partial t}\psi(\alpha,t) = \left[-\frac{\partial^2}{\partial\alpha^2} + u_1(t)\cos(\alpha) + u_2(t)\sin(\alpha)\right]\psi(\alpha,t)\,, \quad \psi(\cdot,t)\in L^2(S^1),$$

where $\alpha \in [0, 2\pi)$ is the coordinate on the circle, related to the Euclidean coordinates through the identities

$$x = \cos(\alpha), \quad y = \sin(\alpha).$$

This equation has been proved to be approximately controllable in [27, Proposition 8.2], using a technique

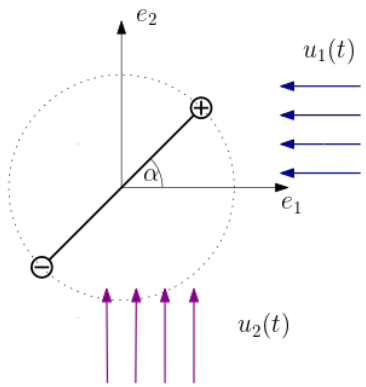


Figure 1.2: Two orthogonal electric fields to control the rotation of a linear bipolar molecule confined to a plane. Its rotation is (approximately) controllable, after [27].

based on the existence of a non-resonant connected chain in the spectrum of the drift $H := -\frac{\partial^2}{\partial\alpha^2}$.

Let us point out that the spectrum of H is given by $\{E_k = k^2 \mid k \in \mathbb{Z}\}$, which is degenerate, as $E_k = E_{-k}$ and an Hilbert basis made of eigenfunctions of H is given by the trigonometric functions $\{e^{\mathrm{i}k\alpha}/\sqrt{2\pi} \mid k \in \mathbb{Z}\}$. The eigenspace corresponding to the degenerate eigenvalue E_k, $k \geq 1$, is spanned by the pair of functions $\{\phi_k := \cos(k\alpha)/\sqrt{\pi}, \phi_{-k} := \sin(k\alpha)/\sqrt{\pi}\}$. The control fields are given by the bounded multiplicative operators $B_1 := \cos(\alpha)$ and $B_2 := \sin(\alpha)$.

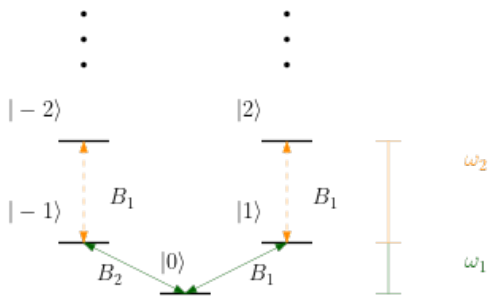


Figure 1.3: Spectral graph associated with a planar linear-top: transitions at frequencies $\omega_1 := |E_1 - E_0|$ and $\omega_2 := |E_2 - E_1|$, between states $|k\rangle := \phi_k$, for $k = -2, \ldots, 2$, driven by B_1 or B_2. Same-shaped arrows correspond to equal spectral gaps.

In the example 3 of chapter 3 we show that this system satisfies the Lie-Galerkin tracking condition. This implies that it is approximately controllable, and also satisfies stronger properties such as approximate controllability in the sense of density matrices, by means of piecewise constant and smooth controls $u_1, u_2 \in [-\delta, \delta]$, for any $\delta > 0$.

- **Linear molecule** The system of a linear bipolar molecule interacting with three orthogonal controls is modelled by the following bilinear controlled Schrödinger equation on the sphere S^2:
(1.3.3)
$$\mathrm{i}\frac{\partial}{\partial t}\psi(\alpha,\beta,t) = \big[-\Delta + u_1(t)\sin(\beta)\cos(\alpha) + u_2(t)\sin(\beta)\sin(\alpha) + u_3(t)\cos(\beta)\big]\psi(\alpha,\beta,t)\,, \quad \psi(\cdot,\cdot,t)\in L^2(S^2),$$

where $(\alpha, \beta) \in [0, 2\pi) \times [0, \pi]$ are the spherical coordinates, related to the Euclidean coordinates through the identities

$$x = \sin(\beta)\cos(\alpha), \quad y = \sin(\beta)\sin(\alpha), \quad z = \cos(\beta),$$

and

$$\Delta = \frac{1}{\sin(\beta)}\frac{\partial}{\partial\beta}\left(\sin(\beta)\frac{\partial}{\partial\beta}\right) + \frac{1}{\sin^2(\beta)}\frac{\partial^2}{\partial\alpha^2}$$

is the Laplace-Beltrami operator of $S^2 \subset \mathbb{R}^3$. The interaction Hamiltonians $B_1 := \sin(\beta)\cos(\alpha), B_2 := \sin(\beta)\sin(\alpha), B_3 := \cos(\beta)$ are sometimes called in the physical and chemical literature, resp., x-,y-, and z-polarization of the electric field.

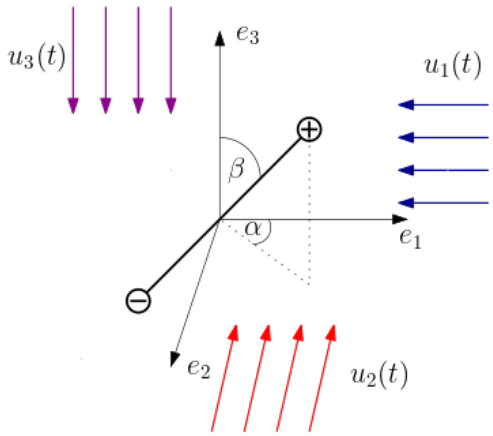


Figure 1.4: Three orthogonal electric fields to control the rotation of a linear molecule in $\mathbb{R}^3$. The diagram represents, e.g., the hydrogen chloride molecule HCl. Its rotation is (approximately) controllable, after [28].

System (1.3.3) has been proved to be approximately controllable, and satisfy stronger properties (e.g., it is a modulus tracker [28, Theorem 3.1]), by means of piecewise constant [28, Theorem 2.8] and smooth [40, Theorem 2.7] controls $u_1, u_2, u_3 \in [-a, a]$, for any $a > 0$. In fact, it has been proved to satisfy the Lie-Galerkin tracking condition in [28, Lemma 3.2]. Let us point out some spectral properties of the drift $-\Delta$: its spectrum is given by the set of eigenvalues $\{E_j := j(j+1) \mid j \in \mathbb{N}\}$, and the associated eigenfunctions are the spherical harmonics $\{Y_m^j(\alpha, \beta) \mid j \in \mathbb{N},\ m = -j, \dots, j\}$. The spherical harmonics satisfy the following partial differential equations:

$$\begin{aligned} -\Delta\, Y_m^j &= j(j+1)\, Y_m^j\,, \quad m = -j, \dots, j \\ J_3\, Y_m^j &= m\, Y_m^j \end{aligned} \tag{1.3.4}$$

where the operator $J_3 := -\mathrm{i}\frac{\partial}{\partial\alpha}$ is the third component of the angular momentum. From (1.3.4) we see that each E_j, $j \geq 1$, is degenerate with associated $(2j+1)$-dimensional eigenspace spanned by $\{Y_m^j(\alpha, \beta) \mid m = -j, \dots, j\}$.

Even if non-resonant chains of connectedness may be constructed for degenerate systems, an unbounded amount of degeneracies make in practice very hard the application of this technique in order to get controllability results, since an unbounded amount of transitions occur at the same frequency.

As we shall see in the next section, system (1.3.3) can be realized as a subsystem of the symmetric molecule.

1.3.2 New results: symmetries and controllability on SO(3)

In this thesis, we study the symmetric- and asymmetric-top as a generalization of the linear one, characterizing its controllability in terms of the position of its electric dipole moment, fixed inside the molecular frame. While for the linear-top two quantum numbers j, m are needed to describe the motion, the main and more evident difference here is the presence of a third quantum number k, which for symmetric-tops classically represents the projection of the total angular momentum on the symmetry axis of the molecule. This should not be a surprise, since the configuration space of a linear-top is the 2-sphere S^2, while symmetric- and asymmetric-tops evolve on the Lie group SO(3), a three-dimensional manifold. As a matter of fact, by fixing $k = 0$, one recovers the linear-top as a subsystem inside the symmetric-top. It is worth mentioning that the general theory developed in [27, 42, 93] is

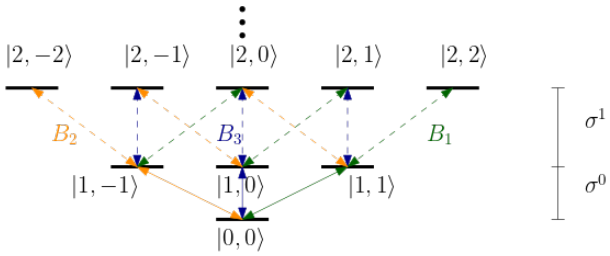


Figure 1.5: Spectral graph associated with a spherical linear-top: transitions at frequencies $\sigma^0 := |E_1 - E_0|$ and $\sigma^1 := |E_2 - E_1|$, between the eigenstates $|j, m\rangle := Y_m^j$, driven by B_1, B_2, and B_3. Same-shaped arrows correspond to equal spectral gaps.

based on non-resonance conditions on the spectrum of the internal Hamiltonian. A major difficulty in studying the controllability properties of the rotational dynamics is that, even in the case of the linear-top, the spectrum of the rotational Hamiltonian has severe degeneracies at the so-called m-levels. The symmetric-top is even more degenerate, due to the additional degeneracy of the so-called k-levels.

We shall first study the symmetric-top, and set $I_1 = I_2$. Anyway, our analysis does not depend on whether $I_3 \geq I_2$ or $I_3 \leq I_2$, so we are actually treating in this way both the cases of a prolate, spherical, or oblate symmetric-top. The principal axis of inertia with associated inertia moment I_3 is then called *symmetry axis* of the molecule. The position of the electric dipole with respect to the symmetry axis plays a crucial role in our controllability analysis: a symmetric molecule with electric dipole collinear to the symmetry axis will be called *genuine*, otherwise it will be called *accidental* ([68, Section 2.6]). Most symmetric molecules present in nature are genuine. The diagram of a genuine symmetric top is given in figure 1.7 and corresponds to the CH_3Cl molecule. Nevertheless, it can happen that two moments of inertia of a real molecule are almost equal, by "accident", although the molecule does not possess a n-fold axis of symmetry with $n \geq 3$.[1]For instance, the inertia moments of the molecule $HSOH$ are $I_1 \sim I_2 \ll I_3$, while its dipole components are $\delta_1 > \delta_2 = \delta_1/2 \gg \delta_3 \neq 0$ [113]. Such slightly asymmetric-tops are often studied in chemistry and physics in their symmetric-top approximations (see, e.g., [113],[68, Section 3.4]), which correspond in general to accidentally symmetric-tops. The diagram of an orthogonal (i.e. $\delta_3 = 0$) accidentally symmetric-top is given in figure 1.3.2 and corresponds to the symmetric top approximation of the D_2S_2 molecule.

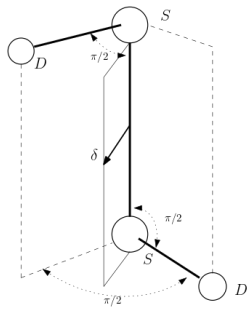


Figure 1.6: Diagram of the orthogonal accidentally symmetric-top approximation of the molecule D_2S_2. Its rotation is not controllable, after Theorem 3.2.11, as the electric dipole δ lies in the orthogonal plane to the symmetry axis.

For the rotational Hamiltonian of a symmetric-top, closed expression for the spectrum and the eigenfunctions are known. Beside its own interest, the accidentally symmetric-top is then used in this thesis to obtain controllability of asymmetric-tops with a perturbative approach. The idea of studying the controllability of quantum systems in general configurations starting from symmetric cases (even if the latter have more degeneracies) has already been exploited, e.g., in [31, 85].

The position of the electric dipole moment turns out to play a decisive role: when it is neither along the symmetry axis, nor orthogonal to it, as in Figure 1.1(c), then approximate controllability holds, under a suitable

[1]The existence of a n-fold axis of symmetry (i.e., an axis such that a rotation of angle $2\pi/n$ about it leaves unchanged the distribution of atoms in the space) with $n \geq 3$, implies that the top is genuine symmetric. This can be visualized by rotating the ellipsoid of inertia: if a rotation of angle $2\pi/n$, with $n \geq 3$, is a symmetry then the planar sections orthogonal to the axis of symmetry are circles, implying the equality of two inertia moments.

non-resonance condition, as it is stated in Theorem 3.2.5 for symmetric-tops; for asymmetric-tops, approximate controllability holds when the dipole is not along any principal axis of inertia, as it is stated in Theorem 3.3.2. To prove both Theorems, we apply the new controllability test for the discrete spectrum Schrödinger equation introduced in Section 1.2.2. The control strategy for the symmetric molecule is based on the excitation of the system with external fields in resonance with three families of frequencies (cf. (3.2.11), (3.2.12), and (3.2.13)), corresponding to internal spectral gaps. One frequency is used to overcome the m-degeneracy in the spectrum (Appendix 3.4.1), and this step is quite similar to the proof of the linear-top approximate controllability [28, proof of Lemma 3.2]. The other two frequencies are used in a next step to break the k-degeneracy, in a three-wave mixing scheme (Appendix 3.4.2) typically addressed in microwave molecular spectroscopy to obtain enantiomer-selective population transfer in chiral molecules (see, e.g., [82]).

Concerning symmetric tops, the two dipole configurations to which Theorem 3.2.5 does not apply are extremely relevant from the physical point of view. Indeed, the dipole moment of a symmetric-top lies usually along its symmetry axis (Figure 1.1(a), see also the diagram of the genuine symmetric molecule CH_3Cl in Fig. 1.7), and if not, for accidentally symmetric-tops, it is often found in the orthogonal plane (Figure 1.1(b), see also the diagram of the orthogonal accidentally symmetric molecule D_2S_2 in Fig. 1.3.2). Here two different symmetries arise, implying the non-controllability of these systems, as we prove, respectively, in Theorems 3.2.1 and 3.2.11.

Concerning asymmetric tops, the three dipole configurations (i.e., dipole along one of the principal axis of inertia) that lead to conserved quantities and lack of controllability (see Theorem 3.3.1) are less relevant from a physical point of view, as asymmetric rotors may naturally be more complex objects and have in general non-vanishing dipole components along the three principal axis of inertia. For example, our numerical simulations of rotational dynamics (cf. Sec. 4.4) are carried on the models of the carvone and the propanediol molecules, which are asymmetric molecules with three non-vanishing dipole components. So, in particular, our study singles out an important obstruction in the controllability problem of symmetric molecules, and gives a positive answer to the controllability problem of asymmetric molecules. Nonetheless, it is worth noting that there exist in nature very simple and important asymmetric molecules whose rotational dynamics we prove to be non-controllable: for example the water molecule H_2O, due to its simple structure, has dipole moment lying along the axis of greatest moment of inertia (Figure 1.9), and it is thus non-controllable after Theorem 3.3.1 (i). It is also worth mentioning the fact that our theoretical and qualitative analysis does not take into account the time needed for the transfer of rotational population: due to the presence of quasi-resonant transitions in the spectrum of asymmetric-top rotational Hamiltonians, this time might be large and experimentally unrealistic w.r.t. the time limit given by decoherence and dissipative phenomena; such a problem deserves to be addressed more in details, starting from finite-dimensional Hilbert subspaces.

Let us discuss more in detail the controlled bilinear Schrödinger PDEs which describe rotating symmetric and asymmetric molecules, and summarize our new results on these systems.

- **Symmetric molecule** The system of a rotating symmetric molecule interacting with three orthogonal controls is modelled via the following bilinear controlled Schrödinger equation on the rotation group SO(3):

$$\begin{aligned} \mathrm{i}\frac{\partial}{\partial t}\psi(\alpha,\beta,\gamma,t) &= \left(\frac{1}{2I_2}P^2+\left(\frac{1}{2I_3}-\frac{1}{2I_2}\right)P_3^2\right)\psi(\alpha,\beta,\gamma,t) \\ &- \sum_{l=1}^{3} u_l(t)\langle R(\alpha,\beta,\gamma)\delta, e_l\rangle\psi(\alpha,\beta,\gamma,t), \quad \psi(\cdot,\cdot,\cdot,t)\in L^2(\mathrm{SO}(3)), \end{aligned} \tag{1.3.5}$$

where $(\alpha,\beta,\gamma)\in[0,2\pi)\times[0,\pi]\times[0,2\pi)$ are the Euler angles, $I_1=I_2, I_3$ are the moments of inertia of the molecule, $\delta=(\delta_1,\delta_2,\delta_3)^T$ is the electric dipole expressed in the rotating frame, and $R(\alpha,\beta,\gamma)\in\mathrm{SO}(3)$ specifies the configuration of the molecule in the space (being $e_1,e_2,e_3\in\mathbb{R}^3$ the canonical basis). The electric dipole is transformed into a vector expressed in the fixed frame through the identities

$$x=-\langle R(\alpha,\beta,\gamma)\delta,e_1\rangle, \quad y=-\langle R(\alpha,\beta,\gamma)\delta,e_2\rangle, \quad z=-\langle R(\alpha,\beta,\gamma)\delta,e_3\rangle,$$

or more explicitly

$$\begin{aligned} x &= -(\cos\alpha\cos\beta\cos\gamma-\sin\alpha\sin\gamma)\delta_1+(\cos\alpha\cos\beta\sin\gamma-\sin\alpha\cos\gamma)\delta_2-(\cos\alpha\sin\beta)\delta_3 \\ y &= -(\sin\alpha\cos\beta\cos\gamma+\cos\alpha\sin\gamma)\delta_1+(\sin\alpha\cos\beta\sin\gamma+\cos\alpha\cos\gamma)\delta_2-(\sin\alpha\sin\beta)\delta_3 \\ z &= (\sin\beta\cos\gamma)\delta_1-(\sin\beta\sin\gamma)\delta_2-(\cos\beta)\delta_3. \end{aligned} \tag{1.3.6}$$

The bounded operators of multiplication $B_i := -\langle R(\alpha,\beta,\gamma)\delta, e_i\rangle$, $i = 1,2,3$, are called the x-, y- and z-polarizations of the electric field. Notice that, if $\delta = (0,0,\delta_3)^T$ (i.e., the dipole is parallel to the symmetry axis of the molecule), we recover the interaction of a linear top with the controls. In particular, the third angular variable γ (which describes the rotation around the symmetry axis) disappears from the controls, suggesting that this configuration of the dipole is non-controllable.

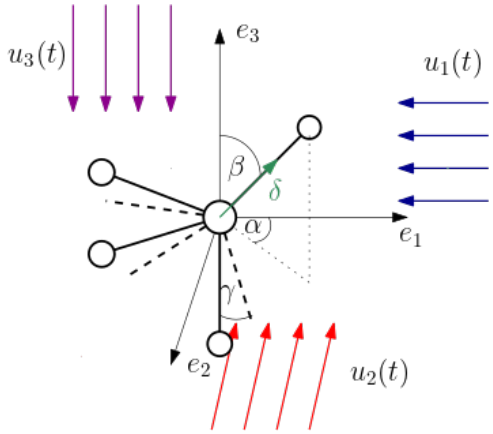


Figure 1.7: Three orthogonal electric fields to control the rotation of a symmetric molecule in $\mathbb{R}^3$. The diagram represents, e.g., the chlorometane molecule CH_3Cl. Its rotation is not controllable, after Theorem 3.2.1, as the electric dipole δ is parallel to the symmetry axis of the molecule.

The drift $H := \left(\frac{1}{2I_2}P^2 + \left(\frac{1}{2I_3} - \frac{1}{2I_2}\right)P_3^2\right)$ is obtained from the rotational Hamiltonian $H = \frac{1}{2}\left(\frac{P_1^2}{I_1} + \frac{P_2^2}{I_2} + \frac{P_3^2}{I_3}\right)$ after having imposed the symmetry condition $I_1 = I_2$ (being $P^2 := P_1^2 + P_2^2 + P_3^2$), and as a differential operator in Euler's coordinates reads

$$H = -\frac{1}{I_2}\left[\frac{1}{\sin(\beta)}\frac{\partial}{\partial\beta}\left(\sin(\beta)\frac{\partial}{\partial\beta}\right) + \frac{1}{\sin^2(\beta)}\left(\frac{\partial^2}{\partial\alpha^2} + \frac{\partial^2}{\partial\gamma^2} - 2\cos(\beta)\frac{\partial^2}{\partial\alpha\partial\gamma}\right)\right] - \left(\frac{1}{2I_3} - \frac{1}{2I_2}\right)\frac{\partial^2}{\partial\gamma^2}.$$

Notice that its action on functions which do not depend on the third angular variable γ is $-1/I_2$-times the action of the Laplace-Beltrami Δ of the sphere S^2. Its spectrum is given by the set of eigenvalues $\{E_k^j := \frac{j(j+1)}{2I_2} + \left(\frac{1}{2I_3} - \frac{1}{2I_2}\right)k^2 \mid j \in \mathbb{N}, k = -j,\dots,j\}$ and the associated eigenfunctions are the Wigner D-functions $\{D_{k,m}^j(\alpha,\beta,\gamma) \mid j \in \mathbb{N},\ m,k = -j\dots,j\}$. The Wigner D-functions satisfy the following partial differential equations:

$$\begin{aligned} P^2\, D_{k,m}^j &= j(j+1)\, D_{k,m}^j, \quad m = -j,\dots,j \\ J_3\, D_{k,m}^j &= m\, D_{k,m}^j, \\ P_3\, D_{k,m}^j &= k\, D_{k,m}^j, \end{aligned}$$

where P^2 is given in the squared brackets of H, $J_3 := -\mathrm{i}\frac{\partial}{\partial\alpha}$, and $P_3 := -\mathrm{i}\frac{\partial}{\partial\gamma}$. In quantum mechanics, P^2 is interpreted as the squared norm of the angular momentum, J_3 is the projection of the angular momentum along the space fixed third axis, and P_3 is the projection of the angular momentum along the molecule fixed third axis. We remark that, as in classical mechanics the rigid body has an additional third degree of freedom (the angle γ) w.r.t. the motion on the sphere, in quantum mechanics this additional degree of freedom is represented by the additional quantum number k. Hence, the eigenvalue equation for the drift reads

$$\left[\frac{1}{2I_2}P^2 + \left(\frac{1}{2I_3} - \frac{1}{2I_2}\right)P_3^2\right] D_{k,m}^j = \left[\frac{j(j+1)}{2I_2} + \left(\frac{1}{2I_3} - \frac{1}{2I_2}\right)k^2\right] D_{k,m}^j, \quad m = -j,\dots,j \tag{1.3.7}$$

from which we see that each E_k^j, $j \geq 1$ and $k \neq 0$, is $(2j+1)$-degenerate w.r.t. m and 2-degenerate w.r.t. k, with associated eigenspace spanned by $\{D_{l,m}^j(\alpha,\beta,\gamma) \mid m = -j\dots,j,\ l = k,-k\}$. We remark that $D_{0,m}^j = Y_m^j$, and in this sense we recover the linear molecule as the evolution described by (1.3.5), w.r.t. the dipole $\delta = (0,0,\delta_3)$, on the Hilbert subspace spanned by the spherical harmonics $\{Y_m^j \mid j \in \mathbb{N},\ m = -j,\dots,j\}$.

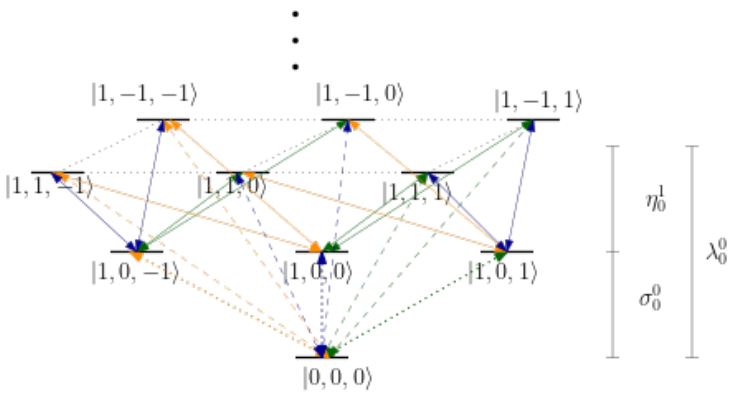


Figure 1.8: Three-dimensional spectral graph associated with a symmetric-top: transitions at frequencies $\lambda_0^0 := |E_1^1 - E_0^0|$, $\sigma_0^0 := |E_0^1 - E_0^0|$, and $\eta_0^1 = |E_1^1 - E_0^1|$ between the eigenstates $|j,k,m\rangle := D^j_{k,m}$, driven by B_1 (green arrows), B_2 (orange arrows), and B_3 (blue arrows). Same-shaped arrows correspond to equal spectral gaps.

In this thesis we classify the controllability and the symmetries of (1.3.5) depending on δ, by applying the controllability test introduced in section 1.2.2 (see also Theorem 3.1.21). More precisely, we prove that:

(i) If $\delta = (0,0,\delta_3)^T$, (1.3.5) is not controllable. More precisely, there exists a decomposition in orthogonal invariant Hilbert sub-spaces $L^2(\mathrm{SO}(3)) = \bigoplus_{k\in\mathbb{Z}} \mathcal{S}_k$ (see Theorem 3.2.1) which are also the simultaneously approximately reachable sets (see Theorem 3.2.3).

(ii) If $\delta = (\delta_1,\delta_2,0)^T$, (1.3.5) is not controllable. More precisely, there exists a decomposition in orthogonal invariant Hilbert sub-spaces $L^2(\mathrm{SO}(3)) = \mathcal{L}_e \oplus \mathcal{L}_o$ (see Theorem 3.2.11) which are also the simultaneously approximately reachable sets (see Theorem 3.2.12), when $\frac{I_2}{I_3} \notin \mathbb{Q}$.

(iii) If $\delta \neq (0,0,\delta_3)^T, (\delta_1,\delta_2,0)^T$, (1.3.5) is a modulus-tracker, when $\frac{I_2}{I_3} \notin \mathbb{Q}$ (see Theorem 3.2.5). In particular, it is approximately controllable in the sense of wave-functions, and in the sense of density matrices, by means of piecewise constant or smooth controls $u_1,u_2,u_3 \in [-a,a]$, for any $a > 0$. It is also approximately controllable in higher H^s-norms.

We remark that our proof does not use a perturbative approach to lift the spectral degeneracies in the drift. Anyway, a perturbation at first order may lead to a result similar to (iii): despite evident difficulties in finding non-resonant chains of connectedness, one may study a first or higher order perturbation of the Lie algebra generated by a perturbed drift and the control operators. In fact, if one considers $\epsilon > 0$ and the Stark effect Hamiltonian $\widetilde{H} := H + \epsilon B_3$, then its spectrum is given by the analytic curves $\{E^j_{k,m}(\epsilon) \mid j \in \mathbb{N}, k,m = -j,\dots,j\}$, and it is less degenerate than the one of H: indeed several degeneracies are lifted at first order, as we have [68, Chapter 10]

$$\frac{d}{d\epsilon}\Big|_{\epsilon=0} E^j_{k,m}(0) = \langle D^j_{k,m}, B_3 D^j_{k,m}\rangle = -\delta_3 \frac{km}{j(j+1)} \,. \tag{1.3.8}$$

Thus, for example, in Figure 1.8 the unperturbed eigenstates $|1,1,1\rangle$ and $|1,-1,1\rangle$ have the same energy $E^1_1 = E^1_{-1}$, but after the application of a constant electric field of magnitude ϵ and polarization z the state $|1,-1,1\rangle$ goes up and $|1,1,1\rangle$ goes down (after (1.3.8)), lifting the degeneracy at $k = 1,-1$. In this way one easily finds non-resonant connected chains in the spectrum of $\widetilde{H}$ for $j = 0,1$, for example, or equivalently a computation shows that the first order Lie algebra generated by $\mathrm{i}(H^{(0,1)}+\epsilon B_3^{(0,1)})$, $\mathrm{i}B_1^{(0,1)}$, $\mathrm{i}B_2^{(0,1)}$ is $\mathfrak{su}(10)$, where $A^{(0,1)}$ denotes the operator $\Pi_{0,1}A\Pi_{0,1}$, and $\Pi_{j,j+1} : L^2(\mathrm{SO}(3)) \to \mathrm{span}\{D^l_{k,m} \mid l = j, j+1,\ k,m = -l,\dots,l\}$ is the orthogonal projection. A general perturbative proof that works for any j is an open challenge.

We finally remark that such a perturbative controllability proof, for the rotational spectrum of rigid rotors, may be interesting for physicists and chemists, as it would represent a mathematical confirmation of a well-established experimental technique. In fact, the application of a small constant electric field in order to detect a splitting in the rotational energies has been widely used in experiments of microwave molecular spectroscopy for more than 70 years [45].

- **Asymmetric molecule** The system of a rotating symmetric molecule interacting with three orthogonal

controls is modelled via the following bilinear controlled Schrödinger equation on the rotation group SO(3):

$$
\begin{aligned}
(1.3.9) \qquad \mathrm{i}\frac{\partial}{\partial t}\psi(\alpha,\beta,\gamma,t) &= \frac{1}{2}\left(\frac{P_1^2}{I_1}+\frac{P_2^2}{I_2}+\frac{P_3^2}{I_3}\right)\psi(\alpha,\beta,\gamma,t) \\
&- \sum_{l=1}^{3} u_l(t)\langle R(\alpha,\beta,\gamma)\delta, e_l\rangle\psi(\alpha,\beta,\gamma,t), \quad \psi(\cdot,\cdot,\cdot,t)\in L^2(\mathrm{SO}(3)),
\end{aligned}
$$

where $I_1 < I_2 < I_3$ are the moments of inertia of the molecule. Everything is defined as for the symmetric molecule, but the drift is more general. The angular momentum operators in Euler's coordinates are given by the differential operators:

$$
\begin{aligned}
P_1 &= -\mathrm{i}\cos\gamma\frac{\cos\beta}{\sin\beta}\frac{\partial}{\partial\gamma} + \mathrm{i}\frac{\cos\gamma}{\sin\beta}\frac{\partial}{\partial\alpha} - \mathrm{i}\sin\gamma\frac{\partial}{\partial\beta}, \\
P_2 &= \mathrm{i}\sin\gamma\frac{\cos\beta}{\sin\beta}\frac{\partial}{\partial\gamma} - \mathrm{i}\frac{\sin\gamma}{\sin\beta}\frac{\partial}{\partial\alpha} - \mathrm{i}\cos\gamma\frac{\partial}{\partial\beta}, \\
P_3 &= -\mathrm{i}\frac{\partial}{\partial\gamma}.
\end{aligned}
$$

(1.3.10)

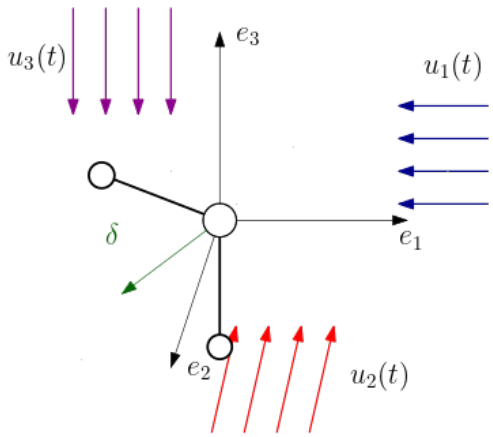


Figure 1.9: Three orthogonal electric fields to control the rotation of an asymmetric molecule in $\mathbb{R}^3$. The diagram represents, e.g., the water molecule H_2O. Its rotation is not controllable, after Theorem 3.3.1 (i), as the electric dipole $\delta = (0,0,\delta_3)^T$ is parallel to the axis of greatest inertia moment.

The spectral properties of the drift $H = \frac{1}{2}\left(\frac{P_1^2}{I_1}+\frac{P_2^2}{I_2}+\frac{P_3^2}{I_3}\right)$ can be deduced via symmetry considerations and perturbation techniques from the ones of the symmetric molecule (see figure 1.10). For a spectral graph of an asymmetric top, with eigenstates transitions at different frequencies, see figure 4.1 in chapter 4. In general, j and m are still good quantum numbers for asymmetric molecules, while k is no longer defined. The spectrum of H is given by the set of eigenvalues $\{E_\tau^j \mid j\in\mathbb{N}, \tau = -j,\dots,j\}$ and each E_τ^j is $(2j+1)$-degenerate w.r.t. m, but the k-degeneracy, typical of symmetric molecules, is lifted. It is worth noting that here τ is an index, and does not represent any physical observable (i.e., it is not a quantum number). The eigenfunctions of H are given by

$$
\Psi_{\tau,m}^j(\alpha,\beta,\gamma) = \sum_{k=-j,\dots,j} c_{k,m}^j(\tau) D_{k,m}^j(\alpha,\beta,\gamma),
$$

and the eigenspace corresponding to the degenerate eigenvalue E_τ^j, $j\geq 1$, is spanned by $\{\Psi_{\tau,m}^j \mid m = -j,\dots,j\}$.

In this thesis we classify the controllability and the symmetries of (1.3.9) depending on δ, by applying the controllability test introduced in section 1.2.2 (see also Theorem 3.1.21) and an analytic perturbative expansion from an associated symmetric molecule. More precisely, we prove that:

(i) If $\delta = (0,0,\delta_3)^T$, (1.3.9) is not controllable. More precisely, there exists a decomposition in orthogonal invariant Hilbert sub-spaces $L^2(\mathrm{SO}(3)) = \mathcal{K}_e \oplus \mathcal{K}_o$ (see Theorem 3.3.1 (i)).

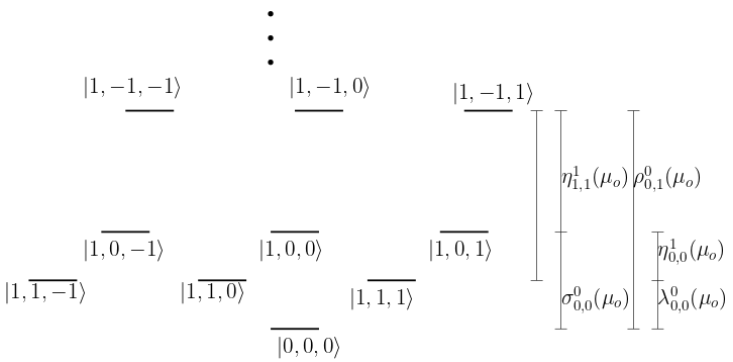


Figure 1.10: Three-dimensional spectral graph associated with an asymmetric-top. The frequencies $\eta^1_{1,1}(\mu_o)$, $\rho^0_{0,1}(\mu_o)$, $\sigma^0_{0,0}(\mu_o)$, $\eta^1_{0,0}(\mu_o)$, and $\lambda^0_{0,0}(\mu_o)$ between the eigenstates $|j,\tau,m\rangle := \Psi^j_{\tau,m}$ are defined in (3.3.10)-(3.3.13) as analytic perturbations, w.r.t. the asymmetry parameter $\mu_o = \frac{A-B}{2C-B-A} \in [-1,0]$, of symmetric top's spectral gaps (where $A = 1/(2I_1)$, $B = 1/(2I_2)$ and $C = 1/(2I_3)$).

(ii) If $\delta = (\delta_1, 0, 0)^T$, (1.3.9) is not controllable. More precisely, there exists a decomposition in orthogonal invariant Hilbert sub-spaces $L^2(\mathrm{SO}(3)) = \mathcal{L}_e \oplus \mathcal{L}_o$ (see Theorem 3.3.1 (ii)).

(iii) If $\delta = (0, \delta_2, 0)^T$, (1.3.9) is not controllable. More precisely, there exists a decomposition in orthogonal invariant Hilbert sub-spaces $L^2(\mathrm{SO}(3)) = \mathcal{G}_e \oplus \mathcal{G}_o$ (see Theorem 3.3.1 (iii)).

(iv) If $\delta \neq (0,0,\delta_3)^T, (\delta_1,0,0)^T, (0,\delta_2,0)^T$, (1.3.9) is a modulus-tracker for almost every value of I_1, I_2, I_3 (see Theorem 3.3.2). In particular, it is approximately controllable in the sense of wave-functions, and in the sense of density matrices, by means of piecewise constant or smooth controls $u_1, u_2, u_3 \in [-a, a]$, for any $a > 0$. It is also approximately controllable in higher s-norms.

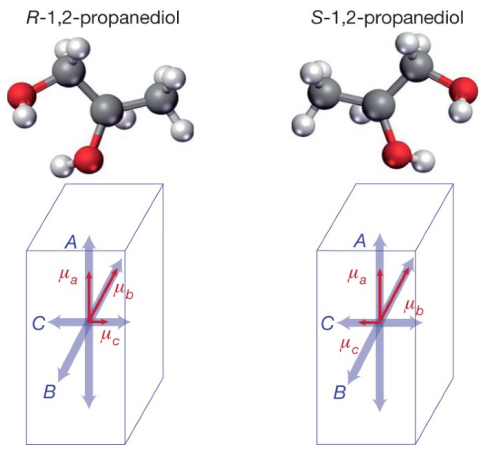


Figure 1.11: Diagram of the propanediol chiral molecule. In any chiral molecule, the two tops are identical and mirrored: that is, the opposite R- and S-enantiomers have the same rotational constants A, B, and C, and the same magnitude of dipole moment components $|\mu_a|$, $|\mu_b|$, and $|\mu_c|$, but the sign of the quantity $\mu_a\mu_b\mu_c$ is distinct for each enantiomer. The rotation of each single enantiomer is (approximately) controllable, after Theorem 3.3.2, since it has three non-vanishing dipole components. Furthermore, the projections (on specific finite-dimensional subspaces) of their rotational dynamics are simultaneously controllable, after Proposition 4.2.1. Numerical simulations for the propanediol rotational dynamics, with the goal of orientational- and enantio-selectivity, are performed in sections 4.4.1 and 4.4.2. Taken from [95].

1.3.3 An application to quantum chemistry: new results on the detection of molecular chirality via controllability

After the study of the Schödinger PDE (1.3.1) describing symmetric and asymmetric molecules, in Chapter 4 we consider the projection of (1.3.1) on some experimentally relevant finite-dimensional subspaces of $L^2(\mathrm{SO}(3))$, defined in terms of the asymmetric-top representation as

$$\mathcal{H}_{j,\tau} \oplus \mathcal{H}_{j+1,\tau'} \oplus \mathcal{H}_{j+1,\tau''} \ ,$$

where $\tau \in \{-j, \dots, j\}$, $\tau', \tau'' \in \{-j-1, \dots, j+1\}$, and

$$\mathcal{H}_{l,r} := \mathrm{span}\{\Psi^l_{r,m} \mid m = -l, \dots, l\}.$$

Such a finite-dimensional Hilbert space can be used to study the so-called problem of enantiomer-selective transfer of population in chiral molecules, via generalized three-wave mixing schemes. We approach it as a simultaneous controllability problem for two rotating asymmetric tops (in this case called enantiomers), identical and mirrored (see Figure 1.11). The two enantiomers cannot be superimposed via rotations: they are *chiral* object, and the two-body composite system is called a chiral molecule.

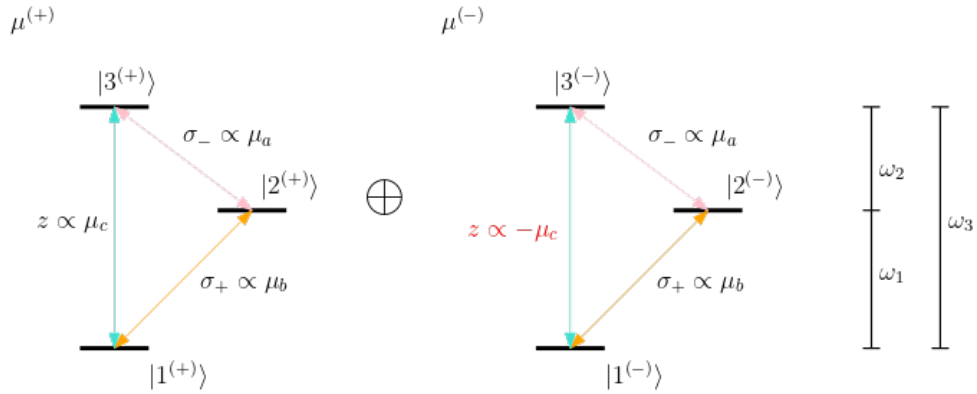


Figure 1.12: Three-wave mixing for a 3+3-level system, describing a simplified model (i.e., without m-degeneracies) of two enantiomers. The dipole moments here are denoted by $\mu^{(\pm)}$. After the three transitions indicated by the three arrows, the rotational population can be distinguished respectively on the two 3-level systems, thanks to the presence of a minus sign in only one dipole component (here denoted as μ_c).

The control target is made so that, at the end of the controlled rotational dynamics, the two enantiomers are distinguished by regarding their rotational population. We prove that simultaneous control is possible and we find, via Lie algebraic computations, combinations of frequencies and polarizations which realize the desired goal (see Propositions 4.2.1 and 4.3.1). Based on these results, we then numerically simulate the rotational dynamics in the second part of Chapter 4, in section 4.4, deriving pulse sequences which lead to the desired goal of enantio-selectivity (see Figure 1.13); it could be used in future microwave molecular experiments, as the implementability of such pulse sequences is at the hand of nowadays technologies. Such an analysis is based and motivated on recent models of three-wave-mixing spectroscopy for chirality detection developed on both theoretical [82] and experimental [95] viewpoints. Our theoretical results generalize some important properties of chiral systems which were proved on simplified models as in Figure 1.12 (that did not include the m-degeneracies): e.g., in [82] three polarizations and three dipole components were found to be necessary to detect chirality.

1.4 The Euler equations on SO(3): new results with external controls

The conserved quantities found in Theorems 3.2.1, 3.2.11, and 3.3.1 for the quantum evolution on SO(3) stimulated and motivated the study of the classical dynamics of symmetric- and asymmetric-tops, presented in Chapter 2 as a prequel of the quantum dynamics. The classical dynamics are given by the equation of motion associated with the Hamiltonian function $H + V$ on $\mathrm{SO}(3) \times \mathbb{R}^3$, where

$$H = \frac{1}{2}\left(\frac{P_1^2}{I_1} + \frac{P_2^2}{I_2} + \frac{P_3^2}{I_3}\right), \quad V(g) = -\sum_{i=1}^{3} u_i \langle (g^{-1}e_i), \delta \rangle.$$

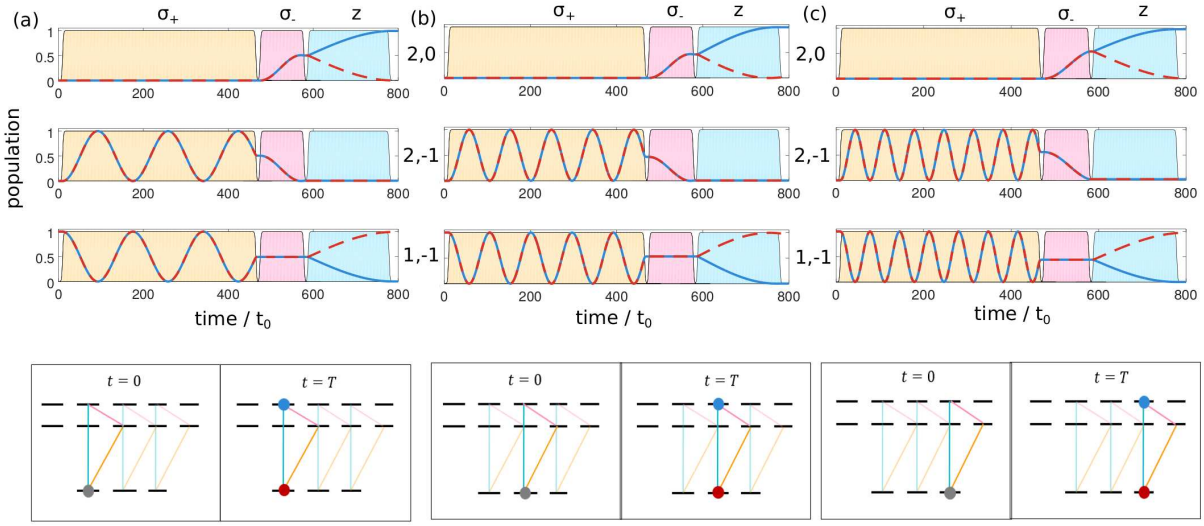


Figure 1.13: Synchronized three-wave mixing, simulated for the rotational dynamics of a carvone molecule, which leads to enantiomer-selective transfer of population. This model, studied in detail in Chapter 4 Section 4.4.3, takes into account the m-degeneracies and is based on the Lie algebraic analysis of Chapter 4, Section 4.3

The free rotational dynamics associated with H are the well-known Euler equations for a rotating rigid body, and V is a control potential. Concerning symmetric-tops, the first conserved quantity, appearing in Theorem 3.2.1, corresponds to a classical observable (i.e., the component of the angular momentum along the symmetry axis of the molecule) and it turns out to be a first integral also for the classical controlled dynamics, as we remark in Theorem 2.2.1. The second conserved quantity, appearing in Theorem 3.2.11, is more challenging, because it does not have a counterpart in the classical dynamics, being due to the superposition of k and $-k$ states in the quantum dynamics. We show in Theorem 2.2.2 that this position of the dipole, and in general any dipole not parallel to the symmetry axis, corresponds to a controllable system for the classical symmetric-top.

Concerning asymmetric-tops, all conserved quantities presented in Theorem 3.3.1 are only quantum, and do not have a classical analogy, as we prove that all dipole configurations are classically controllable for the asymmetric molecule in Theorem 2.3.1.

We notice that hence, as a byproduct of our analysis, we find several examples of systems whose quantum dynamics are not controllable even though the classical dynamics are. The possible discrepancy between quantum and classical controllability has been already noticed, for example, in the harmonic oscillator dynamics [88].

It should be noticed that the classical dynamics of a rigid body controlled with external torques (e.g., opposite pairs of gas jets) or internal torques (momentum exchange devices such as wheels) as studied in the literature mainly concern the control and stabilization problem for spacecrafts and launchers (see, e.g., [7, Section 6.4], [26],[44], [73, Section 4.6]), and differ from the ones considered here, where the controlled fields (i.e., the interactions between the electric fields and the electric dipole) are not left-invariant and their action depends on the configuration of the rigid body in the space.

1.5 Self-adjointness and the existence of quantum dynamics

In Chapters 5 and 6, we study the self-adjointness problem on two-dimensional generalized almost-Riemannian manifolds. The problem of self-adjointness in quantum mechanics has a long history, and finds its roots in the works of Von Neumann, Stone, Friedrichs [94, 104, 58] and many other great mathematicians. We wish to point out first its relation with quantum mechanics. Indeed, the self-adjointness is equivalent to two key concepts in mathematical physics: (i) observables have real spectra, and (ii) the quantum evolution exists, is unique, and is unitary.

Let $H, \mathcal{D}(H)$ be a symmetric operator (i.e., $(Hu, v) = (u, Hv)\ \forall u, v \in \mathcal{D}(H)$), that is closed on its domain of definition (i.e., its graph is closed in $\mathcal{H} \times \mathcal{H}$). We shall always assume that $\mathcal{D}(H)$ is a dense linear subspace of a separable Hilbert space $\mathcal{H}$ (otherwise, the definition of adjoint operator would not be well-posed). The spectrum

of H is defined as the set of complex numbers z such that $H - z$ has not a bounded inverse everywhere defined on $\mathcal{H}$. The self-adjointess of H can be visualized through the following definitions/theorems (see, e.g., [100, 106]):

(i) H is self-adjoint if and only if its spectrum is real;

(ii) H is self-adjoint if and only if there exists a strongly-continuous one-parameter unitary group $\{U(t)\}_{t\in\mathbb{R}}$ acting on $\mathcal{H}$, such that

- $U(t)\mathcal{D}(H) \subset \mathcal{D}(H)$, for all $t \in \mathbb{R}$,
- for any $\psi_0 \in \mathcal{D}(H)$, the function $\psi(t) := U(t)\psi_0$ solves the Schrödinger equation

$$\mathrm{i}\frac{d}{dt}\psi(t) = H\,\psi(t)\,, \qquad \psi(0) = \psi_0. \tag{1.5.1}$$

Moreover, if (i) or equivalently (ii) holds, then $U(t)\psi_0$ is the only solution of (1.5.1), that is explicitly given by the formula

$$\psi(t) = U(t)\psi_0 = e^{-\mathrm{i}tH}\psi_0\,,$$

defined thanks to the spectral theorem of unbounded self-adjoint operators.

On the one hand, a self-adjoint operator defines in a unique way the quantum dynamics. On the other hand, non-self-adjoint operators may be extended in order to create well-defined quantum dynamics. When the Hilbert space $\mathcal{H}$ is identified with $L^2(\Omega)$, the space of square-integrable functions on a domain $\Omega \subset \mathbb{R}^n$, the extensions are realized by imposing additional boundary conditions for $\psi(t)$ on $\partial\Omega$. Non-self-adjoint operators thus generate a variety of different quantum dynamics, each of them specified by different physical behaviours of the wave function while hitting the boundary of a certain domain.

1.5.1 Von Neumann self-adjoint extension theory

The usual definition of essential self-adjoitness for a symmetric, densely defined, linear operator $H, \mathcal{D}(H)$ (it is not assumed to be closed here, but it is always closable being symmetric and densely defined, see Chapter 5 Section 5.3) on an Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle)$, is given in terms of two important objects, that are respectively the domains of the closure and adjoint operator:

$$\mathcal{D}(\overline{H}) = \overline{\mathcal{D}(H)}^{\|\cdot\|_H}, \quad \mathcal{D}(H^*) = \{v \in \mathcal{H} \mid \exists w \in \mathcal{H} \text{ s.t. } (Hu, v) = (u, w),\ \forall u \in \mathcal{D}(H)\},$$

where $\|\cdot\|_H = \|\cdot\| + \|H\cdot\|$. Note that, when $\mathcal{H} = L^2(\Omega)$ and $\mathcal{D}(H) = C_0^\infty(\Omega)$ is the set of smooth functions compactly supported in Ω, the domain of the adjoint corresponds to the set of functions v such that $Hv \in L^2(\Omega)$ in the sense of distributions. One can check that the inclusion $\mathcal{D}(\overline{H}) \subset \mathcal{D}(H^*)$ is always true, for symmetric operators. The operator H is said to be (essentially) self-adjoint if also the converse inclusion holds, that is

$$H, \mathcal{D}(H) \text{ essentially self-adjoint} \Leftrightarrow \mathcal{D}(\overline{H}) = \mathcal{D}(H^*).$$

If the operator under consideration is not essentially self-adjoint, it may have extensions that are self-adjoint: more precisely, a self-adjoint extension H_e of H is a closed symmetric operator which verifies

$$\overline{H} \subset H_e = H_e^* \subset H^*,$$

where the notation $A \subset B$ for two operators A, B means that $\mathcal{D}(A) \subset \mathcal{D}(B)$ and $Bu = Au$, $\forall u \in \mathcal{D}(A)$. The relation between the closure, the adjoint, and the self-adjoint extensions is usually visualized in terms of the fundamental Von Neumann decomposition [100, Chapter X]

$$\mathcal{D}(H^*) = \mathcal{D}(\overline{H}) \oplus_{H^*} \ker(H^* + z) \oplus_{H^*} \ker(H^* + \overline{z})\,, \qquad \forall z \in \mathbb{C} \setminus \mathbb{R}\,,$$

where the sum is an orthogonal sum of vector spaces with respect to the scalar product $(\cdot,\cdot)_{H^*} = (\cdot,\cdot) + (H^*\cdot, H^*\cdot)$. The dimensions of the vector spaces $\ker(H^* + z)$ and $\ker(H^* + \overline{z})$ (called deficiency spaces), which are constant in the lower and upper complex half-planes [100, Theorem X.1], are called *deficiency indices* of H, and measure the codimension of the domain of the closure inside the domain of the adjoint. We can thus fix $z = \mathrm{i}$. If these dimensions are both zero, the operator is essentially self-adjoint. With a further reasoning, if these dimensions are both zero then the spectrum of H does not contain points in the lower and upper complex half-plane ([100, Theorem X.1]). So, if $\mathcal{D}(\overline{H}) = \mathcal{D}(H^*)$, the spectrum of H is a subset of the real line, which is indeed another definition of self-adjointness.

Within this decomposition, if the deficiency spaces $\ker(H^* + z)$ and $\ker(H^* + \overline{z})$ have the same dimension (that is guaranteed, for example, if the operator is semi-bounded [100, Corollary to Theorem X.1] or more generally if it commutes with complex conjugation [100, Theorem X.3]), then self-adjoint extensions exist and are in one-to-one correspondence with the unitary transformations of the deficiency spaces [100, Theorem X.2]:

$$\left\{ \begin{array}{c} \text{Unitary transformations from} \\ \ker(H^* - \mathrm{i}) \text{ to } \ker(H^* + \mathrm{i}) \end{array} \right\} \longleftrightarrow \left\{ \text{ Self-adjoint extensions of } H, \mathcal{D}(H) \right\}$$

$$(U : \ker(H^* - \mathrm{i}) \to \ker(H^* + \mathrm{i})) \quad \longmapsto \quad \begin{cases} \mathcal{D}(H^{(U)}) = \{\psi + \Phi + U\Phi \mid \psi \in \mathcal{D}(\overline{H}),\ \Phi \in \ker(H^* - \mathrm{i})\} \\ H^{(U)}(\psi + \Phi + U\Phi) = \overline{H}\psi + \mathrm{i}\Phi - \mathrm{i}U\Phi. \end{cases}$$

The action of $H^{(U)}$ is, of course, the action of H^* restricted to $\mathcal{D}(H^{(U)})$.

The Von Neumann self-adjoint extension theory, besides being very famous and widely used in the literature, is the most general as it applies to any symmetric densely defined operator with equal deficiency indices.

1.5.2 Kreĭn-Višik-Birman self-adjoint extension theory

A less general approach to self-adjoint extensions is given by the Kreĭn-Višik-Birman (KVB for brevity) theory [78, 110, 23, 10]. It is based on a different decomposition of the adjoint domain, which is available when the operator H is strictly positive (or semi-bounded). In this case, one can consider a canonical self-adjoint extension of H, called the Friedrichs extension H_F ([100, Theorem X.23]), that is also strictly positive if H is so, and thus has an everywhere defined bounded inverse. The KVB decomposition then reads

$$\mathcal{D}(H^*) = \mathcal{D}(\overline{H}) + H_F^{-1} \ker H^* + \ker H^*,$$

where the sum is meant in the sense of vector spaces. Within this different framework, the self-adjoint extensions of $H, \mathcal{D}(H)$ are in one-to-one correspondence with the self-adjoint transformations acting on Hilbert subspaces of $\ker H^*$ [62, Theorem 5]:

$$\left\{ \begin{array}{c} \text{Self-adjoint transformations on} \\ \text{Hilbert subspaces of } \ker H^* \end{array} \right\} \longleftrightarrow \left\{ \text{ Self-adjoint extensions of } H, \mathcal{D}(H) \right\}$$

$$(T : \mathcal{D}(T) \subset \ker H^* \to \ker H^*) \quad \longmapsto \quad \begin{cases} \mathcal{D}(H^{(T)}) = \left\{ \psi + H_F^{-1}(T\xi + \rho) + \xi \;\middle|\; \begin{array}{c} \psi \in \mathcal{D}(\overline{H}),\ \xi \in \mathcal{D}(T), \\ \rho \in \ker H^* \cap \mathcal{D}(T)^\perp \end{array} \right\} \\ H^{(T)}(\psi + H_F^{-1}(T\xi + \rho) + \xi) = \overline{H}\psi + T\xi + \rho. \end{cases}$$

Also here, we notice that the action of $H^{(T)}$ is the action of H^* on $\mathcal{D}(H^{(T)})$.

Let us discuss some examples.

Example 1. .

- **Free quantum particle on the line**
  We consider $\mathcal{H} = L^2(\mathbb{R}), H = -\frac{d^2}{dx^2}, \mathcal{D}(H) = C_0^\infty(\mathbb{R})$. Then,

  $$\mathcal{D}(\overline{H}) = \mathcal{D}(H^*) = H^2(\mathbb{R}),$$

  so the operator is essentially self-adjoint. Note also that the metric space $(\mathbb{R}, |\cdot|)$ is complete, so Gaffney's Theorem applies. The manifold $\mathbb{R}$ is then said to be quantum mechanically and classically complete.

- **Quantum particle on the half-line**
  We consider $\mathcal{H} = L^2(0,\infty), H = -\frac{d^2}{dx^2}, \mathcal{D}(H) = C_0^\infty(0,\infty)$. Then,

  $$\mathcal{D}(\overline{H}) = H_0^2(0,\infty) \subsetneq H^2(0,\infty) = \mathcal{D}(H^*),$$

  so the operator is not essentially self-adjoint. Indeed, boundary conditions at 0 are needed. The self-adjoint extensions form a one-parameter family of operators $\{H_\gamma\}_{\gamma \in (-\infty,\infty]}$ specified by the domains

  $$\mathcal{D}(H_\gamma) = \{\psi \in H^2(0,\infty) \mid \psi'(0) = \gamma\psi(0)\}.$$

  For $\gamma = \infty$ we find the Dirichlet Laplacian on the half-line, and for $\gamma = 0$ we find the Neumann one. The manifold $(0,\infty)$ is neither classically nor quantum mechanically complete.

- **Quantum particle on the line subject to zero-range interaction at the origin**
  We consider $\mathcal{H} = L^2(\mathbb{R}), H = -\frac{d^2}{dx^2}, \mathcal{D}(H) = C_0^\infty(\mathbb{R} \setminus \{0\})$. Then,
  $$\mathcal{D}(\overline{H}) = H_0^2(\mathbb{R} \setminus \{0\}) \subsetneq H^2(\mathbb{R} \setminus \{0\}) = \mathcal{D}(H^*),$$
  so the operator is not essentially self-adjoint. Indeed, boundary conditions at 0 are needed. The self-adjoint extensions form a one-parameter family of operators $\{H_\gamma\}_{\gamma \in (-\infty, \infty]}$ specified by the domains
  $$\mathcal{D}(H_\gamma) = \{\psi \in H^1(\mathbb{R}) \cap H^2(\mathbb{R} \setminus \{0\}) \mid \psi'(0^+) - \psi'(0^-) = \gamma\psi(0)\}.$$
  For $\gamma = \infty$ we find the Friedrichs extension (that is, the unique extension that has domain contained in the form domain of H), and for $\gamma = 0$ we find the bridging one (that is, the unique extension whose functions in its domain have continuous derivative in 0). The manifold $\mathbb{R} \setminus \{0\}$ is neither classically nor quantum mechanically complete. The operators H_γ are the rigorous realizations of the so-called Hamiltonians of zero-range interaction at the origin of strength γ, that is $H_\gamma = -\frac{d^2}{dx^2} + \gamma\delta(x)$. Indeed, by integrating on $(-\epsilon, \epsilon)$ the stationary Schrödinger equation $-\psi''(x) + \gamma\delta(x)\psi(x) = E\psi(x)$, $E \in \mathbb{C}$, and letting $\epsilon \to 0$, one obtains the boundary conditions $\psi'(0^+) - \psi'(0^-) = \gamma\psi(0)$.

1.6 The free Schrödinger equation on almost-Riemannian surfaces

We now turn to the relation between self-adjointness and diffusion phenomena associated with the Schrödinger or the heat equations on singular manifolds. We have already mentioned Gaffney's Theorem [61], which states the following

Theorem 1.6.1. *Let (M, g) be a complete Riemannian manifold with associated Riemannian volume ω. Then, the Laplace-Beltrami operator $\Delta := \mathrm{div}_\omega \circ \mathrm{grad}_g$, defined on $\mathcal{D}(\Delta) = C_0^\infty(M)$, is essentially self-adjoint on $L^2(M, \omega)$.*

We introduce for a moment an almost-Riemannian manifold M as a Riemannian manifold where the volume ω explodes approaching a set $\mathcal{Z}$: we cut out the singular set and obtain the Riemannian manifold $M \setminus \mathcal{Z}$, which is the union of connected Riemannian components. Each component is non-complete, as geodesics can smoothly cross the singularities (as we shall see later on). Then, Gaffney's Theorem does not apply, but we can still wonder whether the self-adjoitness holds or not.

In this thesis we focus on the 2D case. A 2-dimensional almost-Riemannian Structure (2-ARS for short) is a generalized Riemannian structure on a 2-dimensional manifold M, that can be defined locally by assigning a pair of smooth vector fields, which play the role of an orthonormal frame. It is assumed that the vector fields satisfy the Hörmander condition (see Section 5.2 for a more intrinsic definition). 2-ARSs were introduced in the context of hypoelliptic operators [57, 70] and are particular case of rank-varying sub-Riemannian structures (see for instance [4, 19, 71, 89, 109]).

Let us denote by $\mathcal{D}_p$ the linear span of the two vector fields X_1, X_2 at a point p. We can then locally visualize a generic 2D ARS around p in terms of the following normal forms [6]:

(a) $X_1(x, y) = \dfrac{\partial}{\partial x}, \quad X_2(x, y) = e^{\phi(x,y)}\dfrac{\partial}{\partial y},$ (Riemannian point)

(b) $X_1(x, y) = \dfrac{\partial}{\partial x}, \quad X_2(x, y) = xe^{\phi(x,y)}\dfrac{\partial}{\partial y},$ (Grushin Point)

(c) $X_1(x, y) = \dfrac{\partial}{\partial x}, \quad X_2(x, y) = (y - x^2\psi(x))e^{\xi(x,y)}\dfrac{\partial}{\partial y},$ (Tangency point)

where ϕ, ψ, and ξ are smooth functions such that $\phi(0, y) \equiv 0$ and $\psi(0) \neq 0$. A point $p \in M$ is said to be a *Riemannian point* if $\mathcal{D}_p$ is two-dimensional, and hence a local description around p is given by (a). A point p such that $\mathcal{D}_p$ is one-dimensional, and $\mathcal{D}_p + [\mathcal{D}, \mathcal{D}]_p$ is two-dimensional, is called a *Grushin point* and a local description around p is given by (b). A point p such that $\mathcal{D}_p + [\mathcal{D}, \mathcal{D}]_p$ is one-dimensional, and $\mathcal{D}_p + \big[\mathcal{D}, [\mathcal{D}, \mathcal{D}]\big]_p$ is two-dimensional is called a *tangency (or characteristic) point* and a local description around p is given by (c). Structures as in (b), resp. (c), are in particular 2-step, resp. 3-step. Outside of the singular set
$$\mathcal{Z} := \{p \in M \mid \mathrm{span}\mathcal{D}_p \subsetneq T_pM\}$$
the structure is Riemannian and hence the Riemannian volume ω and metric g are well defined. We can then consider the Laplace-Beltrami operator associated with such structures, given by
$$\Delta := \mathrm{div}_\omega \circ \mathrm{grad}_g = \sum_{i=1,2} X_i^2 + (\mathrm{div}_\omega X_i)X_i.$$

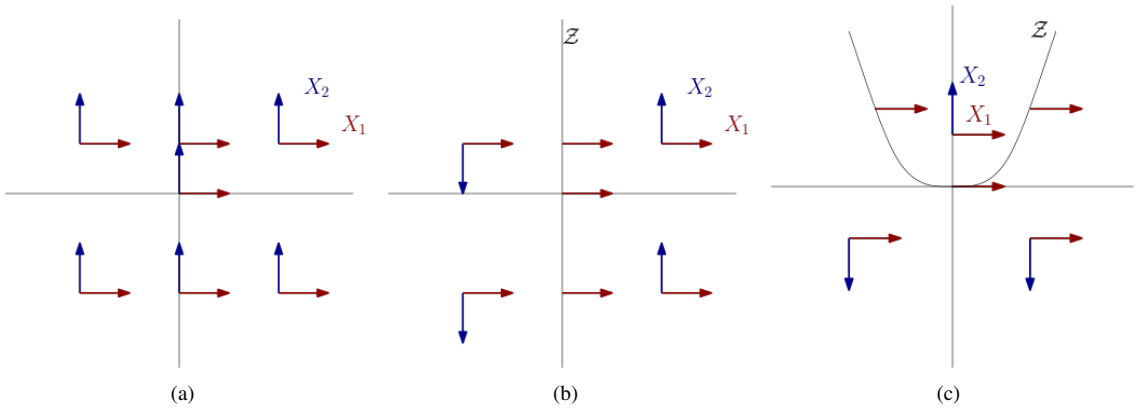


Figure 1.14: Orthonormal frames for generic 2D ARSs: (a) the origin $p = (0, 0)$ and its neighborhood are made of Riemannian points; (b) the origin $p = (0, 0)$ and the vertical axis are made of Grushin points, while the plane minus the vertical axis are made of Riemannian points; (c) the origin $p = (0, 0)$ is a tangency point (indeed $\mathcal{D}_p \subset T_p\mathcal{Z}$), the parabola minus the origin is made of Grushin points, and the plane minus the parabola is made of Riemannian points.

Example 2. .

(a) **Euclidean plane**
We consider the Riemannian structure on $\mathbb{R}^2$ given by

$$X_1(x, y) = \frac{\partial}{\partial x}, \; X_2(x, y) = \frac{\partial}{\partial y} \longleftrightarrow g = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The Laplace-Beltrami operator associated with this structure is of course

$$\Delta = \partial_x^2 + \partial_y^2, \quad \mathcal{D}(\Delta) = C_0^\infty(\mathbb{R}^2),$$

that is known to be essentially self-adjoint on $L^2(\mathbb{R}^2, dxdy)$. For example, Gaffney's Theorem applies. Indeed, this manifold is quantum mechanically and classically complete.

(b) **Grushin plane**
We consider the almost-Riemannian structure on $\mathbb{R}^2$ given by

$$X_1(x, y) = \frac{\partial}{\partial x}, \; X_2(x, y) = x\frac{\partial}{\partial y} \longleftrightarrow g = \begin{pmatrix} 1 & 0 \\ 0 & 1/x^2 \end{pmatrix}.$$

The Riemannian area associated with g is $\omega = \sqrt{\det g}dxdy = \frac{1}{|x|}dxdy$, and the Laplace-Beltrami operator associated with this structure is

$$\Delta = \partial_x^2 + x^2\partial_y^2 - \frac{1}{x}\partial_x, \quad \mathcal{D}(\Delta) = C_0^\infty(\mathbb{R}^2 \setminus \{x = 0\}).$$

Despite Gaffney's Theorem does not apply, as the manifold $(\mathbb{R}^2 \setminus \{x = 0\}, g)$ is not geodesically complete, it is essentially self-adjoint [63].

(c) **Plane with tangency point**
We consider the almost-Riemannian structure on $\mathbb{R}^2$ given by

$$X_1(x, y) = \frac{\partial}{\partial x}, \; X_2(x, y) = (y - x^2)\frac{\partial}{\partial y} \longleftrightarrow g = \begin{pmatrix} 1 & 0 \\ 0 & 1/(y - x^2)^2 \end{pmatrix}.$$

The Riemannian area associated with g is $\omega = \sqrt{\det g}dxdy = \frac{1}{|y-x^2|}dxdy$, and the Laplace-Beltrami operator associated with this structure is

$$\Delta = \partial_x^2 + (y - x^2)^2\partial_y^2 + \frac{2x}{y - x^2}\partial_x + (y - x^2)\partial_y, \quad \mathcal{D}(\Delta) = C_0^\infty(\mathbb{R}^2 \setminus \{y - x^2 = 0\}).$$

Almost nothing is known about this operator. In particular, its self-adjoitness on $L^2(\mathbb{R}^2, \frac{1}{|y-x^2|}dxdy)$ is an open question. The advanced techniques developed in [99] do not apply to this operator because the almost-Riemannian distance from the singular set is not smooth near a tangency point (for further details, see also [55]). Interesting results such as the characterization of the closure operator for geometric perturbations of the Laplace-Beltrami in the presence of tangency points are presented in the very recent paper [20].

One of the main features of 2-ARSs is the fact that geodesics can pass through the singular set, with no singularities even if all Riemannian quantities (as for instance the metric, the Riemannian area, the curvature) explode while approaching $\mathcal{Z}$.

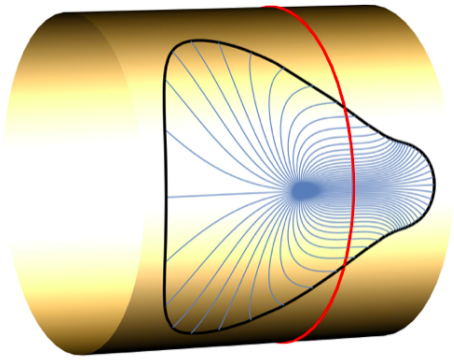


Figure 1.15: Geodesics on the Grushin cylinder, staring from the point $(-1/2, 0)$ with final time $t_f = 1.3$, crossing smoothly the singular set $\mathcal{Z}$ (red circle). The Grushin cylinder is a 2D ARS, defined as the compactification in the y-direction of the Grushin plane, introduced in Example 2 (b)

1.6.1 State-of-the-art: quantum confinement for the Laplacian $H_0 = -\Delta$ on ARSs

Even if geodesics cross the singular set, this is not possible for the Brownian motion or for a quantum particle when they are described by the Laplace-Beltrami operator Δ associated with the 2-ARS. This is due to the explosion of the Riemannian area while approaching $\mathcal{Z}$, which creates highly singular first order terms in Δ.

This phenomenon is described by the following Theorem on the self-adjoitness of 2-step 2D ARSs, proved to hold using the normal forms (b) to compute Δ near Grushin points:

Theorem 1.6.2 ([30])**.** *Let M be a 2-dimensional manifold equipped with a genuine 2-step 2-ARS. Assume that the singular set $\mathcal{Z}$ is compact. Let Ω be a connected component of $M \setminus \mathcal{Z}$. Let g be the Riemannian metric induced by the 2-ARS on Ω and ω be the corresponding Riemannian area. The Laplace-Beltrami operator $\Delta := \mathrm{div}_\omega \circ \mathrm{grad}_g$ with domain $C_0^\infty(\Omega)$, is essentially self-adjoint on $L^2(\Omega, \omega)$.*

Notice that by construction $\partial\Omega$ is diffeomorphic to S^1, Ω is open and (Ω, g) is a non-complete Riemannian manifold. In particular the conclusion of the theorem holds for the Grushin cylinder in figure 1.15.

In light of the classical comparison, the main consequence of Theorem 1.6.2 is that the Cauchy problems for the heat and the Schrödinger equations[2]

$$\begin{aligned} \partial_t \phi(t,p) &= \Delta\, \phi(t,p), & \phi(0,\cdot) = \phi_0 \in L^2(\Omega,\omega), \\ i\hbar\, \partial_t \psi(t,p) &= -\hbar^2 \Delta\, \psi(t,p), & \psi(0,\cdot) = \psi_0 \in L^2(\Omega,\omega), \end{aligned}$$

are well defined in $L^2(\Omega, \omega)$ and hence nothing can flow outside Ω, that is, $e^{t\Delta}\phi_0$ (resp. $e^{it\hbar\Delta}\psi_0$) is supported in Ω, for all $t \geq 0$ (resp. $t \in \mathbb{R}$). This phenomenon is usually known as *quantum confinement* (see [56, 99] and, for similar problems, [91]). Moreover, generalizations of Theorem 1.6.2 to higher dimensional and higher step ARSs exist, as for example the following result:

Theorem 1.6.3 ([99])**.** *Assume that the singular set $\mathcal{Z}$ of an almost-Riemannian manifold M is compact and has no tangency points. Then, the Laplace-Beltrami operator Δ, $\mathcal{D}(\Delta) = C_0^\infty(M \setminus \mathcal{Z})$ is essentially self-adjoint on $L^2(\Omega, \omega)$, where $\Omega = M$ or a connected component of $M \setminus \mathcal{Z}$.*

[2]In these equations all constant are normalized to 1 except for the Planck constant $\hbar$, since its role is important for further discussions.

1.6.2 New result: no quantum confinement for the curvature Laplacian $H_0 = -\Delta + cK$ on 2D-ARSs of step 2

Given that the geodesics cross the singular set with no singularities, the impossibility for the heat or for a quantum particle to flow through $\mathcal{Z}$ implied by Theorem 1.6.2 is quite surprising. For what concerns the heat, a satisfactory interpretation of Theorem 1.6.2 in terms of Brownian motion/Bessel processes has been provided for the Grushin cylinder in [32] and from [5] one can extract an interpretation of Theorem 1.6.2 in terms of random walks. Roughly speaking random particles are lost in the infinite area accumulated along $\mathcal{Z}$ that, as a consequence, acts as a barrier.

Although for the heat-equation the situation is relatively well-understood, this is not the case for the Schrödinger equation since semiclassical analysis (see for instance [116]) roughly says that for $\hbar \to 0$ sufficiently concentrated solutions of the Schrödinger equation move approximately along classical geodesics. Clearly semiclassical analysis breaks down on the singularity $\mathcal{Z}$.

It is then natural to come back on the quantization procedure that permits to pass from the description of a free classical particle moving on a Riemannian manifold to the corresponding Schrödinger equation.

This is a complicated subject that has no unique answer. The resulting evolution equation for quantum particles depends indeed from the chosen quantization procedure.

Most of coordinate invariant quantization procedures provide in the Laplace-Beltrami operator a correction term depending on the Gaussian curvature K, i.e., they provide a Schrödinger equation of the form

$$\mathrm{i}\hbar\, \partial_t \psi(t,p) = \hbar^2\Big(-\Delta + cK(p)\Big)\psi(t,p),$$

where Δ is the Laplace-Beltrami operator and $c \geq 0$ is a constant. Values given in the literature include:

- path integral quantization: $c = 1/6$ and $c = 1/4$ in [50], $c = 1/3$ in [49];
- covariant Weyl quantization: $c \in [0, 1/3]$ including conventional Weyl quantization ($c = 0$) in [60];
- geometric quantization for a real polarization: $c = 1/6$ in [114];
- finite dimensional approximations to Wiener Measures $c = 1/3$ in [13].

We refer to [13, 60] for interesting discussions on the subject.[3]

In Chapter 5 we study the self-adjointness of the *curvature Laplacian* $-\Delta + cK$ in function of c to understand if quantum confinement holds for the dynamics induced by this operator. Before stating the main result, let us remark that the curvature term cK interacts with the diverging first order term in Δ.

For instance for the Grushin cylinder a unitary transformation (see Section 5.4.1, (5.4.1)) permits to transform the operator

$$\Delta = \frac{\partial^2}{\partial x^2} + x^2\frac{\partial^2}{\partial y^2} - \frac{1}{x}\frac{\partial}{\partial x} \text{ on } L^2(\mathbb{R}\times S^1, \frac{1}{|x|}dx\,dy)$$

in

$$\tilde{\Delta} = \frac{\partial^2}{\partial x^2} + x^2\frac{\partial^2}{\partial y^2} - \frac{3}{4}\frac{1}{x^2} \text{ on } L^2(\mathbb{R}\times S^1, dx\,dy)$$

and hence the adding of a term of the form $-cK = -c\big(-2\frac{1}{x^2}\big)$ (that remains untouched by the unitary transformation) to $\tilde{\Delta}$ changes the diverging behaviour around $x = 0$. In particular for $c = 3/8$ the diverging potential disappears and $-\tilde{\Delta} + cK$ is not essentially self-adjoint in $L^2(\mathbb{R}^+\times S^1, dx\,dy)$ while $-\tilde{\Delta}$ does. The same conclusion applies to $-\Delta + cK$ in $L^2(\mathbb{R}^+\times S^1, \frac{1}{|x|}dx\,dy)$.

The main result of Chapter 5 is that the perturbation term given by the curvature destroys the essential self-adjointness of the Laplace-Beltrami operator.

Theorem 1.6.4. *Let M be a compact oriented 2-dimensional manifold equipped with a genuine 2-step 2-ARS. Let Ω be $M \setminus \mathcal{Z}$ or one of its connected component, where $\mathcal{Z}$ is the singular set. Let g be the Riemannian metric induced by the 2-ARS on Ω, ω be the corresponding Riemannian area, K the corresponding Gaussian curvature and $\Delta = \mathrm{div}_\omega \circ \mathrm{grad}_g$ the Laplace-Beltrami operator. Let $c \geq 0$. The curvature Laplacian $-\Delta + cK$ with domain $C_0^\infty(\Omega)$, is essentially self-adjoint on $L^2(\Omega,\omega)$ if and only if c=0. Moreover, if $c > 0$, the curvature Laplacian has infinite deficiency indices.*

[3]There are also other approaches to the quantization process on Riemannian manifolds that provide correction terms depending on the curvature. For instance if one considers the Laplacian on a ϵ-tubular neighborhood of a surface in $\mathbb{R}^3$ with Dirichlet boundary conditions, then for $\epsilon \to 0$ after a suitable renormalization, one gets an operator containing a correction term depending on the Gaussian curvature and the square of the mean curvature (see [79, 80]).

The non-self-adjointness of $-\Delta + cK$ implies that one can construct self-adjoint extensions of this operator that permit to the solution to the Schrödinger equation to flow out of the set Ω, in the same spirit of Chapter 6 (see also [34]). The study of these self-adjoint extension and how semiclassical analysis applies to them is a subject that deserves to be studied in detail.

Remark 1.6.5. We remark that in Theorem 1.6.4 one can also consider the case $c < 0$. In this case, one can prove that the curvature Laplacian is essentially self-adjoint (applying for example the criterion for the self-adjointes of operators of the form $-\Delta + V$ on non-complete Riemannian manifolds, found in [99]). However, if this case admits a physical interpretation is not known to the authors.

As in Theorem 1.6.2 the compactness hypothesis is useful to simplify the statement of the theorem. A version without the compactness hypothesis is given here where also the orientability assumption of M is not necessary.

Theorem 1.6.6. *Let M be a 2-dimensional manifold equipped with a genuine 2-step 2-ARS.*
Assume that

- *the singular set $\mathcal{Z}$ is compact;*
- *the 2-ARS is geodesically complete.*

Let Ω be a connected component of $M \setminus \mathcal{Z}$, and $c \geq 0$. With the same notations of Theorem 5.1.1, the curvature Laplacian $-\Delta + cK$ with domain $C_0^\infty(\Omega)$, is essentially self-adjoint on $L^2(\Omega, \omega)$ if and only if c=0. Moreover, if $c > 0$, the curvature Laplacian has infinite deficiency indices.

For the sake of simplicity, in Chapter 5 we prove Theorem 1.6.4 only. Theorem 1.6.6 can be proved following the same ideas.

Theorem 1.6.6 applies in particular to the Grushin cylinder with curvature Laplacian $-\Delta + cK = -(\partial_x^2 + x^2\partial_y^2 - \frac{1}{x}\partial_x) + \frac{2c}{x^2}$. For this case, the fact that the deficiency indices are infinite means that all Fourier components of $-\Delta + cK$ are not self-adjoint.

Notice that under the hypothesis of the theorem, each connected component of $\partial\Omega$ is diffeomorfic to S^1. Of course if $c > 0$, the manifold does not need to be geodesically complete.

If one removes the 2-step hypothesis the situation is more complicated since tangency points [6, 8] may appear. In presence of tangency points even the essential self-adjointness of the standard Laplace-Beltrami operator (without the term $-cK$) is an open question [30]. Without the 2-step hypothesis results can indeed be very different. To illustrate this, in Chapter 5 we also study the α-Grushin cylinder for which computations can be done explicitly.

Proposition 1.6.7. *Fix $\alpha \in \mathbb{R}$. On $\mathbb{R} \times S^1$ consider the generalized Riemannian structure for which an orthonormal frame is given by*

$$X_1(x, y) = \frac{\partial}{\partial x}, \qquad X_2^{(\alpha)}(x, y) = |x|^\alpha \frac{\partial}{\partial y}, \qquad \text{here } x \in \mathbb{R}, \ \ y \in S^1. \tag{1.6.1}$$

Let $c \geq 0$. On $\mathbb{R}^+ \times S^1$ the structure is Riemannian with Riemannian area $\frac{1}{|x|^\alpha} dx\, dy$. Let $-\Delta_\alpha + cK_\alpha$ be the curvature Laplacian with domain $C_0^\infty(\mathbb{R}^+ \times S^1)$ acting on $L^2(\mathbb{R}^+ \times S^1, \frac{1}{|x|^\alpha} dx\, dy)$. Denote by

$$\alpha_{c,\pm} = \frac{(-2c+1) \pm 2\sqrt{(c-2+\sqrt{3})(c-2-\sqrt{3})}}{4c-1}.$$

- *If $0 \leq c < 1/4$,* $\quad -\Delta_\alpha + cK_\alpha$ *is essentially self-adjoint if and only if $\alpha \geq \alpha_{c,+}$ or $\alpha \leq \alpha_{c,-}$;*
- *if $c = 1/4$,* $\quad -\Delta_\alpha + cK_\alpha$ *is essentially self-adjoint if and only if $\alpha \geq 3$;*
- *if $1/4 < c \leq 2 - \sqrt{3}$,* $\quad -\Delta_\alpha + cK_\alpha$ *is essentially self-adjoint if and only if $\alpha_{c,-} \leq \alpha \leq \alpha_{c,+}$;*
- *if $2 - \sqrt{3} < c < 2 + \sqrt{3}$,* $\quad -\Delta_\alpha + cK_\alpha$ *is not essentially self-adjoint $\forall \alpha \in \mathbb{R}$;*
- *if $c \geq 2 + \sqrt{3}$,* $\quad -\Delta_\alpha + cK_\alpha$ *is essentially self-adjoint if and only if $\alpha_{c,-} \leq \alpha \leq \alpha_{c,+}$.*

The regions where $-\Delta_\alpha + cK_\alpha$ is essentially self-adjoint are plotted in Figure 1.16. Note that for some of the quantizations listed earlier, $-\Delta_\alpha + cK_\alpha$ is essentially self-adjoint for $|\alpha|$ sufficiently big. Hence, for such structures quantum confinement still holds for the curvature Laplacian.

The α-Grushin cylinder is an interesting geometric structure studied in [32, 34, 64]; its analogous version on $\mathbb{R}_x \times \mathbb{R}_y$ has been studied in [63, 98]. In Chapter 6 we present an original classification of its local self-adjoint

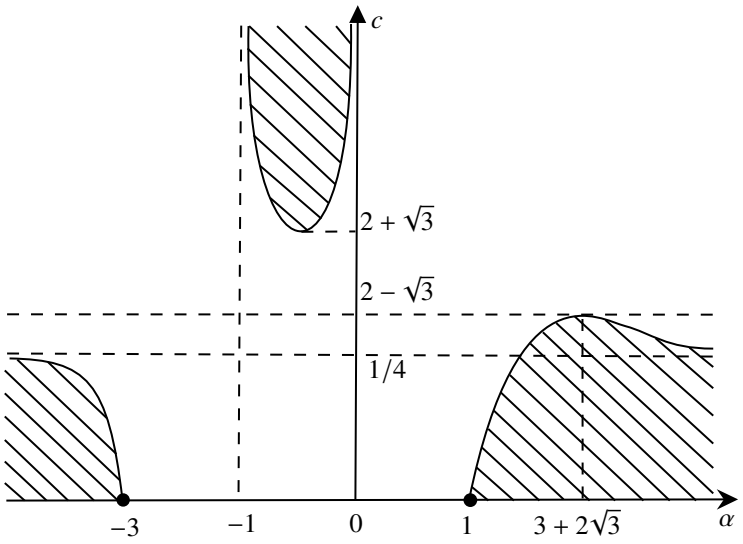


Figure 1.16: Regions of the (α, c) parameter space where the operator $-\Delta_\alpha + cK_\alpha$ is essentially self-adjoint.

extensions. For $\alpha = 0$ it is a flat cylinder, for α positive integer is a $(\alpha + 1)$-step 2-ARS; for α negative it describes a conic-like surface (see Figure 1.17).

We conclude the presentation of Chapter 5 with a remark on the heat equation: while an operator of the form $-\Delta + cK(p)$ is useful to describe a quantum particle in a Riemannian manifold, it is not meaningful in the description of the heat evolution; indeed a heat equation of the form $\partial_t \phi = (-\Delta + cK(p))\phi$ would describe the evolution of a random particle on a Riemannian manifold with a rate of killing proportional to the Gaussian curvature.

1.6.3 State-of-the-art: self-adjointness on α-Grushin structures

In Chapter 6 we present a classification of the uniformly fibred self-adjoint extensions of the Laplace-Beltrami operator associated with the α-Grushin structure on the cylinder, for $\alpha \in [0, 1)$. This structure is defined for any $\alpha \in \mathbb{R}$ via the pair of vector fields introduced in (1.6.1), globally defined on $\mathbb{R} \times S^1 =: M$. When $\alpha \in \mathbb{N}$, (1.6.1) defines a smooth almost-Riemannian structure of step $(\alpha + 1)$. Notice that the same structure is considered in Chapter 5 as an example of higher-step ARS, and the self-adjointness of its associated curvature Laplacian is studied (cf. Proposition 1.6.7 above). For $\alpha \notin \mathbb{N}$, it defines a generalized almost-Riemannian structure, that is not smooth and does not verify the Hörmander condition in general. By cutting out from the manifold $\mathbb{R} \times S^1$ the singular set $\{x = 0\}$ where X_1 and X_2 become collinear, we obtain a Riemannian structure on $\mathbb{R} \setminus \{0\} \times S^1$ with the associated Riemannian metric, volume and Gaussian curvature given respectively by

$$g_\alpha = \mathrm{d}x \otimes \mathrm{d}x + \frac{1}{|x|^{2\alpha}}\,\mathrm{d}y \otimes \mathrm{d}y, \quad \omega_\alpha = \frac{1}{|x|^\alpha}\,\mathrm{d}x \wedge \mathrm{d}y, \quad K_\alpha = -\frac{\alpha(\alpha+1)}{x^2}.$$

In particular, when $\alpha > 0$, all geometric quantities are singular on $\mathcal{Z}$.

The Laplace-Beltrami operator

$$H_\alpha = -\Delta_\alpha := \mathrm{div}_{\omega_\alpha} \circ \mathrm{grad}_{g_\alpha}, \quad \mathcal{D}(\Delta_\alpha) = C_0^\infty\Big(\mathbb{R} \setminus \{0\} \times S^1\Big)$$

of the α-Grushin structure is equivalent, via the unitary transformation $L^2(\mathbb{R} \times S^1, \omega_\alpha) \to L^2(\mathbb{R} \times S^1, \mathrm{d}x\mathrm{d}y)$, to the singular differential operator

$$\mathsf{H}_\alpha \psi = \Big(-\frac{\partial^2}{\partial x^2} - |x|^{2\alpha}\frac{\partial^2}{\partial y^2} + \frac{\alpha(2+\alpha)}{4x^2}\Big)\psi, \quad \psi \in C_0^\infty\Big(\mathbb{R} \setminus \{0\} \times S^1\Big) \subset L^2(\mathbb{R} \times S^1, \mathrm{d}x\mathrm{d}y). \tag{1.6.2}$$

The classification of the self-adjointness problem for these operators is well-known (notice that this result is also recovered in Proposition 1.6.7 and corresponds to $c = 0$):

Theorem 1.6.8 (Self-adjoitness in α-Grushin conic and anti-conic surfaces, [34])**.**

(i) If $\alpha \in (-\infty, -3] \cup [1, +\infty)$, then H_α is essentially self-adjoint.

(ii) If $\alpha \in (-3,-1]$, then H_α is not essentially self-adjoint and it has deficiency index 2.

(iii) If $\alpha \in (-1,1)$, then H_α is not essentially self-adjoint and it has infinite deficiency index.

Theorem 1.6.8 is not contradicting Theorem 1.6.3, as (1.6.1) defines an almost-Riemannian manifold only if $\alpha \in \mathbb{N}$. To better visualize Theorem 1.6.8, let us formally decompose the operator (1.6.2) in its Fourier modes w.r.t.

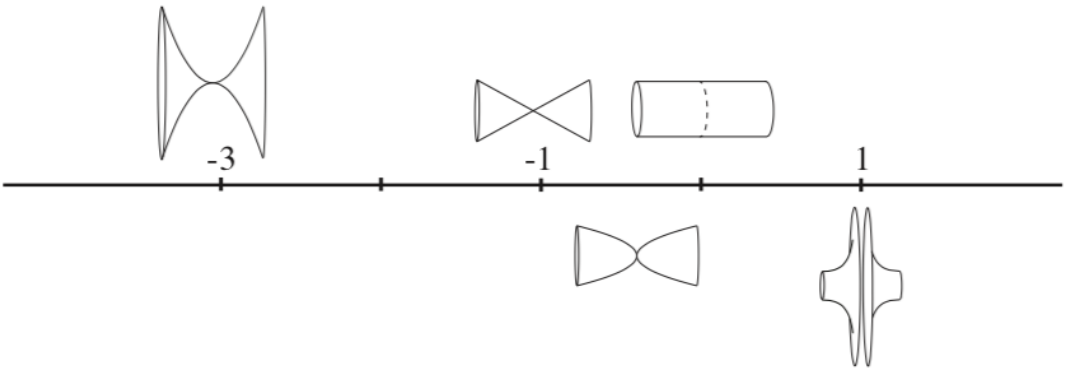


Figure 1.17: Geometric interpretation of α-Grushin surfaces. It is conic for $\alpha < 0$, a cylinder for $\alpha = 0$, and anti-conic for $\alpha > 0$. Taken from [34].

to $y \in S^1$. This gives

$$\bigoplus_{k\in\mathbb{Z}} (\mathsf{H}_\alpha)_k, \quad (\mathsf{H}_\alpha)_k := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + |x|^{2\alpha}k^2 + \frac{\alpha(2+\alpha)}{4x^2},$$

acting on the Hilbert space $\ell^2(\mathbb{Z}, L^2(\mathbb{R}, \mathrm{d}x))$, with constant mode domains $\mathcal{D}\Big((\mathsf{H}_\alpha)_k\Big) = C_0^\infty(\mathbb{R}\setminus\{0\})$ for all k. Then, the self-adjointness of each $(\mathsf{H}_\alpha)_k$ can be studied using Sturm-Liouville theory for 1D inverse square potential Schrödinger operators of the form $-\frac{d^2}{dx^2} + V(x)$. We can reinterprete the statements on the deficiency indices as follow:

(i) If $\alpha \in (-\infty,-3] \cup [1,+\infty)$, then $(\mathsf{H}_\alpha)_k$ is essentially self-adjoint for all $k \in \mathbb{Z}$. That is, nothing can flow through $\mathcal{Z}$.

(ii) If $\alpha \in (-3,-1]$, then $(\mathsf{H}_\alpha)_k$ is essentially self-adjoint for all $k \in \mathbb{Z}\setminus\{0\}$, while $(H_\alpha)_0$ is non-self-adjoint. That is, only the average of the wave function

$$\widehat{\psi}_0(x) = \frac{1}{2\pi}\int_0^{2\pi} \psi(x,y)\mathrm{d}y$$

can flow through $\mathcal{Z}$.

(iii) If $\alpha \in (-1,1)$, then $(\mathsf{H}_\alpha)_k$ is non-self-adjoint for all $k \in \mathbb{Z}$. That is, all modes can flow though $\mathcal{Z}$.

1.6.4 New results: self-adjoint extensions on α-Grushin structures and their Sobolev regularity at the boundary

A natural question regarding the region of α such that H_α is not self-adjoint, is then the following: which boundary conditions at the singularity $\{x = 0\}$ are allowed for the Schrödinger equation $\mathrm{i}\partial_t\psi = H_\alpha\psi$ to be well-posed across the two halves of the cylinder? In other words, when H_α is not self-adjoint, how do its self-adjoint extensions look like? In Chapter 6 we partly answer this question, applying KVB extension theory, and the main results read as follows

Theorem 1.6.9. *Let $\alpha \in [0,1)$. The operator H_α admits the following families of self-adjoint extensions in $L^2(M,\omega_\alpha)$:*

- *<u>Friedrichs extension</u>: $H_{\alpha,F}$;*
- *<u>Family $\mathrm{I_R}$</u>: $\{H^{[\gamma]}_{\alpha,R} \mid \gamma \in \mathbb{R}\}$;*

- *Family* $\mathrm{I_L}$: $\{H^{[\gamma]}_{\alpha,L} \mid \gamma \in \mathbb{R}\}$;
- *Family* II_a *with* $a \in \mathbb{C}$: $\{H^{[\gamma]}_{\alpha,a} \mid \gamma \in \mathbb{R}\}$;
- *Family* III: $\{H^{[\Gamma]}_{\alpha} \mid \Gamma \equiv (\gamma_1, \gamma_2, \gamma_3, \gamma_4) \in \mathbb{R}^4\}$.

Each operator belonging to any such family is a restriction of H^*_α*, and hence its differential action is given by* $-\Delta_\alpha$*. The domain of each of the above extensions is qualified as the space of the functions* $f \in L^2(M, \omega_\alpha)$ *satisfying the following properties:*

(i) Integrability and regularity:

$$\int_M \left|\Delta_\alpha f\right|^2 \omega_\alpha \;<\; +\infty\,. \tag{1.6.3}$$

(ii) Boundary condition: The limits

$$f_0^{\pm}(y) \;=\; \lim_{x\to 0^\pm} f(x,y) \tag{1.6.4}$$

$$f_1^{\pm}(y) \;=\; \pm(1+\alpha)^{-1} \lim_{x\to 0^\pm} \left(\frac{1}{|x|^\alpha}\,\frac{\partial f(x,y)}{\partial x}\right) \tag{1.6.5}$$

exist and are finite for almost every $y \in S^1$*, and depending on the considered type of extension, and for almost every* $y \in S^1$*, they satisfy*

$$f_0^{\pm}(y) \;=\; 0 \qquad \text{if } f \in \mathcal{D}(H_{\alpha,F}), \tag{1.6.6}$$

$$\begin{cases} f_0^-(y) = 0 \\ f_1^+(y) = \gamma f_0^+(y) \end{cases} \qquad \text{if } f \in \mathcal{D}(H^{[\gamma]}_{\alpha,R}), \tag{1.6.7}$$

$$\begin{cases} f_1^-(y) = \gamma f_0^-(y) \\ f_0^+(y) = 0 \end{cases} \qquad \text{if } f \in \mathcal{D}(H^{[\gamma]}_{\alpha,L}), \tag{1.6.8}$$

$$\begin{cases} f_0^+(y) = a\, f_0^-(y) \\ f_1^-(y) + \overline{a}\, f_1^+(y) = \gamma f_0^-(y) \end{cases} \qquad \text{if } f \in \mathcal{D}(H^{[\gamma]}_{\alpha,a}), \tag{1.6.9}$$

$$\begin{cases} f_1^-(y) = \gamma_1 f_0^-(y) + (\gamma_2 + \mathrm{i}\gamma_3) f_0^+(y) \\ f_1^+(y) = (\gamma_2 - \mathrm{i}\gamma_3) f_0^-(y) + \gamma_4 f_0^+(y) \end{cases} \qquad \text{if } f \in \mathcal{D}(H^{[\Gamma]}_{\alpha})\,. \tag{1.6.10}$$

As a byproduct of the theorem above, we can deduce the regularity of the wave-function at the boundary, depending on the different physics imposed by different self-adjoint extensions.

Corollary 1.6.10. *Let* f *belong to the domain of one of the self-adjoint extension of* H_α *listed in Theorem 1.6.9. Then,*

$$f_0^{\pm} \in H^{s_{0,\pm}}(S^1, \mathrm{d}y) \qquad \text{and} \qquad f_1^{\pm} \in H^{s_{1,\pm}}(S^1, \mathrm{d}y) \tag{1.6.11}$$

with

- $s_{1,\pm} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$ *for the Friedrichs extension,*
- $s_{1,-} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$, $s_{0,+} = s_{1,+} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type* I_R*,*
- $s_{1,+} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$, $s_{0,-} = s_{1,-} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type* I_L*,*
- $s_{1,\pm} = s_{0,\pm} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$ *for extensions of type* II_a*,*
- $s_{1,\pm} = s_{0,\pm} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type* III.

The last Corollary, in particular, extends the Sobolev-regularity $\frac{1}{2}\frac{1-\alpha}{1+\alpha}$ proved for the deficiency spaces of H_α in [97] (which corresponds to the regularity of the Friedrichs extension) to the domains of the other self-adjoint extensions.

We remark that requirement (1.6.3) only means that all the considered extensions are contained in H^*_α. Each of the requirements (1.6.6)-(1.6.10) then expresses the corresponding condition of self-adjointness.

The common feature of all such extensions is that their boundary conditions as $x \to 0$ have the same form independently of $y \in S^1$. In this sense, those are *local* extensions.

It is also clear that the Friedrichs extension, as well as type-$\mathrm{I_R}$ and type-$\mathrm{I_L}$ extensions, are reduced with respect to the Hilbert space decomposition

$$L^2(M, \omega_\alpha) = L^2(\mathbb{R}^+ \times S^1, \omega_\alpha) \oplus L^2(\mathbb{R}^- \times S^1, \omega_\alpha) =: L^2(M^+, \omega_\alpha) \oplus L^2(M^-, \omega_\alpha).$$

Each such operator is the orthogonal sum of two self-adjoint operators, respectively on $L^2(M^+, \omega_\alpha)$ and $L^2(M^-, \omega_\alpha)$, characterised by independent boundary conditions at the singularity region $\mathcal{Z}$ from the right and from the left. On the contrary, type-II_a (with $a \neq 0$) and type-III extensions are not reduced *in general*: the boundary condition couples the behaviour as $x \to 0^+$ and $x \to 0^-$.

The left-right reducibility

$$\widetilde{H}_\alpha \;\cong\; \widetilde{H}^-_\alpha \oplus \widetilde{H}^+_\alpha \tag{1.6.12}$$

of the extension $\widetilde{H}_\alpha = H_{\alpha,F}$, or $\widetilde{H}_\alpha = H^{[\gamma]}_{\alpha,R}$, or $\widetilde{H}_\alpha = H^{[\gamma]}_{\alpha,L}$, results in a decoupled independent Schrödinger evolution of the two components f^+ and f^- of the solution $f \in C^1(\mathbb{R}_t, L^2(M, \omega_\alpha))$ to the Cauchy problem

$$\begin{cases} \mathrm{i}\,\partial_t f \;=\; \widetilde{H}_\alpha\, f \\ f|_{t=0} \;=\; u_0 \;\in\; \mathcal{D}(\widetilde{H}_\alpha)\,. \end{cases}$$

This means that, separately on each half-cylinder,

$$f^\pm(t) \;=\; e^{-\mathrm{i}t\widetilde{H}^\pm_\alpha} u^\pm_0\,, \tag{1.6.13}$$

where $u^\pm_0 \in L^2(M^\pm, \omega_\alpha)$, with no exchange between left and right at the interface $\mathcal{Z}$.

The picture is then the following.

- Friedrichs extension $H_{\alpha,F}$: quantum confinement on each half of the Grushin cylinder, with no interaction of the particle with the boundary and no dynamical transmission between the two halves.
- Type-$\mathrm{I_R}$ and type-$\mathrm{I_L}$ extensions: no dynamical transmission across $\mathcal{Z}$, but possible non-trivial interaction of the quantum particle with the boundary respectively from the right or from the left, with quantum confinement on the opposite side. (Thus, for instance, a quantum particle governed by $H^{[\gamma]}_{\alpha,R}$ may 'touch' the boundary from the right, but not from the left, and moreover it cannot trespass the singularity region.)
- Type-II_a and type-III extensions: in general, dynamical transmission through the boundary.

Among the latter group of extensions, a special status is deserved by the Laplace-Beltrami realisation

$$H_{\alpha,B} \;:=\; H^{[\gamma]}_{\alpha,a} \qquad \text{with } a = 1 \text{ and } \gamma = 0\,.$$

In this case the boundary condition (1.6.9) takes the form

$$\begin{aligned} \lim_{x\to 0^-} f(x,y) \;&=\; \lim_{x\to 0^+} f(x,y) \\ \lim_{x\to 0^-} \Big(\frac{1}{|x|^\alpha}\,\frac{\partial f(x,y)}{\partial x}\Big) \;&=\; \lim_{x\to 0^+} \Big(\frac{1}{|x|^\alpha}\,\frac{\partial f(x,y)}{\partial x}\Big) \end{aligned} \tag{1.6.14}$$

for almost every $y \in S^1$. Quantum-mechanically, (1.6.14) are interpreted as the continuity of the spatial probability density of the particle in the region around $\mathcal{Z}$ and of the momentum in the direction orthogonal to $\mathcal{Z}$, defined with respect to the weight $|x|^{-\alpha}$ induced by the degenerate metric. The extension $H_{\alpha,B}$ is usually called the *bridging extension* of H_α. This particular extension, and the Friedrichs extension, were firstly found in [34, Proposition 3.11]. It is easily seen by inspection of (1.6.6)-(1.6.10) that no other boundary condition of self-adjointness allows for such a two-fold continuity for any other weight.

1.7 Conclusion

We resume here the main contributions of this thesis:

- In chapter 2 we show that the classical rotation of a symmetric rigid body controlled with three external orthogonal fields is: (i) controllable if the dipole is not parallel to the symmetry axis; (ii) not controllable if the dipole is parallel to the symmetry axis, due to the conservation of the angular momentum component along that axis (and we compute the reachable sets in this non-controllable case). We then show that the classical rotation of an asymmetric rigid body is controllable with three external orthogonal fields, for all configuration of the dipole. W.r.t. previous known results: the problem of controlling the rotation of a rigid body has been extensively studied, and the available results (to the best of the author knowledge) involve different strategies of control (e.g., internal torques or wheels [44]) that in particular result in controls which do not depend on the configuration of the rigid body in the space (i.e., left invariant control fields), which is not the case in our problem.

- In chapter 3 we present an original (approximate) controllability test for the multi-input bilinear infinite-dimensional discrete spectrum Schrödinger equation, and an original (approximate) simultaneous controllability test for evolutions that are decomposed in invariant subspaces. Both results apply also to density matrix approximate controllability, and controllability in finer norms. We apply this technique to study the Schrödinger equation on SO(3), controlled with three orthogonal electric fields. We show that the quantum rotation of a symmetric rigid molecule is: (i) approximately controllable if the electric dipole is not parallel nor orthogonal to the symmetry axis of the molecule; (ii) not controllable if the dipole is parallel to the symmetry axis due to the conservation of the angular momentum operator component along that axis (and we compute the reachable sets in this non-controllable case, where in particular the system decomposes in an infinite direct sum decomposition of invariant orthogonal subspaces); (iii) not controllable if the dipole is orthogonal to the symmetry axis (and we compute the reachable sets in this non-controllable case, where in particular the system decomposes in a direct sum decomposition of two invariant orthogonal subspaces). We then show that the quantum rotation of an asymmetric rigid molecule is: (i) approximately controllable if the electric dipole is not parallel to any of the principal axis of inertia of the molecule; (ii) not controllable if the dipole is parallel to any of the principal axis of inertia (where in particular the system decomposes in a direct sum decomposition of two invariant orthogonal subspaces, depending on which principal axis is parallel to the dipole). These results hold under a non-resonant assumption and for almost all value of the inertia moments of the molecule. W.r.t. previous known results: our new controllability test is a close variation of the Lie-Galerkin tracking condition introduced in the paper [28], where it is also proved the approximate controllability of the quantum rotation of a linear molecule using this condition. The approximate controllability of a linear molecule was already known from [72] also. The quantum controllability of symmetric and asymmetric rotating molecules was proposed as an open question in [77], and the operator controllability was conjectured for finite-dimensional subspaces of linear molecules in [72].

- In chapter 4 we show the simultaneous (operator) control in finite-dimensional subspaces of two chiral asymmetric molecules, pointing out the (minimal) combinations of spectral gaps (frequencies) and directions of the field (polarizations) which control the system. Based on this insight, we perform numerical simulations of microwave rotational dynamics for propanediol and carvone molecules that confirm our controllability results. W.r.t previous known results: in [82] the authors show, on a simplified model, that three dipole components and three polarizations are necessary for the simultaneous control, as it is confirmed in our results.

- In chapter 5 we prove the non-self-adjointness of curvature Laplacians, on 2D almost-Riemannian manifolds of step 2. This implies in particular that the free Schrödinger evolution on step 2 2D-ARSs generated by the operator $-\Delta + cK$ needs boundary conditions at the singular sets of the structure to be well-defined, for any $c > 0$. We also show with an example (the α-Grushin 2D-structures) that results are in general different without the step 2 assumption. W.r.t. previous known results: the Laplace-Beltrami operator on 2D ARS of step 2 (which corresponds to the case $c = 0$) has been proved to be essentially self-adjoint in the paper [30], and more in general in the paper [99] the authors proved the same result on any ARS when the singular sets are compact and have no tangency points.

- In chapter 6 we present a classification of four different families of local self-adjoint extensions of the Laplace-Beltrami operator in α-Grushin anti-conic surfaces, described in terms of different boundary conditions for the wave function to be imposed at the singularity of the structure. As a consequence of our analysis, we also obtain the Sobolev-regularity of the local boundary conditions allowed for a well-posed Schrödinger evolution

on such singular Riemannian structures. We also mention an estimate of the double derivative in the vertical direction in terms of the α-Grushin Laplace-Beltrami operator (see Lemma 6.6.11), that we obtain using the inverse of the Friedrichs extension. W.r.t. previous known results: the self-adjointness of the α-Grushin surfaces and the Friedrichs and bridging extensions were firstly studied in [34]. The Sobolev-regularity of the deficiency spaces of the Laplace-Beltrami on α-Grushin sufaces (which corresponds to the regularity of the boundary conditions for the Friedrichs extension) was already found in [97]. A similar estimate of powers of the derivative in the vertical direction in terms of Baouendi-Grushin-type operators has been obtained in the very recent paper [84, Lemma 2.1], with a different technique based on elliptic estimates: it is interesting to remark that both techniques rely on the positivity of these operators.

Chapter 2

Classical controllability of a rotating molecule

In this chapter we study the controllability problem for the Hamilton equations of a rotating symmetric- and asymmetric-top molecule. The molecule is assumed to be rigid, and the Hamilton equation thus corresponds to the well-known Euler equations of a rigid body rotating around its center of mass. The molecule is controlled through three orthogonal electric fields interacting with its electric dipole.

Concerning the symmetric-top, the controllability is characterized in terms of the dipole position, which is fixed inside the molecular frame: when it lies along the symmetry axis of the molecule the rotations are not controllable, due to the presence of a conserved quantity, the third component of the total angular momentum; if the dipole is not along the symmetry axis, we show controllability of the rotational dynamics.

Concerning the asymmetric-top, we prove that the rotational dynamics are controllable for all dipole configurations.

The chapter is organized as follows: in Section 2.1 we recall abstract results from geometric control theory; in Section 2.2 we apply this framework to a rotating symmetric-top; in Section 2.3 the framework is applied to a rotating asymmetric-top.

The main original results of this Chapter are: for symmetric-tops, Theorems 2.2.1 and 2.2.2, where we prove, respectively, the non-controllability when the dipole lies along the symmetry axis of the body (computing also its reachable sets in Theorem 2.2.4) and the controllability in any other case; for asymmetric-tops, Theorem 2.3.1, where we prove that the rotational dynamics are controllable for all dipole configurations.

The results on the classical symmetric-top system are in the paper [33].

2.1 Controllability of control-affine systems with recurrent drift

We recall in this section some useful results on the controllability properties of (finite-dimensional) control-affine systems.

Let M be an n-dimensional manifold, $X_0, X_1, \dots, X_\ell$ a family of smooth (i.e., C^∞) vector fields on M, $U \subset \mathbb{R}^\ell$ a set of control values which is a neighborhood of the origin. We consider the control system

$$\dot{q} = X_0(q) + \sum_{i=1}^{\ell} u_i(t) X_i(q), \qquad q \in M, \tag{2.1.1}$$

where the control functions u are taken in $L^\infty(\mathbb{R}, U)$. The vector field X_0 is called the *drift*. The *reachable set* from $q_0 \in M$ is

$$\begin{aligned}\mathrm{Reach}(q_0) :=\{&q \in M \mid \exists\, u, T \text{ s.t. the solution to (2.1.1) with } q(0) = q_0 \\ &\text{satisfies } q(T) = q\}.\end{aligned}$$

System (2.1.1) is said to be *controllable* if $\mathrm{Reach}(q_0) = M$ for all $q_0 \in M$.

The family of vector fields $X_0, X_1, \dots, X_\ell$ is said to be *Lie bracket generating* if

$$\dim(\mathrm{Lie}_q\{X_0, X_1, \dots, X_\ell\}) = n$$

for all $q \in M$, where $\mathrm{Lie}_q\{X_0, X_1, \dots, X_\ell\}$ denotes the evaluation at q of the Lie algebra generated by $X_0, X_1, \dots, X_\ell$.

The following is a basic result in geometric control theory (see, for example, [73, Section 4.6]). Recall that a complete vector field X on M is said to be *recurrent* if for every open nonempty subset V of M and every time $t > 0$, there exists $\tilde{t} > t$ such that $\phi_{\tilde{t}}(V) \cap V \neq \emptyset$, where $\phi_{\tilde{t}}$ denotes the flow of X at time $\tilde{t}$.

Theorem 2.1.1. *Let $U \subset \mathbb{R}^m$ be a neighborhood of the origin. If X_0 is recurrent and the family $X_0, X_1, \dots, X_\ell$ is Lie bracket generating, then system (2.1.1) is controllable.*

A useful test to check that the Lie bracket generating condition holds true is given by the following simple lemma, whose proof is given for completeness.

Lemma 2.1.2. *If the family of analytic vector fields $X_0, X_1, \dots, X_\ell$ is Lie bracket generating on the complement of a subset $N \subset M$ and* $\mathrm{Reach}(q) \not\subset N$*, for all $q \in N$, then the family is Lie bracket generating on M.*

Proof. Let $q \in N$ and $q_1 \in \mathrm{Reach}(q) \setminus N$. By the Orbit theorem applied to the case of analytic vector fields (see, e.g., [7, Chapter 5]) the dimension of $\mathrm{Lie}_q\{X_0, X_1, \dots, X_\ell\}$ and $\mathrm{Lie}_{q_1}\{X_0, X_1, \dots, X_\ell\}$ coincide. By assumption the latter is equal to n, which implies that the same is true for the former. □

2.2 Symmetric molecule

2.2.1 The classical dynamics of a molecule subject to electric fields

Since the translational motion (of the center of mass) of a rigid body is decoupled from the rotational motion, we shall assume that the molecule can only rotate around its center of mass. In detail, for any vector $v \in \mathbb{R}^3$, denoting by e_1, e_2, e_3 a fixed orthonormal frame of $\mathbb{R}^3$ and by a_1, a_2, a_3 a moving orthonormal frame with the same orientation, both attached to the rigid body's center of mass, the configuration of the molecule is identified with the unique $g \in \mathrm{SO}(3)$ such that $g\ (x, y, z)^T = (X, Y, Z)^T$, where (x, y, z) are the coordinates of v with respect to a_1, a_2, a_3, and (X, Y, Z) are the coordinates of v with respect to e_1, e_2, e_3. In order to describe the equations on the tangent bundle $\mathrm{SO}(3) \times \mathfrak{so}(3)$, we shall make use of the isomorphism of Lie algebras

$$a : (\mathbb{R}^3, \times) \to (\mathfrak{so}(3), [\cdot, \cdot]), \quad P = \begin{pmatrix} P_1 \\ P_2 \\ P_3 \end{pmatrix} \mapsto a(P) = \begin{pmatrix} 0 & -P_3 & P_2 \\ P_3 & 0 & -P_1 \\ -P_2 & P_1 & 0 \end{pmatrix} \tag{2.2.1}$$

where $\times$ is the vector product. As external forces to control the rotation of the molecule, we consider three orthogonal electric fields with intensities $u_1(t), u_2(t), u_3(t)$ and directions e_1, e_2, e_3. We assume that

$$(u_1, u_2, u_3) \in U \subset \mathbb{R}^3, \quad (0, 0, 0) \in \mathrm{Interior}(U),$$

that is, the set $U \subset \mathbb{R}^3$ of admissible values for the triple (u_1, u_2, u_3) is a neighborhood of the origin. Denoting by δ the dipole of the molecule written in the moving frame, the three forces due to the interaction with the electric fields are $u_i(t)(g^{-1}(t)e_i) \times \delta$, $i = 1, 2, 3$. Then, the equations for the classical rotational dynamics of a molecule with inertia moments I_1, I_2, I_3 controlled with electric fields read

$$\begin{pmatrix} \dot{g} \\ \dot{P} \end{pmatrix} = X(g, P) + \sum_{i=1}^{3} u_i(t) Y_i(g, P), \quad (g, P) \in \mathrm{SO}(3) \times \mathbb{R}^3,\ u \in U, \tag{2.2.2}$$

where

$$X(g, P) := \begin{pmatrix} g\, a(\rho P) \\ P \times (\rho P) \end{pmatrix}, \quad Y_i(g, P) := \begin{pmatrix} 0 \\ (g^{-1} e_i) \times \delta \end{pmatrix}, \quad i = 1, 2, 3, \tag{2.2.3}$$

and $P = (P_1, P_2, P_3)^T$, $\rho P = (P_1/I_1, P_2/I_2, P_3/I_3)^T$. Similarly to [73, Section 12.2] (where this is done for the heavy rigid body), these equations can be derived as Hamilton equations corresponding to the Hamiltonian

$$H = \frac{1}{2}\left(\frac{P_1^2}{I_1} + \frac{P_2^2}{I_2} + \frac{P_3^2}{I_3}\right) + V(g), \quad V(g) = -\sum_{i=1}^{3} u_i \langle (g^{-1} e_i), \delta \rangle$$

on $\mathrm{SO}(3) \times \mathbb{R}^3$. System (2.2.2) can be seen as a control-affine system with $\ell = 3$ controlled fields.

Rotating molecule dynamics can also be represented in terms of quaternions, lifting the dynamics from $\mathrm{SO}(3)$ to the 3-sphere S^3, as follows. We denote by $\mathbb{H}$ the space of quaternions and we identify $S^3 \subset \mathbb{R}^4$ with

$\{q_0+\mathrm{i}q_1+\mathrm{j}q_2+\mathrm{k}q_3 \in \mathbb{H} \mid q_0^2+q_1^2+q_2^2+q_3^2 = 1\}$. We also identify $\mathbb{R}^3$ with $\{\mathrm{i}P_1+\mathrm{j}P_2+\mathrm{k}P_3 \in \mathbb{H} \mid (P_1, P_2, P_3) \in \mathbb{R}^3\}$. Via this identification, the vector product $P \times \Omega$ becomes $\frac{1}{2}[P, \Omega] := \frac{1}{2}(P\Omega - \Omega P)$, for any $P, \Omega \in \mathbb{R}^3$. Moreover, given $q = \cos(\alpha) + (q_1, q_2, q_3)\sin(\alpha) \in S^3$ and $P \in \mathbb{R}^3$, the quaternion product $qP\overline{q}$ is in $\mathbb{R}^3$ and corresponds to the rotation of P of angle 2α around the axis (q_1, q_2, q_3). Hence, S^3 can be seen as a double covering space of SO(3) (see [1, Section 5.2] for further details). System (2.2.2) is lifted to $S^3 \times \mathbb{R}^3$ to the system

$$\begin{cases} \dfrac{dq(t)}{dt} = q(t)\rho P(t), \\ \dfrac{dP(t)}{dt} = \dfrac{1}{2}[P(t), \rho P(t)] + \dfrac{u_1(t)}{2}[\overline{q(t)}\mathrm{i}q(t), \delta] + \dfrac{u_2(t)}{2}[\overline{q(t)}\mathrm{j}q(t), \delta] \\ \qquad\qquad + \dfrac{u_3(t)}{2}[\overline{q(t)}\mathrm{k}q(t), \delta]. \end{cases} \tag{2.2.4}$$

We are going to use the quaternion representation in order to prove that the vector fields characterizing (2.2.4) form a Lie bracket generating family. As a consequence, the same will be true for (2.2.2).

2.2.2 Non-controllability of the classical genuine symmetric-top

In most cases of physical interest, the electric dipole δ of a symmetric-top molecule lies along the symmetry axis of the molecule. If $I_1 = I_2$, the symmetry axis is the third one, and we have that $\delta = (0, 0, \delta_3)^T$, $\delta_3 \neq 0$, in the body frame. The corresponding molecule is called a *genuine symmetric-top* ([68, Section 2.6]).

Theorem 2.2.1. *The third angular momentum P_3 is a conserved quantity for the controlled motion* (2.2.2) *of the genuine symmetric-top molecule.*

Proof. In order to compute the equation satisfied by P_3 in (2.2.2), notice that

$$P(t) \times \rho P(t) = \begin{pmatrix} P_1(t) \\ P_2(t) \\ P_3(t) \end{pmatrix} \times \begin{pmatrix} P_1(t)/I_2 \\ P_2(t)/I_2 \\ P_3(t)/I_3 \end{pmatrix} = \begin{pmatrix} \left(\frac{1}{I_3} - \frac{1}{I_2}\right)P_2(t)P_3(t) \\ \left(\frac{1}{I_2} - \frac{1}{I_3}\right)P_1(t)P_3(t) \\ 0 \end{pmatrix}.$$

Moreover, $u_i(t)(g^{-1}(t)e_i) \times \delta = u_i(t)(g^{-1}(t)e_i) \times (0, 0, \delta_3)^T = (\star, \star, 0)^T$. Hence, for a genuine symmetric-top, the equation for P_3 becomes $\frac{dP_3(t)}{dt} = 0$. □

As a consequence, the controlled dynamics live in the hypersurfaces $\{P_3 = \text{const}\}$ and hence system (2.2.2) is not controllable in the 6-dimensional manifold $\mathrm{SO}(3) \times \mathbb{R}^3$.

2.2.3 Controllability of the classical accidentally symmetric-top

In Theorem 2.2.1 we proved that P_3 is a first integral for equations (2.2.2), using both the symmetry of the mass and the symmetry of the charge, meaning that $I_1 = I_2$ and $\delta = (0, 0, \delta_3)^T$. We consider now a symmetric-top molecule with electric dipole δ not along the symmetry axis of the body, that is, $\delta = (\delta_1, \delta_2, \delta_3)^T$, with $\delta_1 \neq 0$ or $\delta_2 \neq 0$. This system is usually called *accidentally symmetric-top* ([68, Section 2.6]).

Theorem 2.2.2. *For an accidentally symmetric-top molecule system* (2.2.2) *is controllable.*

Proof. The drift X is recurrent, as observed in [7, Section 8.4]. Thus, by Theorem 2.1.1, to prove controllability it suffices to show that, for any $(g, P) \in \mathrm{SO}(3) \times \mathbb{R}^3$, $\dim\Big(\mathrm{Lie}_{(g,P)}\{X, Y_1, Y_2, Y_3\}\Big) = 6$. Actually, we will find six vector fields in $\mathrm{Lie}\{X, Y_1, Y_2, Y_3\}$ whose span is six-dimensional everywhere but on a set of positive codimension, and we will conclude by applying Lemma 2.1.2. Notice that $[X, Y_i](g, P) = \begin{pmatrix} -g\, a(\rho[(g^{-1})e_i \times \delta]) \\ \star \end{pmatrix}$. Denote by $\Pi_{\mathrm{SO}(3)}$ the projection onto the SO(3) part of the tangent bundle, that is, $\Pi_{\mathrm{SO}(3)} : T(\mathrm{SO}(3) \times \mathbb{R}^3) \to T\mathrm{SO}(3)$. Then we have

$$\begin{aligned} &\mathrm{span}\{\Pi_{\mathrm{SO}(3)}X(g, P), \Pi_{\mathrm{SO}(3)}[X, Y_1](g, P), \Pi_{\mathrm{SO}(3)}[X, Y_2](g, P), \Pi_{\mathrm{SO}(3)}[X, Y_3](g, P)\} \\ &\quad = g\, a\Big(\rho[\{\delta\}^\perp \oplus \mathrm{span}\{P\}]\Big). \end{aligned}$$

Hence, if $\langle P, \delta\rangle \neq 0$, we have

$$\begin{aligned} &\dim\Big(\mathrm{span}\{\Pi_{\mathrm{SO}(3)}X(g, P), \Pi_{\mathrm{SO}(3)}[X, Y_1](g, P), \Pi_{\mathrm{SO}(3)}[X, Y_2](g, P), \\ &\qquad \Pi_{\mathrm{SO}(3)}[X, Y_3](g, P)\}\Big) = 3. \end{aligned} \tag{2.2.5}$$

To go further in the analysis, it is convenient to use the quaternion parametrization (2.2.4) in which every field is polynomial. We have, in coordinates $q = (q_0, q_1, q_2, q_3) \in S^3$, $P = (P_1, P_2, P_3) \in \mathbb{R}^3$,

$$X(q,P) = \begin{pmatrix} q\rho P \\ \frac{1}{2}[P, \rho P] \end{pmatrix} = \begin{pmatrix} -q_1\frac{P_1}{I_2} - q_2\frac{P_2}{I_2} - q_3\frac{P_3}{I_3} \\ q_0\frac{P_1}{I_2} + q_2\frac{P_3}{I_3} - q_3\frac{P_2}{I_2} \\ q_0\frac{P_2}{I_2} - q_1\frac{P_3}{I_3} + q_3\frac{P_1}{I_2} \\ q_0\frac{P_3}{I_3} + q_1\frac{P_2}{I_2} - q_2\frac{P_1}{I_2} \\ \left(\frac{1}{I_3} - \frac{1}{I_2}\right)P_2P_3 \\ \left(\frac{1}{I_2} - \frac{1}{I_3}\right)P_1P_3 \\ 0 \end{pmatrix},$$

$$Y_1(q,P) = \begin{pmatrix} 0 \\ \frac{1}{2}[\overline{q}\mathrm{i}q, \delta] \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ (q_1q_2 - q_0q_3)\delta_3 - (q_1q_3 + q_0q_2)\delta_2 \\ (q_1q_3 + q_0q_2)\delta_1 - \frac{1}{2}(q_0^2 + q_1^2 - q_2^2 - q_3^2)\delta_3 \\ \frac{1}{2}(q_0^2 + q_1^2 - q_2^2 - q_3^2)\delta_2 - (q_1q_2 - q_0q_3)\delta_1 \end{pmatrix},$$

$$Y_2(q,P) = \begin{pmatrix} 0 \\ \frac{1}{2}[\overline{q}\mathrm{j}q, \delta] \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \frac{1}{2}(q_0^2 - q_1^2 + q_2^2 - q_3^2)\delta_3 - (q_2q_3 - q_0q_1)\delta_2 \\ (q_2q_3 - q_0q_1)\delta_1 - (q_1q_2 + q_0q_3)\delta_3 \\ (q_1q_2 + q_0q_3)\delta_2 - \frac{1}{2}(q_0^2 - q_1^2 + q_2^2 - q_3^2)\delta_1 \end{pmatrix}.$$

Let us consider the six vector fields $X, Y_1, Y_2, [X, Y_1], [X, Y_2], [[X, Y_1], Y_1]$: we have that the determinant of the matrix obtained by removing the first row from the 7×6 matrix

$$(X(q,P), Y_1(q,P), Y_2(q,P), [X,Y_1](q,P), [X,Y_2](q,P), [[X,Y_1],Y_1](q,P))$$

is equal to $D(q,P) := S(q)\langle P, \delta\rangle$, where $S(q) = S_1(q)S_2(q)S_3(q)S_4(q)$ and

$$\begin{aligned}
S_1(q) &:= \frac{I_2 - I_3}{32 I_2^3 I_3^2} q_1, \\
S_2(q) &:= (-2q_1q_2\delta_1 + 2q_0q_3\delta_1 + q_0^2\delta_2 + q_1^2\delta_2 - (q_2^2 + q_3^2)\delta_2), \\
S_3(q) &:= (q_0(-2q_2\delta_1 + 2q_1\delta_2) + 2q_3(q_1\delta_1 + q_2\delta_2) + (q_0^2 - q_1^2 - q_2^2 + q_3^2)\delta_3)^2, \\
S_4(q) &:= (-2(q_0q_2 + q_1q_3)(\delta_1^2 + \delta_2^2) + ((q_0^2 + q_1^2 - q_2^2 - q_3^2)\delta_1 + 2(q_1q_2 - q_0q_3)\delta_2)\delta_3), \\
\langle P, \delta\rangle &= P_1\delta_1 + P_2\delta_2 + P_3\delta_3.
\end{aligned}$$

Remark 2.2.3. As a byproduct of this computation, we notice that when $\delta = (0, 0, \delta_3)$ then $S_2 \equiv 0$ and thus $D \equiv 0$. This is a signature of the non-controllability of the genuine symmetric-top, proved in Theorem 2.2.1.

Hence, for all (q, P) such that $D(q, P) \neq 0$,

$$\begin{aligned}
\dim \Big(\mathrm{span}\{&X(q,P), Y_1(q,P), Y_2(q,P), [X,Y_1](q,P), [X,Y_2](q,P), \\
&[[X,Y_1],Y_1](q,P)\}\Big) = 6,
\end{aligned}$$

that is, outside the set $N := \{(q,P) \in S^3 \times \mathbb{R}^3 \mid D(q,P) = 0\}$ the family X, Y_1, Y_2 is Lie bracket generating.

Now we are left to prove that $\mathrm{Reach}(q,P) \not\subset N$ for every $(q,P) \in N$, and then to apply Lemma 2.1.2. Let us start by considering the factor $\langle P, \delta\rangle$ of D and notice that, for any fixed $q \in S^3$, $Q := \{P = (P_1, P_2, P_3) \in \mathbb{R}^3 \mid \langle P, \delta\rangle = 0\}$ defines a surface inside $\{q\} \times \mathbb{R}^3$. Denote by $\Pi_{\mathbb{R}^3} : T(S^3 \times \mathbb{R}^3) \to T\mathbb{R}^3$ the projection onto the $\mathbb{R}^3$ part of the tangent bundle. The vector field $\Pi_{\mathbb{R}^3}X$ is tangent to $Q = \{\langle P, \delta\rangle = 0\}$ if and only if

$$\langle \Pi_{\mathbb{R}^3}X|_Q, \nabla D|_Q\rangle = 0 \Leftrightarrow \langle [P, \rho P]|_Q, \delta\rangle = 0 \Leftrightarrow \delta \in \mathrm{span}\{P|_Q, \rho P|_Q\} \Leftrightarrow \delta \in \mathrm{span}\{\rho P|_Q\},$$

where in the second equivalence we used that $\operatorname{rank}(P, \rho P) = 2$ as long as the top is not spherical, i.e., as long as the inertia contants do not satisfy $I_1 = I_2 = I_3$, and in the last equivalence we used that $\langle P, \delta\rangle|_Q = 0$. Then, we obtain that $\Pi_{\mathbb{R}^3} X$ is tangent to Q if and only if

$$P = t\begin{pmatrix}\delta_1 I_1\\ \delta_2 I_2\\ \delta_3 I_3\end{pmatrix}, \quad t \in \mathbb{R}.$$

Using again that $\langle P, \delta\rangle|_Q = 0$, we see that $\langle t(\delta_1 I_1, \delta_2 I_2, \delta_3 I_3)^T, (\delta_1, \delta_2, \delta_3)^T\rangle = 0$, implying $t = 0$. Finally, we have seen that $\Pi_{\mathbb{R}^3} X$ is tangent to Q if and only if $P = 0$; as $\Pi_{\mathbb{R}^3} Y_i(q, P = 0) \neq 0$, for any $i = 1, 2, 3$, we conclude that the distribution spanned by $\{\Pi_{\mathbb{R}^3} X, \Pi_{\mathbb{R}^3} Y_i\}$ is not tangent to Q. Summarizing, we have

$$\operatorname{Reach}(q, P) \not\subset \{\langle P, \delta\rangle = 0\}, \quad \forall (q, P) \in \{\langle P, \delta\rangle = 0\}.$$

To conclude, if $(q, P) \in \{S_i = 0\}$, $i = 1, \dots, 4$, then we fix P and we get two-dimensional strata $\{q \in S^3 \mid S_i(q) = 0\} \subset S^3$. Now the projections of the vector fields $X, [X, Y_1], [X, Y_2], [X, Y_3]$ on the base part of the bundle span a three-dimensional vector space if $\langle P, \delta\rangle \neq 0$, as observed in (2.2.5). So, by possibly steering P to a point where $\langle P, \delta\rangle \neq 0$, it is possible to exit from the union of $\{S_i = 0\}$. This concludes the proof of the theorem. □

2.2.4 Reachable sets of the classical genuine symmetric-top

Theorem 2.2.1 states that each hypersurface $\{P_3 = \text{const}\}$ is invariant for the controlled motion. Next we prove that the restriction of system (2.2.2) to any such hypersurface is controllable.

Theorem 2.2.4. *Let $I_1 = I_2$ and $\delta = (0, 0, \delta_3)^T$, $\delta_3 \neq 0$. Then for $(g_0, P_0) \in \mathrm{SO}(3) \times \mathbb{R}^3$, $P_0 = (P_{01}, P_{02}, P_{03})$, one has*

$$\operatorname{Reach}(g_0, P_0) = \{(g, P) \in \mathrm{SO}(3) \times \mathbb{R}^3 \mid P_3 = P_{03}\}.$$

Proof. From Theorem 2.2.1 we know that $\{P_3 = \text{const}\}$ is invariant. Since the drift X is recurrent, it suffices to prove that system (2.2.2) is Lie bracket generating on the 5-dimensional manifold $\{P_3 = \text{const}\}$.

We recall from (2.2.5) that, if $\langle P, \delta\rangle \neq 0$, that is, if $P_3 \neq 0$, we have

$$\begin{aligned}\dim\Big(\operatorname{span}\{&\Pi_{\mathrm{SO}(3)} X(g, P), \Pi_{\mathrm{SO}(3)}[X, Y_1](g, P), \Pi_{\mathrm{SO}(3)}[X, Y_2](g, P),\\ &\Pi_{\mathrm{SO}(3)}[X, Y_3](g, P)\}\Big) = 3.\end{aligned}$$

Moreover, since $\Pi_{\mathbb{R}^3} Y_i(q, P) = (g^{-1} e_i) \times \delta$ for $i = 1, 2, 3$, we have that

$$\dim\Big(\operatorname{span}\{\Pi_{\mathbb{R}^3} Y_1, \Pi_{\mathbb{R}^3} Y_2, \Pi_{\mathbb{R}^3} Y_3\}\Big) = 2 \tag{2.2.6}$$

everywhere. Thus, if $P_3 \neq 0$, it follows that

$$\begin{aligned}\dim\Big(\operatorname{span}\{&X(g, P), Y_1(g, P), Y_2(g, P), Y_3(g, P), [X, Y_1](g, P), [X, Y_2](g, P),\\ &[X, Y_3](g, P)\}\Big) = 5.\end{aligned}$$

So the system is Lie bracket generating on the manifold $\{P_3 = \text{const} \neq 0\}$.

We are left to consider the case $P_3 = 0$. Notice that $\Pi_{\mathbb{R}^3} Y_1, \Pi_{\mathbb{R}^3} Y_2, \Pi_{\mathbb{R}^3} Y_3$ span a two-dimensional distribution for any value of P_3. So we consider in the quaternion parametrization the projections of $X, [X, Y_1], [X, Y_2], [[X, Y_1], X]$ on the S^3 part of the bundle and we obtain

$$\begin{aligned}\dim\Big(\operatorname{span}\{&\Pi_{S^3} X(q, P), \Pi_{S^3}[X, Y_1](q, P), \Pi_{S^3}[X, Y_2](q, P),\\ &\Pi_{S^3}[[X, Y_1], X](q, P)\}\Big) = 3,\end{aligned}$$

for $P_3 = 0$, except when $q_3[2P_2(q_1 q_2 - q_0 q_3) + P_1(q_0^2 + q_1^2 - q_2^2 - q_3^2)] = 0$. This equation defines the union of two surfaces inside S^3. (Notice that we can assume $P_1 \neq 0$ and $P_2 \neq 0$ because (2.2.6) gives local controllability in (P_1, P_2)). On $\{q_3 = 0\}$, we have that $\Pi_{S^3} X$ is tangent if and only if $q_1 P_2 - q_2 P_1 = 0$. On the curve $\gamma \subset S^3$ of equation

$$\begin{cases} q_3 = 0,\\ q_1 P_2 - q_2 P_1 = 0,\end{cases}$$

we can consider the two-dimensional distribution spanned by $\Pi_{S^3}[X, Y_1], \Pi_{S^3}[X, Y_2], \Pi_{S^3}[X, Y_3]$, which is clearly not tangent to γ. Following Lemma 2.1.2, the system is Lie bracket generating also on $\{q_3 = 0\}$.

Analogously, on $\{2P_2(q_1q_2 - q_0q_3) + P_1(q_0^2 + q_1^2 - q_2^2 - q_3^2) = 0\}$ we consider the vector field $\Pi_{S^3}[[[X, Y_1], X], Y_2]$ which is tangent if and only if $(q_0q_2 + q_1q_3)(P_1q_0q_1 + P_2q_0q_2 - P_2q_1q_3 + P_1q_2q_3) = 0$. Again, since the distribution spanned by $\Pi_{S^3}[X, Y_1], \Pi_{S^3}[X, Y_2], \Pi_{S^3}[X, Y_3]$ is two-dimensional, we can exit from the set of equations

$$\begin{cases} 2P_2(q_1q_2 - q_0q_3) + P_1(q_0^2 + q_1^2 - q_2^2 - q_3^2) = 0, \\ (q_0q_2 + q_1q_3)(P_1q_0q_1 + P_2q_0q_2 - P_2q_1q_3 + P_1q_2q_3) = 0, \end{cases}$$

whose strata have dimension at most one. Thus, applying again Lemma 2.1.2, we can conclude that the restriction of the system to the manifold $\{P_3 = 0\}$ is Lie bracket generating. □

2.3 Asymmetric molecule

Here we prove the following:

Theorem 2.3.1. *Let $\delta \neq 0$. Assume that the molecule is asymmetric, that is, $0 < I_1 < I_2 < I_3$. Then,* (2.2.2) *is controllable.*

Proof. We follow the proof of Theorem 2.2.2 on the controllability of an accidentally symmetric top, pointing out the main differences. In quaternions parametrization (q, P) of $S^3 \times \mathbb{R}^3$ (as a double cover of $\mathrm{SO}(3) \times \mathbb{R}^3$) the determinant D of the 6×6 matrix obtained by removing the first row from the 7×6 matrix

$$(X(q, P), Y_1(q, P), Y_2(q, P), [X, Y_1](q, P), [X, Y_2](q, P), [[X, Y_1], Y_1](q, P))$$

now gives

$$D(q, P) = \langle P, \delta \rangle \, S_{\delta,(I_1,I_2,I_3)}(q),$$

where

$$\begin{aligned} S_{\delta,(I_1,I_2,I_3)}(q) = {} & (4I_1I_2I_3)^{-1} q_0 \big\{ q_0(-2q_2\delta_1 + 2q_1\delta_2) + 2q_3(q_1\delta_1 + q2\delta_2) + q_0^2\delta_3 - (q_1^2 + q_2^2 - q_3^2)\delta_3 \big\}^2 \\ & \times \big\{ (2I_1I_2I_3)[q_0q_2\delta_2 + q_1q_3\delta_2 - q_1q_2\delta_3 + q_0q_3\delta_3][2q_0\delta_1(q_3\delta_2 - q_2\delta_3) - 2q_1\delta_1(q_2\delta_2 + q_3\delta_3) \\ & + q_0^2(\delta_2^2 + \delta_3^2) + q_1^2(\delta_2^2 + \delta_3^2) - (q_2^2 + q_3^2)(\delta_2^2 + \delta_3^2)] \\ & + I_1 \big[I_2(-2q_1q_2\delta_1 + 2q_0q_3\delta_1 + q_0^2\delta_2 + q_1^2\delta_2 - (q_2^2 + q_3^2)\delta_2) \\ & \times [-2(q_0q_2 + q_1q_3)(\delta_1^2 + \delta_2^2) + (q_0^2\delta_1 + q_1^2\delta_1 - (q_2^2 + q_3^2)\delta_1 + 2q_1q_2\delta_2 - 2q_0q_3\delta_2)\delta_3] \\ & - I_3[-2(q_0q_2 + q_1q_3)\delta_1 + (q_0^2 + q_1^2 - q_2^2 - q_3^2)\delta_3][q_0^2\delta_1\delta_2 + q_1^2\delta_1\delta_2 - (q_2^2 + q_3^2)\delta_1\delta_2 + 2q_1q_3\delta_2\delta_3 \\ & - 2q_1q_2(\delta_1^2 + \delta_3^2) + 2q_0\{q_2\delta_2\delta_3 + q_3(\delta_1^2 + \delta_3^2)\}] \big] \big\} \end{aligned}$$

Remark 2.3.2. The main difference here w.r.t. the symmetric top case ($I_1 = I_2$ for, e.g., oblate symmetry) is that $S_{(0,0,\delta_3),(I_1,I_2,I_3)} \not\equiv 0$ if $I_1 < I_2 < I_3$, while $S_{(0,0,\delta_3),(I_2,I_2,I_3)} \equiv 0$ (cf. Remark 2.2.3): this means that this way we will also prove controllability for the case $\delta = (0, 0, \delta_3)^T$ (which is not controllable for a symmetric top, cf. Theorem 2.2.1).

Now the same proof of Theorem 2.2.2 shows that

$$\mathrm{Reach}(q, P) \not\subset \{\langle P, \delta \rangle = 0\}, \quad \forall (q, P) \in \{\langle P, \delta \rangle = 0\}.$$

We then conclude exactly as in the last part of the proof of Theorem 2.2.2: by possibly steering P to a point where $\langle P, \delta \rangle \neq 0$, the projection on TS^3 of the distribution spanned by the vector fields $X, [X, Y_1], [X, Y_2], [X, Y_3]$ is three-dimensional (as it is proven in (2.2.5), which always holds also in the asymmetric case $I_1 < I_2 < I_3$), and thus it cannot be tangent to the two-dimensional strata of $\{q \in S^3 \mid S_{\delta,(I_1,I_2,I_3)}(q) = 0\}$. Hence, $\mathrm{Reach}(q, P) \not\subset N$ for every $(q, P) \in N$, and the proof is concluded thanks to Lemma 2.1.2. □

Chapter 3

Quantum controllability of a rotating molecule

In this chapter we present a study on the controllability of the bilinear Schrödinger equation of a rotating symmetric- and asymmetric-top molecule. The molecule is modelled as a rigid rotor and is controlled through three orthogonal electric fields interacting with its electric dipole.

Both for the symmetric and the asymmetric system, we characterize the controllability in terms of the dipole configuration, fixed inside the molecular frame.

Concerning the symmetric-top, we summarize our findings in the following facts: if the dipole lies along the symmetry axis of the molecule, the rotations are not controllable, due to the presence of a conserved quantity, the third component of the angular momentum (it corresponds to the phenomenon already observed for the classical dynamics in Theorem 2.2.1); if the dipole is orthogonal to the symmetry axis, the rotations are not controllable, due to the superposition of degenerate states (it has no classical counterpart); if the dipole is not along the symmetry axis nor orthogonal to it, approximate controllability and stronger properties of the Schrödinger equation are proved to hold for the rotational dynamics, under a non-resonant assumption on the inertia moments.

Concerning the asymmetric-top, we prove that the rotational dynamics are not controllable if the dipole is parallel to any of the principal axis of inertia, and that any other configuration of the dipole yields approximately controllable rotational dynamics and stronger properties, for almost all values of the inertia moments.

The chapter is organized as follows: in Section 3.1 we recall some notions of controllability and present some criteria to prove the approximate controllability and stronger properties of the multi-input bilinear Schrödinger equation; in Section 3.2 we apply this framework to a rotating symmetric-top; in Section 3.3 the framework is applied to a rotating asymmetric-top. In the Appendix 3.4 we give the proof of two important propositions.

In Section 3.1 we also present two original sufficient conditions for the approximate controllability of the bilinear Schrödinger equation, that are Corollary 3.1.20 and Theorem 3.1.21, which can be seen as consequences of the main controllability criteria stated in Corollary 3.1.16, and whose proof can be found in [28]. The results of Sections 3.2 and 3.3 are original, and in particular the approximate controllability of accidentally symmetric-tops and asymmetric-tops, for almost all values of the inertia moments, are proved resp. in Theorems 3.2.5 and 3.3.2.

The results on the quantum symmetric-top system are in the papers [33] and [35].

3.1 Controllability of the multi-input bilinear Schrödinger equation

3.1.1 Notions of controllability

Let $\ell \in \mathbb{N}$ and $U \subset \mathbb{R}^\ell$ be a neighborhood of the origin. Let $\mathcal{H}$ be an infinite-dimensional Hilbert space with scalar product $\langle \cdot, \cdot \rangle$ (linear in the first entry and conjugate linear in the second), $H, B_1, \dots, B_\ell$ be (possibly unbounded) self-adjoint operators on $\mathcal{H}$, with domains $D(H), D(B_1), \dots, D(B_\ell)$. We consider the controlled Schrödinger equation

$$\mathrm{i}\frac{d\psi(t)}{dt} = (H + \sum_{j=1}^{\ell} u_j(t)B_j)\psi(t), \quad \psi(t) \in \mathcal{H}, \quad u(t) \in U. \tag{3.1.1}$$

Definition 3.1.1. • We say that the operator H satisfies ($\mathbb{A}1$) if it has discrete spectrum with infinitely many distinct eigenvalues (possibly degenerate).
Denote by $\mathcal{B}$ a Hilbert basis $(\phi_k)_{k\in\mathbb{N}}$ of $\mathcal{H}$ made of eigenvectors of H associated with the family of eigenvalues $(\lambda_k)_{k\in\mathbb{N}}$ and let $\mathcal{L}$ be the set of finite linear combination of eigenstates, that is,

$$\mathcal{L} = \operatorname{span}\{\phi_k \mid k \in \mathbb{N}\}.$$

- We say that $(H, B_1, \dots, B_\ell, \mathcal{B})$ satisfies ($\mathbb{A}2$) if $\phi_k \in D(B_j)$ for every $k \in \mathbb{N}$, $j = 1, \dots, \ell$.
- We say that $(H, B_1, \dots, B_\ell, \mathcal{B})$ satisfies ($\mathbb{A}3$) if

$$H + \sum_{j=1}^{\ell} u_j B_j : \mathcal{L} \to \mathcal{H}$$

  is essentially self-adjoint for every $u \in U$.
- We say that $(H, B_1, \dots, B_\ell, \mathcal{B})$ satisfies ($\mathbb{A}$) if H satisfies ($\mathbb{A}1$) and $(H, B_1, \dots, B_\ell, \mathcal{B})$ satisfies ($\mathbb{A}2$) and ($\mathbb{A}3$).

If $(H, B_1, \dots, B_\ell, \mathcal{B})$ satisfies ($\mathbb{A}$) then, for every $(u_1, \dots, u_\ell) \in U$, $H + \sum_{j=1}^{\ell} u_j B_j$ generates a one-parameter group $e^{-\mathrm{i}t(H+\sum_{j=1}^{\ell} u_j B_j)}$ inside the group of unitary operators $U(\mathcal{H})$. It is therefore possible to define the propagator Γ_T^u at time T of system (3.1.1) associated with a piecewise constant control law $u(\cdot) = (u_1(\cdot), \dots, u_\ell(\cdot))$ by composition of flows of the type $e^{-\mathrm{i}t(H+\sum_{j=1}^{\ell} u_j B_j)}$.

Definition 3.1.2. Let $(H, B_1, \dots, B_\ell, \mathcal{B})$ satisfy ($\mathbb{A}$).

- Given ψ_0, ψ_1 in the unit sphere $\mathcal{S}$ of $\mathcal{H}$, we say that ψ_1 is reachable from ψ_0 if there exist a time $T > 0$ and a piecewise constant control law $u : [0, T] \to U$ such that $\psi_1 = \Gamma_T^u(\psi_0)$. We denote by $\operatorname{Reach}(\psi_0)$ the set of reachable points from ψ_0.
- We say that (3.1.1) is approximately controllable if for every $\psi_0 \in \mathcal{S}$ the set $\operatorname{Reach}(\psi_0)$ is dense in $\mathcal{S}$.

By fully exploiting the geometric control theory behind our technique, we will actually obtain a stronger controllability property for (3.1.1). For this reason, let us introduce the notion of module-tracker (m-tracker, for brevity) that is, a system for which any given curve can be tracked up to (relative) phases. The identification up to phases of elements of $\mathcal{H}$ in the basis $\mathcal{B} = (\phi_k)_{k\in\mathbb{N}}$ can be accomplished by the projection

$$\mathcal{M} : \psi \mapsto \sum_{k\in\mathbb{N}} |\langle \phi_k, \psi\rangle| \phi_k.$$

Definition 3.1.3. Let $(H, B_1, \dots, B_\ell, \mathcal{B})$ satisfy ($\mathbb{A}$). We say that system (3.1.1) is an *m-tracker* if, for every $r \in \mathbb{N}$, $\psi_1, \dots, \psi_r$ in $\mathcal{H}$, $\widehat{\Gamma} : [0, T] \to U(\mathcal{H})$ continuous with $\widehat{\Gamma}_0 = \mathrm{Id}_{\mathcal{H}}$, and $\epsilon > 0$, there exists an invertible increasing continuous function $\tau : [0, T] \to [0, T_\tau]$ and a piecewise constant control $u : [0, T_\tau] \to U$ such that

$$\|\mathcal{M}(\widehat{\Gamma}_t \psi_k) - \mathcal{M}(\Gamma^u_{\tau(t)} \psi_k)\| < \epsilon, \qquad k = 1, \dots, r,$$

for every $t \in [0, T_\tau]$.

Remark 3.1.4. We recall that if system (3.1.1) is an m-tracker, then it is also approximately controllable, as noticed in [28, Remark 2.9].

If a system is an m-tracker and the control system is weakly coupled, then approximate controllability holds also in higher norms. Thanks to spectral calculus, we define for $s > 0$

$$|H|^s \psi = \sum_{n\in\mathbb{N}} |\lambda_n|^s \langle \psi, \phi_n\rangle \phi_n$$

for every ψ belonging to

$$\mathcal{D}(|H|^s) := \left\{ \psi \in \mathcal{H} \mid \sum_{n\in\mathbb{N}} |\lambda_n|^{2s} |\langle \psi, \phi_n\rangle|^2 < \infty \right\}.$$

We consider the s-norm defined on $\mathcal{D}(|H|^s)$ as $\|\cdot\|_s := \||H|^s \cdot\|$.

Definition 3.1.5. We say that (3.1.1) is *approximately controllable in the s-norm* if, for every $\psi^{\text{in}}, \psi^{\text{fin}} \in \mathcal{D}(|H|^s)$ of norm one, and $\epsilon > 0$, there exists a piecewise constant control $u : [0,T] \to U$ such that

$$\|\Gamma_T^u(\psi^{\text{in}}) - \psi^{\text{fin}}\|_s < \epsilon.$$

We say that $(H, B_1, \dots, B_\ell, \mathcal{B})$ satisfies $(\mathbb{A}')$ if it satisfies $(\mathbb{A})$ and

- the operator $H + \sum_{j=1}^{\ell} u_j B_j$ is bounded from below for every $u \in \mathbb{R}^\ell$;
- the sequence $(\lambda_k)_{k\in\mathbb{N}}$ of eigenvalues of H is positive non-decreasing and accumulates at ∞.

Definition 3.1.6. Let $(H, B_1, \dots, B_\ell, \mathcal{B})$ satisfy $(\mathbb{A}')$ and let $s > 0$. We say that $(H, B_1, \dots, B_\ell)$ is s-weakly coupled if $\mathcal{D}(|H + \sum_{j=1}^{\ell} u_j B_j|^{s/2}) = \mathcal{D}(|H|^{s/2})$ for every $u \in \mathbb{R}^\ell$ and there exists C such that

$$|\Re\langle |H|^s\psi, B_j\psi\rangle| \le C|\langle |H|^s\psi, \psi\rangle|,$$

for every $j = 1, \dots, \ell$ and $\psi \in \mathcal{D}(|H|^s)$.

Remark 3.1.7. We recall that if system (3.1.1) satisfies $(\mathbb{A}')$, is an m-tracker and is s-weakly coupled, then it is also approximately controllable in the $s/2$-norm for every $s > 0$ [28, Corollary 2.13] (see also [37, Proposition 5]). We notice that if the controls B_i are bounded operators and $(\lambda_k)_{k\in\mathbb{N}}$ is positive non-decreasing and accumulates at ∞, then (3.1.1) is s-weakly coupled for every $s > 0$.

Another useful notion of controllability for quantum mechanical systems is given in the sense of density matrices. Recall that a density matrix ρ is a non-negative, self-adjoint operator of trace class, whose trace is normalized to one. Its time evolution is determined by

$$\rho(t) = \Gamma_t^u \rho(0) \Gamma_t^{u*},$$

where Γ_t^{u*} is the adjoint of Γ_t^u. After the above definition of time evolution for the density matrix, $\rho(t)$ is necessarily unitary equivalent to $\rho(0)$.

Definition 3.1.8. Let $(H, B_1, \dots, B_\ell, \mathcal{B})$ satisfy $(\mathbb{A})$. We say that (3.1.1) is approximately controllable is the sense of density matrices if for every pair of unitary equivalent density matrices ρ_0, ρ_1 and every $\epsilon > 0$ there exists a piecewise constant control $u : [0,T] \to U$ such that

$$\|\rho_1 - \Gamma_T^u \rho_0 \Gamma_T^{u*}\|_{\mathcal{L}(\mathcal{H})} < \epsilon,$$

for the operator norm on the set of bounded operators $\mathcal{L}(\mathcal{H})$ acting on the Hilbert space $\mathcal{H}$.

Remark 3.1.9. We recall that if system (3.1.1) is an m-tracker, then it is also approximately controllable in the sense of density matrices, as it follows from [28, Remark 2.9, Theorem 2.6] and [27, Proposition A.1].

Our notion of solution to (3.1.1) is given for piecewise constant controls u as a composition of time-independent flows. Hence, our definitions of controllability are given by means of piecewise constant controls. We can extend the notion of solution to (3.1.1) also for different classes of controls.

Definition 3.1.10.

- We say that $u \in L^\infty([0,T], \mathbb{R}^\ell)$ is admissible for (3.1.1) if $u(t) \in U$ for almost every $t \in [0,T]$ and, for every $\psi_0 \in \mathcal{H}$, there exists $\psi : [0,T] \to \mathcal{H}$ such that $\psi(0) = \psi_0$, the function $t \mapsto \langle \psi(t), \phi_k\rangle$ is absolutely continuous for every $k \in \mathbb{N}$, and satisfies

$$\mathrm{i}\frac{d}{dt}\langle \phi_k, \psi(t)\rangle = \langle (H + \sum_{j=1}^{\ell} u_j(t) B_j)\phi_k, \psi(t)\rangle$$

  for almost every $t \in [0,T]$. The function $t \mapsto \psi(t)$ is called the solution of (3.1.1) with initial condition $\psi_0 \in \mathcal{H}$ associated with the control u.
- If $u \in L^\infty([0,T], \mathbb{R}^\ell)$ is admissible for (3.1.1), we call the propagator of (3.1.1) associated with u the map $[0,T] \ni t \mapsto \Gamma_t^u$, where, for any $\psi_0 \in \mathcal{H}$, $\Gamma_t^u\psi_0$ is the evaluation at time t of the solution of (3.1.1) having ψ_0 as initial condition.

Remark 3.1.11.

- If $u : [0,T] \to U$ is piecewise constant, then u is admissible for (3.1.1) and we recover the notion of propagator as a composition of time-independent flows.
- Let $a > 0$ such that $[-a,a]^\ell \subset U$. If $u \in C^1([0,T], [-a,a]^\ell)$ and $B_1, \dots, B_\ell$ are H-small with H-bound smaller than $1/a$ (see (5.3.2) for the definition of H-smallness), then u is admissible for (3.1.1), as a consequence of the Kato-Rellich theorem [100, Theorem X.12], and [100, Theorem X.70]. In particular, it applies if the control operators B_i are bounded.

As a consequence of the previous remark, the notions of controllability previously introduced can be extended to the class of smooth controls u, and all the following results hold in the class of piecewise constant controls and also in the class of smooth controls under the additional smallness assumption on the B_i.

3.1.2 Lie-Galerkin tracking condition

In this section we mostly follow [28] and [40] in order to state a sufficient condition for a system to be an m-tracker. At the end of this section we propose an original simultaneous approximate controllability result, particularly suited for controlled evolutions in the presence of symmetries.

For any $n \in \mathbb{N}$, we consider the projection

$$\Pi_n : \mathcal{H} \ni \psi \mapsto \sum_{j=1,\dots,n} \langle \phi_j, \psi \rangle \phi_j \in \mathcal{H}.$$

and we define $H^{(n)} = \Pi_n H \Pi_n$, $B_j^{(n)} = \Pi_n B_j \Pi_n$, $j = 1, \dots, \ell$. The set of spectral gaps of H for the n-dimensional truncation of the spectrum is defined as $\Sigma_n := \{|\lambda_i - \lambda_j|, i, j = 1, \dots, n\}$.

For every $\sigma \geq 0$, and every square matrix M of dimension m, let

$$\mathcal{E}_\sigma(M) = (M_{l,k} \delta_{\sigma, |\lambda_l - \lambda_k|})_{l,k=1,\dots,m},$$

where $\delta_{l,k}$ is the Kronecker delta. The $n \times n$ matrix $\mathcal{E}_\sigma(B_i^{(n)})$ corresponds to the activation in $B_i^{(n)}$ of the spectral gap $\sigma \in \Sigma_j$: every element is 0 except for the (l, k)-elements such that $|\lambda_l - \lambda_k| = \sigma$. We introduce

$$\Xi_n := \{(\sigma, l) \in \Sigma_n \times \{1, \dots, l\} \mid (B_j)_{k,l} \delta_{\sigma, |\lambda_l - \lambda_k|} = 0, \text{ for every } k = 1, \dots, n \text{ and } l > n\}.$$

To give a picture of the set Ξ_n, we notice that, if $(\sigma, l) \in \Xi_n$, then for every $N > n$

$$\mathcal{E}_\sigma(\mathrm{i}B_i^{(N)}) = \left[\begin{array}{c|c} \mathcal{E}_\sigma(\mathrm{i}B_i^{(n)}) & 0 \\ \hline 0 & * \end{array}\right],$$

and hence Ξ_n is the set of frequencies which preserve the finite-dimensional truncations of (3.1.1). We then define an operator which acts on the vector space of square matrices, W_ξ, $\xi \in S^1 \subset \mathbb{C}$, defined by

$$(W_\xi(M))_{l,k} = \begin{cases} \xi M_{l,k}, & \lambda_l < \lambda_k, \\ 0, & \lambda_l = \lambda_k, \\ \bar{\xi} M_{l,k}, & \lambda_l > \lambda_k. \end{cases} \tag{3.1.2}$$

We remark that the definition of W_ξ is motivated by the following formula of Lie algebraic nature

$$\sigma W_{\mathrm{i}} \mathcal{E}_\sigma(B_j^{(n)}) = \left[\mathcal{E}_\sigma(B_j^{(n)}), H^{(n)}\right]. \tag{3.1.3}$$

Then, we consider the set of effective auxiliary matrices

$$\nu_n := \{W_\xi(\mathcal{E}_\sigma(\mathrm{i}B_i^{(n)})) \mid (\sigma, i) \in \Xi_n, \sigma \neq 0, \xi \in S^1\}$$

acting on $\Pi_n \mathcal{H} \cong \mathbb{C}^n$. Denote by $\|\cdot\|_{L(\Pi_n \mathcal{H}, \mathcal{H})}$ the norm on the space of linear operators from $\Pi_n \mathcal{H}$ to $\mathcal{H}$. We have the following averaging result on periodic excitations, proved in [40, Lemma 3.2] and inspired by [41, Theorem 1]:

Lemma 3.1.12. *Let $n \in \mathbb{N}$, $j \in \{1, \dots, l\}$ and $\sigma > 0$ such that $(\sigma, l) \in \Xi_n$. Fix also $0 < a < b$ and an admissible periodic control of period $T = 2\pi/\sigma$ that is non-vanishing at the j-th component only: $u = (0, \dots, 0, v, 0, \dots, 0) \in \mathbb{R}^l$. Assume moreover that $\int_0^T v(t)dt = 0$, $\int_0^T v(t)e^{\mathrm{i}\sigma t}dt = \alpha$ and $\int_0^T v(t)e^{\mathrm{i}m\sigma t}dt = 0$ for every $m \geq 2$ such that $m\sigma \in \Sigma_n$. Then*

$$\lim_{K \to \infty} \|\Gamma_{KT}^{\tau u/K} - e^{-\mathrm{i}KTH} \exp(\tau\alpha \mathcal{E}_\sigma(\mathrm{i}B_j^{(n)}))\|_{L(\Pi_n \mathcal{H}, \mathcal{H})} = 0,$$

uniformly w.r.t. $\tau \in [a, b]$

Thus, under the assumption that a given frequency $\sigma := |\lambda_i - \lambda_k|$ is non-resonant (in the sense of the set Ξ_n) and that $(B_j)_{i,k} \neq 0$, by applying a control (that has only j-th non vanishing component) of the form $(0, \dots, 0, \cos(\sigma t)/K, 0, \dots, 0)$ in (3.2.4), the system is approximating (modulo a phase) the transfer of population from state ϕ_j to state ϕ_k, with an error that goes to 0 as the amplitude of the control $1/K$ goes to 0.

The last lemma suggests to consider the effective problem:

$$\frac{d}{dt}\psi = M(t)\psi, \quad M(t) \in \nu_n, \quad \psi \in \mathbb{C}^n. \tag{3.1.4}$$

The next lemma (whose proof can be found in [40, Proposition 4.1]) tells that any propagator of (3.1.4) can be approximated by a propagator of (3.1.1).

Lemma 3.1.13. *Let $n, k \in \mathbb{N}$, and fix $0 < a < b$. Consider $M_1, \dots, M_k \in \nu_n$. Then, for every $\epsilon > 0$ and $\tau_1, \dots, \tau_k \in [a, b]$ there exist an admissible control u, $T_u > 0$ and $\gamma \geq 0$ such that*

$$\|\Gamma^u_{T_u} - e^{-\mathrm{i}\gamma H} \circ e^{\tau_k M_k} \circ \cdots \circ e^{\tau_1 M_1}\|_{L(\Pi_n \mathcal{H}, \mathcal{H})} < \epsilon.$$

One can then let evolve the system freely for a time τ (that is, consider $e^{-\mathrm{i}\tau H}\Gamma^u_{T_u}$) to correct the dephasing term $e^{-\mathrm{i}\gamma H}$, as it is proved in [40, Lemma 4.2] :

Lemma 3.1.14. *Let $\psi \in \mathcal{H}$, $\mu > 0$, $N \in \mathbb{N}$, and $\mathcal{N}$ be a neighborhood of $\Pi_N(e^{-\mathrm{i}\mu H}\psi)$ in $\mathrm{span}\{\phi_1, \dots, \phi_N\}$.Then there exists $\tau \geq 0$ such that $e^{-\mathrm{i}\tau H}\mathcal{N}$ is a neighborhood of $\Pi_N\psi$ in $\mathrm{span}\{\phi_1, \dots, \phi_N\}$.*

Now we can state an important consequence:

Definition 3.1.15. We say that (3.1.1) satisfies the Lie-Galerkin tracking condition if for every n_0 there exists $n > n_0$ such that $\mathrm{Lie}(\nu_n) = \mathfrak{su}(n)$.

Corollary 3.1.16 ([28])**.** *If* (3.1.1) *satisfies the Lie-Galerkin tracking condition, then it is an m-tracker.*

Example 3. We give here two examples of physically relevant systems: the first one does not satisfy the Lie-Galerkin tracking condition, and the second one does.

- **Quantum harmonic oscillator** We consider the controlled bilinear Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = \frac{1}{2}\left(-\frac{\partial^2}{\partial x^2} + x^2\right)\psi(x,t) + u(t)x\psi(x,t)\,, \quad \psi(\cdot,t) \in L^2(\mathbb{R}). \tag{3.1.5}$$

  This system represents an example where any finite n-dimensional truncation is controllable [59], while the whole infinite-dimensional system is known to be noncontrollable, neither exactly nor approximately [88, 72].

  An Hilbert basis made of eigenfunctions of the drift $-\frac{\partial^2}{\partial x^2} + x^2$ is given by the Hermite functions $\{\phi_n\}_{n\in\mathbb{N}}$, and the spectrum of the drift is given by the set of eigenvalues $\{E_n = n - 1/2 \mid n \in \mathbb{N}\}$. In this basis, the control field $B_1 = x$ is given by

$$\langle \phi_j, B\phi_k\rangle = \begin{cases} \sqrt{k-1} & \text{if } j = k-1, \\ \sqrt{k} & \text{if } j = k+1, \\ 0 & \text{otherwise.} \end{cases}$$

  For any $n \in \mathbb{N}$, as $\Sigma_n = \{0, 1, \dots, n\}$ and $\Xi_n := \Sigma_n \setminus \{1\}$, we see that $\mathcal{E}_\sigma(B_1)$ is the zero matrix for all $\sigma \in \Xi_n$. Thus, system (3.1.5) does not satisfy the Lie-Galerkin tracking condition. For further interesting remarks on the relation between (3.1.5) and its finite-dimensional truncations, see also [37, Section IV.D].

- **Planar molecule** The system of a planar bipolar molecule interacting with two orthogonal controls is modelled by the following bilinear controlled Schrödinger equation on the circle S^1:

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\alpha,t) = \left[-\frac{\partial^2}{\partial \alpha^2} + u_1(t)\cos(\alpha) + u_2(t)\sin(\alpha)\right]\psi(\alpha,t)\,, \quad \psi(\cdot,t) \in L^2(S^1). \tag{3.1.6}$$

  Let us show here that (3.1.6) satisfies the Lie-Galerkin tracking condition. An Hilbert basis of $L^2(S^1)$ that diagonalizes the drift $\frac{\partial^2}{\partial\alpha^2} =: H$ is given by the exponential trigonometric functions: $\{e^{\mathrm{i}k\alpha}/\sqrt{2\pi} \mid k \in \mathbb{Z}\}$. The spectrum of the drift H is given by $\{E_k = k^2 \mid k \in \mathbb{Z}\}$, which is degenerate, as $E_k = E_{-k}$. We take as basis for the eigenspace corresponding to the degenerate eigenvalue E_k, $k \geq 1$, the pair of functions $\{\phi_k := \cos(k\alpha)/\sqrt{\pi}, \phi_{-k} := \sin(k\alpha)/\sqrt{\pi}\}$, and we set $\phi_0 = 1/\sqrt{2\pi}$. Denoting by $B_1 = \cos(\alpha), B_2 = \sin(\alpha)$ the two multiplicative control operators, we have the following selection rules:

$$\langle \phi_k, B_l\phi_j\rangle = 0, \quad \text{if } |j-k| > 1,\ l = 1, 2.$$

  Moreover, the pairings

$$\begin{aligned}
\langle \phi_k\,, B_1\phi_{k+1}\rangle &= 1/2, \quad k \in \mathbb{Z}\setminus\{-1,0\}, \\
\langle \phi_0\,, B_1\phi_1\rangle &= 1/\sqrt{2}, \\
\langle \phi_{-1}\,, B_1\phi_0\rangle &= 0, \\
\langle \phi_{-1}\,, B_2\phi_0\rangle &= 1/\sqrt{2}, \\
\langle \phi_k\,, B_2\phi_{k+1}\rangle &= 0, \quad k \in \mathbb{Z}\setminus\{-1\},
\end{aligned}$$

imply that the operators B_1, B_2 projected in the Galerkin approximation $L^2(S^1)^{(n)} = \mathrm{span}\{\phi_0, \phi_k, \phi_{-k} \mid k = 1, \dots, n\}$ read

$$\begin{aligned} \mathrm{i}B_1^{(n)} := \Pi_n \mathrm{i}B_1 \Pi_n &= \frac{1}{\sqrt{2}} F_{0,1} + \frac{1}{2} \sum_{\substack{k=-n,\dots,n-1 \\ k \neq 0,-1}} F_{k,k+1} \,, \\ \mathrm{i}B_2^{(n)} := \Pi_n \mathrm{i}B_2 \Pi_n &= \frac{1}{\sqrt{2}} F_{-1,0} \,, \end{aligned}$$

where $\Pi_n : L^2(S^1) \ni \psi \mapsto \sum_{j=-n,\dots,n} \langle \phi_j, \psi \rangle \phi_j \in L^2(S^1)^{(n)}$, $F_{j,k} = \mathrm{i}e_{j,k} + \mathrm{i}e_{k,j}$ is a generalized Pauli $(2n+1) \times (2n+1)$-matrix, and $e_{j,k}$ is the $(2n+1) \times (2n+1)$-matrix whose entries are all zero except for the entry at (row j, column k) which is equal to one. Because of the selection rules, we only need to consider spectral gaps of the form $\omega_k = |E_k - E_{k-1}|$, $k \in \mathbb{Z}$, and we easily see that the only resonance is

$$\omega_k = \omega_j \Leftrightarrow j = k \text{ or } j = -k + 1 \,,$$

which is due to the degeneracy $E_k = E_{-k}$: $|E_k - E_{k-1}| = |E_{-k} - E_{-k+1}| = |2k - 1|$. So we can consider the spectral gaps ω_k for positive $k = 1, \dots, \infty$ only, and write

$$\begin{aligned} \mathcal{E}_{\omega_k}(\mathrm{i}B_1^{(n)}) &= \frac{1}{2}(F_{k-1,k} + F_{-k,-k+1}) \,, \quad k = 2, \dots, n \,, \\ \mathcal{E}_{\omega_1}(\mathrm{i}B_1^{(n)}) &= \frac{1}{\sqrt{2}} F_{0,1} \,, \\ \mathcal{E}_{\omega_k}(\mathrm{i}B_2^{(n)}) &= 0 \,, \quad k = 2, \dots, n \\ \mathcal{E}_{\omega_1}(\mathrm{i}B_2^{(n)}) &= \frac{1}{\sqrt{2}} F_{-1,0} \,. \end{aligned} \tag{3.1.7}$$

Our claim is that

$$\mathrm{Lie}\{W_\xi \mathcal{E}_{\omega_k}(\mathrm{i}B_1^{(n)}), W_\xi \mathcal{E}_{\omega_1}(\mathrm{i}B_2^{(n)}) \mid k = 1, \dots, n, \ \xi = 1, \mathrm{i}\} = \mathfrak{su}(2n+1), \tag{3.1.8}$$

being $2n + 1 = \dim L^2(S^1)^{(n)}$. Recall the commutation rules of the Lie algebra $\mathfrak{su}$:

$$[G_{j,k}, G_{k,n}] = G_{j,n}, \quad [F_{j,k}, F_{k,n}] = -G_{j,n}, \quad [G_{j,k}, F_{k,n}] = F_{j,n}, \tag{3.1.9}$$

$$[G_{j,k}, F_{j,k}] = 2D_{j,k}, \quad [F_{j,k}, D_{j,k}] = 2G_{j,k}. \tag{3.1.10}$$

and

$$[Y_{j,k}, Z_{j',k'}] = 0 \qquad \text{if } \{j,k\} \cap \{j',k'\} = \emptyset, \tag{3.1.11}$$

with $Y, Z \in \{G, F, D\}$, where $F_{j,k} = \mathrm{i}e_{j,k} + \mathrm{i}e_{k,j}$, $G_{j,k} = e_{j,k} - e_{k,j}$, and $D_{j,k} = \mathrm{i}e_{j,j} - \mathrm{i}e_{k,k}$ is a basis of $\mathfrak{su}$, and $e_{j,k}$ is the $(2n+1) \times (2n+1)$-matrix whose entries are all zero except for the entry at (row j, column k) which is equal to one. Moreover,

$$[\mathrm{i}H, G_{j,k}] = -|E_j - E_k| F_{j,k} \,, \quad [\mathrm{i}H, F_{j,k}] = |E_j - E_k| G_{j,k}. \tag{3.1.12}$$

The main issue here is breaking the sum in (3.1.7), due to the degeneracy $E_k = E_{-k}$, in order to get the transitions $k - 1 \leftrightarrow k$ and $-k \leftrightarrow -k + 1$ independently: noticing that

$$\Big[\big[\mathcal{E}_{\omega_2}(\mathrm{i}B_1^{(n)}), \mathcal{E}_{\omega_1}(\mathrm{i}B_2^{(n)})\big], \mathcal{E}_{\omega_2}(\mathrm{i}B_1^{(n)})\Big] = -\frac{1}{4} F_{-2,-1} \,,$$

we obtain also

$$\mathcal{E}_{\omega_2}(\mathrm{i}B_1^{(n)}) + \Big[\big[\mathcal{E}_{\omega_2}(\mathrm{i}B_1^{(n)}), \mathcal{E}_{\omega_1}(\mathrm{i}B_2^{(n)})\big], \mathcal{E}_{\omega_2}(\mathrm{i}B_1^{(n)})\Big] = \frac{1}{2} F_{1,2}.$$

From here, it is easy to break the sum in (3.1.7) for $k \geq 3$, and using the commutation rules prove the claim (3.1.8). Finally, as $\omega_n \neq \omega_{n+1}$, we see that $(\omega_k, l) \in \Xi_n$ for all $k = 1, \dots, n$ and $l = 1, 2$, and hence we proved that the system (3.1.6) verifies the Lie-Galerkin tracking condition.

As another application of Lemma 3.1.13, we would like to point out an interesting spectral Lie-algebraic fact on finite-dimensional quantum systems. Suppose that $\dim \mathcal{H} = N < \infty$. Then, it is well-known from the theory of control systems on Lie groups that (3.1.1) is operator controllable (that is, the equation lifted on the group $SU(N)$ is controllable) if and only if the Lie algebra has maximal rank, that is, $\mathrm{Lie}\{\mathrm{i}H, \mathrm{i}B_1, \dots, \mathrm{i}B_l\} = \mathfrak{su}(N)$ [75]. We can actually check this maximal rank condition on the decoupled Hamiltonians:

Corollary 3.1.17. *Suppose that* $\dim \mathcal{H} = N < \infty$*, and denote by* Σ *the set of spectral gaps of* H*.*
If $\mathrm{Lie}\{\mathrm{i}H, \mathcal{E}_\sigma(\mathrm{i}B_1), \dots, \mathcal{E}_\sigma(\mathrm{i}B_l) \mid \sigma \in \Sigma, \sigma \neq 0\} = \mathfrak{su}(N)$*, then* $\mathrm{Lie}\{\mathrm{i}H, \mathrm{i}B_1, \dots, \mathrm{i}B_l\} = \mathfrak{su}(N)$*. Conversely, if* $\mathrm{Lie}\{\mathrm{i}H, \mathrm{i}B_1, \dots, \mathrm{i}B_l\} = \mathfrak{su}(N)$*, then* $\mathrm{Lie}\{\mathrm{i}H, \mathcal{E}_\sigma(\mathrm{i}B_1), \dots, \mathcal{E}_\sigma(\mathrm{i}B_l) \mid \sigma \in \Sigma\} = \mathfrak{su}(N)$*.*

Proof. If $\mathrm{Lie}\{\mathrm{i}H, \mathcal{E}_\sigma(\mathrm{i}B_1), \dots, \mathcal{E}_\sigma(\mathrm{i}B_l) \mid \sigma \in \Sigma, \sigma \neq 0\} = \mathfrak{su}(N)$, then (3.1.1) is approximately controllable on $SU(N)$, thanks to Lemma 3.1.13. Since any finite-dimensional approximately controllable quantum system is exactly controllable [29, Theorem 17] (see also [103]), we get that $\mathrm{Lie}\{\mathrm{i}H, \mathrm{i}B_1, \dots, \mathrm{i}B_l\} = \mathfrak{su}(N)$. Conversely, if $\mathrm{Lie}\{\mathrm{i}H, \mathrm{i}B_1, \dots, \mathrm{i}B_l\} = \mathfrak{su}(N)$, since we can write any $B_i = \sum_{\sigma \in \Sigma} \mathcal{E}_\sigma(B_i)$, we conclude that $\mathrm{Lie}\{\mathrm{i}H, \mathcal{E}_\sigma(\mathrm{i}B_1), \dots, \mathcal{E}_\sigma(\mathrm{i}B_l) \mid \sigma \in \Sigma\} = \mathfrak{su}(N)$. □

In Corollary 3.1.16 we see that, under some non-resonant assumptions on the spectral gaps (in the sense of the set Ξ_n), controllability properties of the finite-dimensional truncations imply approximate controllability properties of the infinite-dimensional system.

We present now an original application/corollary in terms of simultaneous controllability over invariant subspaces, that will be useful later on for applications on quantum systems with symmetries (for similar results, see also [43]). Suppose that $\mathcal{H} = \bigoplus_{k \in \mathbb{N}} \mathcal{H}_k$ is an orthogonal decomposition, and each $\mathcal{H}_k$ is an infinite-dimensional Hilbert space that is invariant for $H, B_1, \dots, B_\ell$.[1] For any $n \in \mathbb{N}$, denote by $\mathcal{H}_k^n := (\Pi_n \mathcal{H}) \cap \mathcal{H}_k$ and $n_k := \dim \mathcal{H}_k^n$. Of course, as each $\mathcal{H}_k$ is invariant for $H, B_1, \dots, B_l$, we have $\nu_n \subset \mathfrak{su}(n_{k_1}) \oplus \cdots \oplus \mathfrak{su}(n_{k_r})$, where $\Pi_n \mathcal{H} = \bigoplus_{i=1,\dots,r} \mathcal{H}_{k_i}^n$ and $n = \sum_{i=1,\dots,r} n_{k_i}$.

Definition 3.1.18. Suppose that there exists an orthogonal decomposition $\mathcal{H} = \bigoplus_{k \in \mathbb{Z}} \mathcal{H}_k$ in invariant subspaces for $H, B_1, \dots, B_l$. We say that (3.1.1) is *approximately simultaneously controllable* if, for every $r \in \mathbb{N}$, $\psi_{k_j}^{\mathrm{in}}, \psi_{k_j}^{\mathrm{fin}} \in \mathcal{H}_{k_j}$ of norm one, $j = 1, \dots, r$, and $\epsilon > 0$, there exists a piecewise constant control $u : [0, T_u] \to U$ such that

$$\|\Gamma_{T_u}^u \psi_{k_j}^{\mathrm{in}} - \psi_{k_j}^{\mathrm{fin}}\| < \epsilon, \qquad \forall j = 1, \dots, r.$$

Definition 3.1.19. Suppose that there exists an orthogonal decomposition $\mathcal{H} = \bigoplus_{k \in \mathbb{Z}} \mathcal{H}_k$ in invariant subspaces for $H, B_1, \dots, B_l$. We say that (3.1.1) satisfies the Lie-Galerkin simultaneous control condition if for every n_0 there exists $n > n_0$ such that $\mathrm{Lie}(\nu_n) = \mathfrak{su}(n_{k_1}) \oplus \cdots \oplus \mathfrak{su}(n_{k_r})$, with $\sum_{i=1,\dots,r} n_{k_i} = n$.

Corollary 3.1.20. *If* (3.1.1) *satisfies the Lie-Galerkin simultaneous control condition, then it is approximately simultaneously controllable.*

Proof. Let $r \in \mathbb{N}$ and $\psi_{k_j}^{\mathrm{in}}, \psi_{k_j}^{\mathrm{fin}} \in \mathcal{H}_{k_j}$ of norm one, $j = 1, \dots, r$. For $\epsilon > 0$, consider $n_0 \in \mathbb{N}$ such that

$$\left\| \psi_{k_j}^{\mathrm{in}} - \frac{\Pi_{n_0} \psi_{k_j}^{\mathrm{in}}}{\|\Pi_{n_0} \psi_{k_j}^{\mathrm{in}}\|} \right\| < \frac{\epsilon}{3}, \quad \left\| \psi_{k_j}^{\mathrm{fin}} - \frac{\Pi_{n_0} \psi_{k_j}^{\mathrm{fin}}}{\|\Pi_{n_0} \psi_{k_j}^{\mathrm{fin}}\|} \right\| < \frac{\epsilon}{3}, \quad \forall j = 1, \dots, r.$$

The Lie-Galerkin simultaneous control condition ensures the existence of $n > n_0$ such that system (3.1.4) is simultaneously controllable in $\bigoplus_{j=1,\dots,r} \mathcal{H}_{k_j}^n$. By Lemma 3.1.13 there exists an admissible control u, $T_u \geq 0$, and $\gamma \geq 0$ such that

$$\left\| \Gamma_{T_u}^u \left(\frac{\Pi_{n_0} \psi_{k_j}^{\mathrm{in}}}{\|\Pi_{n_0} \psi_{k_j}^{\mathrm{in}}\|} \right) - e^{-\mathrm{i}\gamma H} \frac{\Pi_{n_0} \psi_{k_j}^{\mathrm{fin}}}{\|\Pi_{n_0} \psi_{k_j}^{\mathrm{fin}}\|} \right\| < \frac{\epsilon}{3}, \quad \forall j = 1, \dots, r.$$

Then, by the triangular inequality we conclude that

$$\|\Gamma_{T_u}^u (\psi_{k_j}^{\mathrm{in}}) - e^{-\mathrm{i}\gamma H} \psi_{k_j}^{\mathrm{fin}}\| < \epsilon, \quad \forall j = 1, \dots, r.$$

Finally, the phase tuning can be handled following the same argument of [27, Section 6.2] □

[1] This happens, for example, when there exists a self-adjoint operator P that commutes with all the Hamiltonians $H, B_1, \dots, B_\ell$: such an operator P is called a symmetry of (3.1.1).

3.1.3 A block-wise version of the Lie-Galerkin tracking condition

In this section we propose another sufficient condition for a system to be an m-tracker. The main difference w.r.t. the Lie-Galerkin tracking condition is that, instead of testing a sequence of finite-dimensional properties on an increasing sequence of linear subspaces of $\mathcal{H}$, we test them on a sequence of overlapping finite-dimensional spaces, not necessarily ordered by inclusion. This allows the sufficient condition to be checked block-wise, and it is particularly suited for systems with high degree of symmetries, such as rotating molecules.

Let $\{I_j \mid j \in \mathbb{N}\}$ be a family of finite subsets of $\mathbb{N}$ such that $\cup_{j\in\mathbb{N}} I_j = \mathbb{N}$. Denote by n_j the cardinality of I_j. Consider the subspaces

$$\mathcal{M}_j := \operatorname{span}\{\phi_n \mid n \in I_j\} \subset \mathcal{H}$$

and their associated orthogonal projections

$$\Pi_{\mathcal{M}_j} : \mathcal{H} \ni \psi \mapsto \sum_{n\in I_j} \langle \phi_n, \psi\rangle \phi_n \in \mathcal{H}.$$

Given a linear operator Q on $\mathcal{H}$ we identify the linear operator $\Pi_{\mathcal{M}_j} Q \Pi_{\mathcal{M}_j}$ preserving $\mathcal{M}_j$ with its complex matrix representation with respect to the basis $(\phi_n)_{n\in I_j}$. The set $\Sigma_j = \{|\lambda_l - \lambda_{l'}| \mid l, l' \in I_j\}$ is then the collection of the spectral gaps of $\Pi_{\mathcal{M}_j} H \Pi_{\mathcal{M}_j}$. We define $B_i^{(j)} := \Pi_{\mathcal{M}_j} B_i \Pi_{\mathcal{M}_j}$ for every $i = 1, \dots, \ell$.

If the element $(B_i)_{l,k}$ is different from zero, then a control u_i oscillating at frequency $|\lambda_l - \lambda_k|$ induces a population transfer between the states ϕ_l and ϕ_k ([41]). The dynamics of such a population transfer depend on the other pairs of states $\phi_{l'}$, $\phi_{k'}$ having the same spectral gap and whose corresponding element $(B_i)_{l',k'}$ is different from zero. We are interested in controlling the induced population dynamics within a space $\mathcal{M}_j$. This motivates the definition of the sets

$$\begin{aligned}\Xi_j^0 = \{(\sigma, i) \in \Sigma_j \times \{1, \dots, \ell\} \mid (B_i)_{l,k} = 0 \text{ for every } l \in \mathbb{N},\ k \in \mathbb{N} \setminus I_j \\ \text{such that } |\lambda_l - \lambda_k| = \sigma\},\end{aligned}$$

and

$$\begin{aligned}\Xi_j^1 = \{(\sigma, i) \in \Sigma_j \times \{1, \dots, \ell\} \mid (B_i)_{l,k} = 0 \text{ for every } l \in I_j,\ k \in \mathbb{N} \setminus I_j \\ \text{such that } |\lambda_l - \lambda_k| = \sigma\}.\end{aligned}$$

While the set Ξ_j^1 compares only with pairs of states ϕ_l, ϕ_k with ϕ_l in $\mathcal{M}_j$, such a requirement is not present in the definition if Ξ_j^0. This means that for $(\sigma, i) \in \Xi_j^0$ the induced population dynamics obtained by a control u_i oscillating at frequency σ not only does not produce population transfer out of $\mathcal{M}_j$, but also is trivial within the orthogonal complement to $\mathcal{M}_j$.

Let us consider the sets of excited modes

$$\nu_j^s := \{W_\xi(\mathcal{E}_\sigma(\mathrm{i}B_i^{(j)})) \mid (\sigma, i) \in \Xi_j^s, \sigma \neq 0, \xi \in S^1\}, \quad s = 0, 1. \tag{3.1.13}$$

Notice that $\nu_j^0 \subset \nu_j^1 \subset \mathfrak{su}(n_j)$. Indeed, we have the following picture:

$$\mathcal{E}_\sigma(\mathrm{i}B_i^{(j)}) \in \nu_j^0 \Rightarrow \mathcal{E}_\sigma(\Pi_{j-1,j,j+1}\mathrm{i}B_i\Pi_{j-1,j,j+1}) = \left[\begin{array}{c|c|c} 0 & 0 & 0 \\ \hline 0 & \mathcal{E}_\sigma(\mathrm{i}B_i^{(j)}) & 0 \\ \hline 0 & 0 & 0 \end{array}\right]$$

$$\mathcal{E}_\sigma(\mathrm{i}B_i^{(j)}) \in \nu_j^1 \Rightarrow \mathcal{E}_\sigma(\Pi_{j-1,j,j+1}\mathrm{i}B_i\Pi_{j-1,j,j+1}) = \left[\begin{array}{c|c|c} * & 0 & * \\ \hline 0 & \mathcal{E}_\sigma(\mathrm{i}B_i^{(j)}) & 0 \\ \hline * & 0 & * \end{array}\right]$$

where $\Pi_{j-1,j,j+1}$ denotes the projection onto $\mathcal{M}_{j-1} \oplus \mathcal{M}_j \oplus \mathcal{M}_{j+1}$.

We denote by $\operatorname{Lie}(\nu_j^s)$ the Lie subalgebra of $\mathfrak{su}(n_j)$ generated by the matrices in ν_j^s, $s = 0, 1$, and define $\mathcal{T}_j$ as the minimal ideal of $\operatorname{Lie}(\nu_j^1)$ containing ν_j^0.

Finally, we introduce the graph $\mathcal{G}$ with vertices $\mathcal{V} = \{I_j \mid j \in \mathbb{N}\}$ and edges $\mathcal{E} = \{(I_j, I_k) \mid j, k \in \mathbb{N},\ I_j \cap I_k \neq \emptyset\}$. We are now in a position to state a new sufficient condition for a system to be an m-tracker, and thus, approximately controllable.

Theorem 3.1.21. *Assume that ($\mathbb{A}$) holds true. If the graph $\mathcal{G}$ is connected and $\mathcal{T}_j = \mathfrak{su}(n_j)$ for every $j \in \mathbb{N}$, then* (3.1.1) *is an m-tracker.*

Proof. The proof works by showing that the Lie-Galerkin tracking condition holds true, which guarantees that (3.1.1) is an m-tracker (Corollary 3.1.16, see [28, Theorem 2.8] for the proof). In terms of the notation introduced here, the Lie-Galerkin tracking condition is true if there exists a sequence $\{\widetilde{I_j} \mid j \in \mathbb{N}\}$ of finite subsets of $\mathbb{N}$, strictly increasing with respect to the inclusion, such that $\cup_{j\in\mathbb{N}}\widetilde{I_j} = \mathbb{N}$ and $\mathcal{T}_j = \mathfrak{su}(n_j)$ for every $j \in \mathbb{N}$.

Up to reordering the sets I_j, we can assume that

$$I_{j+1} \cap (\cup_{k=1}^{j} I_k) \neq \emptyset, \qquad \forall j \in \mathbb{N}. \tag{3.1.14}$$

For $j \in \mathbb{N}$, let $\widetilde{I_j} = \cup_{i=1}^{j} I_i$ and $\mathcal{Z}_j = \sum_{k=1}^{j} \mathcal{M}_k$.

The Lie–Galerkin tracking condition holds true if

$$\mathrm{Lie}(\cup_{j=1}^{m}\widetilde{\mathcal{T}_j}) = \mathfrak{su}(\dim(\mathcal{Z}_m)), \qquad m \in \mathbb{N}, \tag{3.1.15}$$

where the set of operators $\widetilde{\mathcal{T}_j}$ is obtained similarly to $\mathcal{T}_j$, replacing ν_j^s, $s = 0, 1$, by

$$\{W_\xi(\mathcal{E}_\sigma(\mathrm{i}\Pi_{\mathcal{Z}_m} B_i \Pi_{\mathcal{Z}_m})) \mid (\sigma, i) \in \Xi_j^s, \sigma \neq 0, \xi \in S^1\}, \quad s = 0, 1.$$

We proceed by induction on m. For $m = 1$, (3.1.15) is true, since we have that $\mathrm{Lie}(\mathcal{T}_1) = \mathcal{T}_1 = \mathfrak{su}(n_1) = \mathfrak{su}(\dim(\mathcal{Z}_1))$. Assume now that (3.1.15) is true for m, and consider the vertex $I_{m+1} \in \mathcal{V}$. Consider $t, p \in \cup_{j=1}^{m+1} I_j$ and let us prove that $G_{t,p} := e_{t,p} - e_{p,t}$ is in $\mathrm{Lie}(\cup_{j=1}^{m+1}\widetilde{\mathcal{T}_j})$, where $e_{a,b}$ is the matrix with all entries equal to 0 except for the one in row a and column b, which is equal to 1 (and the indices in $\cup_{j=1}^{m+1} I_j$ are identified with the elements of $\{1, \dots, \dim(\mathcal{Z}_{m+1})\}$). Decomposing $\mathcal{Z}_{m+1}$ as a direct orthogonal sum $V_1 \oplus (\mathcal{Z}_m \cap \mathcal{M}_{m+1}) \oplus V_2$ with $V_1 \subset \mathcal{Z}_m$ and $V_2 \subset \mathcal{M}_{m+1}$, a matrix in $\widetilde{\mathcal{T}_{m+1}}$ has the form

$$\left[\begin{array}{c|c|c} 0 & 0 & 0 \\ \hline 0 & Q_{11} & Q_{12} \\ \hline 0 & Q_{21} & Q_{22} \end{array}\right], \qquad \left[\begin{array}{c|c} Q_{11} & Q_{12} \\ \hline Q_{21} & Q_{22} \end{array}\right] \in \mathfrak{su}(n_{m+1}),$$

as it follows from the definition of Ξ_j^0 and Ξ_j^1 and the fact that $\widetilde{\mathcal{T}_{m+1}}$ is the ideal generated by ν_j^0 inside $\mathrm{Lie}(\nu_j^1)$. Similarly, a matrix in $\cup_{j=1}^{m}\widetilde{\mathcal{T}_j}$ has the form

$$\left[\begin{array}{c|c|c} Q_{11} & Q_{12} & 0 \\ \hline Q_{21} & Q_{22} & 0 \\ \hline 0 & 0 & 0 \end{array}\right], \qquad \left[\begin{array}{c|c} Q_{11} & Q_{12} \\ \hline Q_{21} & Q_{22} \end{array}\right] \in \mathfrak{su}(\dim(\mathcal{Z}_m)).$$

If $t, p \in \cup_{j=1}^{m} I_j$ or $t, p \in I_{m+1}$ the conclusion follows from the induction hypothesis and the identity $\mathcal{T}_{m+1} = \mathfrak{su}(n_{m+1})$. Let then $t \in I_{m+1} \setminus (\cup_{j=1}^{m} I_j)$ and $p \in \cup_{j=1}^{m} I_j$. Fix, moreover, $r \in I_{m+1} \cap (\cup_{j=1}^{m} I_j)$, whose existence is guaranteed by (3.1.14). Again by the induction hypothesis and the identity $\mathcal{T}_{m+1} = \mathfrak{su}(n_{m+1})$, we have that $G_{p,r}$ and $G_{r,t}$ are in $\mathrm{Lie}(\cup_{j=1}^{m+1}\widetilde{\mathcal{T}_j})$. The bracket $[G_{p,r}, G_{r,t}] = G_{p,t}$ is therefore also in $\mathrm{Lie}(\cup_{j=1}^{m+1}\widetilde{\mathcal{T}_j})$. By similar arguments, we deduce that every element of a basis of $\mathfrak{su}(\dim(\mathcal{Z}_{m+1}))$ is in $\mathrm{Lie}(\cup_{j=1}^{m+1}\widetilde{\mathcal{T}_j})$. □

3.2 Symmetric molecule

3.2.1 The Schrödinger equation of a rotating molecule subject to electric fields

We recall in this section some general facts about Wigner D-functions and the theory of angular momentum in quantum mechanics (see, for instance, [22, 108]).

We use Euler's angles $(\alpha, \beta, \gamma) \in [0, 2\pi) \times [0, \pi] \times [0, 2\pi)$ to describe the configuration space SO(3) of the molecule. More precisely, the coordinates of a vector change from the body fixed frame a_1, a_2, a_3 to the space fixed frame e_1, e_2, e_3 via three rotations

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = R_{e_3}(\alpha) R_{e_2}(\beta) R_{e_3}(\gamma) \begin{pmatrix} x \\ y \\ z \end{pmatrix} =: R(\alpha, \beta, \gamma) \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{3.2.1}$$

where $(x, y, z)^T$ are the coordinates of the vector in the body fixed frame, $(X, Y, Z)^T$ are the coordinates of the vector in the space fixed frame and $R_{e_i}(\theta) \in \mathrm{SO}(3)$ is the rotation of angle θ around the axis e_i. The explicit expression of the matrix $R(\alpha, \beta, \gamma) \in \mathrm{SO}(3)$ is

$$R = \begin{pmatrix} \cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma & -\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma & \cos\alpha\sin\beta \\ \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma & \sin\alpha\sin\beta \\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta \end{pmatrix}. \tag{3.2.2}$$

In Euler coordinates, the angular momentum operators are given by

$$\begin{cases} J_1 = \mathrm{i}\cos\alpha\cot\beta\dfrac{\partial}{\partial\alpha} + \mathrm{i}\sin\alpha\dfrac{\partial}{\partial\beta} - \mathrm{i}\dfrac{\cos\alpha}{\sin\beta}\dfrac{\partial}{\partial\gamma}, \\ J_2 = \mathrm{i}\sin\alpha\cot\beta\dfrac{\partial}{\partial\alpha} - \mathrm{i}\cos\alpha\dfrac{\partial}{\partial\beta} - \mathrm{i}\dfrac{\sin\alpha}{\sin\beta}\dfrac{\partial}{\partial\gamma}, \\ J_3 = -\mathrm{i}\dfrac{\partial}{\partial\alpha}. \end{cases} \tag{3.2.3}$$

These are linear operators acting on the Hilbert space $L^2(\mathrm{SO}(3))$, self-adjoint with respect to the Haar measure $\frac{1}{8}d\alpha d\gamma\sin\beta d\beta$. Using (3.2.3), the self-adjoint operator $P_3 := -\mathrm{i}\frac{\partial}{\partial\gamma}$ can be written as $P_3 = \sin\beta\cos\alpha j_1 + \sin\beta\sin\alpha j_2 + \cos\beta j_3$, that is,

$$P_3 = \sum_{i=1}^{3} R_{i3}(\alpha,\beta,\gamma)J_i,$$

where $R = (R_{ij})_{i,j=1}^3$ is given in (3.2.2).

In the same way we define $P_1 = \sum_{i=1}^3 R_{i1}(\alpha,\beta,\gamma)J_i$, $P_2 = \sum_{i=1}^3 R_{i2}(\alpha,\beta,\gamma)j_i$. The operators J_i and P_i, $i = 1,2,3$, are the angular momentum operators expressed in the fixed and in the body frame, respectively. The rotational Hamiltonian of a molecule with inertia moments $I_1, I_2, I_3 > 0$ is given by

$$H = \frac{1}{2}\Big(\frac{P_1^2}{I_1} + \frac{P_2^2}{I_2} + \frac{P_3^2}{I_3}\Big),$$

which is seen here as a self-adjoint operator acting on the Hilbert space $L^2(\mathrm{SO}(3))$. The interaction Hamiltonian between the dipole δ inside the molecule and the external electric field in the direction e_i, $i = 1,2,3$, is given by the Stark effect ([68, Chapter 10])

$$B_i(\alpha,\beta,\gamma) = -\langle R(\alpha,\beta,\gamma)\delta, e_i\rangle,$$

seen as a multiplicative self-adjoint operator acting on $L^2(\mathrm{SO}(3))$. Then, the rotational Schrödinger equation for a rigid molecule subject to three orthogonal electric fields reads

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\alpha,\beta,\gamma;t) = H\psi(\alpha,\beta,\gamma;t) + \sum_{l=1}^{3} u_l(t)B_l(\alpha,\beta,\gamma)\psi(\alpha,\beta,\gamma;t), \tag{3.2.4}$$

with $\psi(t) \in L^2(\mathrm{SO}(3))$ and $u(t) \in U$, for some neighborhood U of 0 in $\mathbb{R}^3$.

We also consider the square norm operator $J^2 := J_1^2 + J_2^2 + J_3^2 = P_1^2 + P_2^2 + P_3^2$. The self-adjoint operators J^2, J_3, P_3 can be considered as the three commuting observables needed to describe the quantum motion of a molecule. Indeed,

$$[J^2, J_3] = [J^2, P_3] = [J_3, P_3] = 0,$$

and hence there exists an orthonormal Hilbert basis of $L^2(\mathrm{SO}(3))$ which diagonalizes simultaneously J^2, J_3 and P_3. In terms of Euler coordinates, this basis is made by the so-called Wigner functions

$$D^j_{k,m}(\alpha,\beta,\gamma) := e^{\mathrm{i}(m\alpha+k\gamma)}d^j_{k,m}(\beta), \qquad j \in \mathbb{N}, \quad k,m = -j,\dots,j, \tag{3.2.5}$$

where the function $d^j_{k,m}$ solves a suitable Legendre differential equation, obtained by separation of variables (see, e.g., [68, Section 2.5] for the separation of variables ansatz and [108, Chapter 4] for a detailed description of the properties of these functions).

Summarizing, the family of Wigner functions $\{D^j_{k,m} \mid j \in \mathbb{N}, k,m = -j,\dots,j\}$ forms an orthonormal Hilbert basis for $L^2(\mathrm{SO}(3))$. Moreover,

$$J^2 D^j_{k,m} = j(j+1)D^j_{k,m}, \quad J_3 D^j_{k,m} = mD^j_{k,m}, \quad P_3 D^j_{k,m} = kD^j_{k,m}. \tag{3.2.6}$$

Thus, m and k are the quantum numbers which correspond to the projections of the angular momentum on the third axis of, respectively, the fixed and the body frame. In this section we treat the symmetric molecule, so we impose the symmetry relation $I_1 = I_2$, which implies that one can write the rotational Hamiltonian in the following form

$$H = \frac{J^2}{2I_2} + \Big(\frac{1}{2I_3} - \frac{1}{2I_2}\Big)P_3^2.$$

Thus,

$$HD^j_{k,m} = \Big(\frac{j(j+1)}{2I_2} + \Big(\frac{1}{2I_3} - \frac{1}{2I_2}\Big)k^2\Big)D^j_{k,m} =: E^j_k D^j_{k,m}. \tag{3.2.7}$$

implying that the Wigner functions are also the eigenfunctions of the rotational Hamiltonian of the symmetric molecule. Since the eigenvalues of H do not depend on m, the energy level E^j_k is $(2j+1)$-degenerate with respect to m. This property is common to every molecule in nature: the spectrum $\sigma(H)$ does not depend on m, just like in classical mechanics the kinetic energy does not depend on the direction of the angular momentum. Moreover, when $k \neq 0$ the energy level E^j_k is also 2-degenerate with respect to k. This extra degeneracy is actually a characterizing property of symmetric molecules. Breaking this k-symmetry will be one important feature of our controllability analysis.

3.2.2 Non-controllability and reachable sets of the quantum genuine symmetric-top

We recall that the genuine symmetric-top molecule is a symmetric rigid body with electric dipole δ along the symmetry axis: $\delta = (0,0,\delta_3)^T$ in the principal axis frame on the body. We then introduce for any $k \in \mathbb{Z}$ the subspaces $\mathcal{S}_k := \overline{\text{span}}\{D^j_{k,m} \mid j \in \mathbb{N}, j \geq |k|, m = -j, \dots, j\}$, where $\overline{\text{span}}$ denotes the closure of the linear hull in $L^2(\text{SO}(3))$.

Theorem 3.2.1. *The quantum number k is invariant in the controlled motion of the genuine symmetric-top molecule. That is, if $I_1 = I_2$ and $\delta = (0,0,\delta_3)^T$, the subspaces $\mathcal{S}_k$, $k \in \mathbb{Z}$, are invariant for any propagator of the Schrödinger equation (3.2.4).*

Proof. We have to show that H and B_1, B_2, B_3, do not couple different levels of k, that is,

$$\begin{cases} \langle D^j_{k,m}, \mathrm{i}HD^{j'}_{k',m'}\rangle_{L^2(\text{SO}(3))} = 0, & k \neq k', \\ \langle D^j_{k,m}, \mathrm{i}B_l D^{j'}_{k',m'}\rangle_{L^2(\text{SO}(3))} = 0, & k \neq k',\ l = 1,2,3. \end{cases} \tag{3.2.8}$$

The first equation of (3.2.8) is obvious since the orthonormal basis $\{D^j_{k,m}\}$ diagonalizes H. Under the genuine symmetric-top assumption, the second equation of (3.2.8) is also true: for $l = 1$ and $k \neq k'$ we compute

$$\begin{aligned} &\langle D^j_{k,m}, \mathrm{i}B_1 D^{j'}_{k',m'}\rangle_{L^2(\text{SO}(3))} \\ &= -\int_0^{2\pi} d\alpha \int_0^{2\pi} d\gamma \int_0^{\pi} d\beta \sin(\beta) D^j_{k,m}(\alpha,\beta,\gamma)\mathrm{i}B_1(\alpha,\beta,\gamma)\overline{D^{j'}_{k',m'}}(\alpha,\beta,\gamma) \\ &= \mathrm{i}\delta_3 \left(\int_0^{2\pi} d\gamma e^{\mathrm{i}k\gamma} e^{-\mathrm{i}k'\gamma}\right)\left(\int_0^{2\pi} d\alpha \cos(\alpha) e^{\mathrm{i}m\alpha} e^{-\mathrm{i}m'\alpha}\right) \\ &\quad \times \left(\int_0^{\pi} d\beta \sin^2(\beta) d^j_{k,m}(\beta)\overline{d^{j'}_{k',m'}}(\beta)\right) = 0, \end{aligned}$$

using the orthogonality of the functions $e^{ik\gamma}$ and the explicit form (3.2.2) of the matrix R, which yields

$$B_1(\alpha,\beta,\gamma) = -\langle R(\alpha,\beta,\gamma)\begin{pmatrix}0\\0\\\delta_3\end{pmatrix}, \begin{pmatrix}1\\0\\0\end{pmatrix}\rangle = -\delta_3 \cos\alpha \sin\beta.$$

The computations for $l = 2,3$ are analogous, since the multiplicative potentials B_l do not depend on γ. □

Remark 3.2.2. Equation (3.2.8) also shows that, for a genuine symmetric-top, the third component of the angular momentum P_3 commutes with H and B_l, $l = 1,2,3$, hence

$$\Big[P_3, H + \sum_{l=1}^{3} u_l B_l\Big] = 0, \quad \forall u \in U.$$

Thus, $\langle \psi(t), P_3\psi(t)\rangle$ is a conserved quantity, where ψ is the solution of (3.2.4).

In (3.2.8) we see that, when $\delta = (0,0,\delta_3)^T$, transitions $k \to k'$ are forbidden if $k \neq k'$. Thus, if the quantum system is prepared in the initial state $\psi(0)$ with $P_3\psi(0) = k\psi(0)$, the wave function ψ evolves in the subspaces $\mathcal{S}_k = \overline{\text{span}}\{D^j_{k,m} \mid j \in \mathbb{N}, j \geq |k|, m = -j, \dots, j\}$. The next theorem tells us that the restriction of (3.2.4) to this subspace is approximately controllable, and that it is simultaneously approximately controllable w.r.t. k, with the exception of $-k$. Recall that $\mathcal{S}$ denotes the unit sphere of $L^2(\text{SO}(3))$.

Theorem 3.2.3. *Let $I_1 = I_2$. If $\delta = (0, 0, \delta_3)^T$, $\delta_3 \neq 0$, then*

(i) the Schrödinger equation (3.2.4) is an m-tracker in the Hilbert space $\mathcal{S}_k$, for any $k \in \mathbb{Z}$. In particular, $\mathrm{Reach}(\psi)$ *is dense in $\mathcal{S}_k \cap \mathcal{S}$ for all $\psi \in \mathcal{S}_k \cap \mathcal{S}$.*

(ii) the Schrödinger equation (3.2.4) is simultaneously approximately controllable w.r.t. the orthogonal decomposition $L^2(\mathrm{SO}(3)) = \bigoplus_{k\in\mathbb{N}}(\mathcal{S}_k \oplus \mathcal{S}_{-k})$, while the evolution in $\mathcal{S}_{-k}$ is completely determined by the evolution in $\mathcal{S}_k$. In particular, denoting by $\Phi : \mathcal{S}_k \to \mathcal{S}_{-k}$ the linear transformation that acts as $\Phi(D^j_{k,m}) = D^j_{-k,m}$ on the basis elements, if $\psi \in \mathcal{S}$ decomposes as $\psi = \sum_{k\in\mathbb{Z}} p_k\psi_k$, $\psi_k \in \mathcal{S}_k \cap \mathcal{S}$, $\sum_{k\in\mathbb{Z}} |p_k|^2 = 1$, with $\psi_{-k} = \Phi(\psi_k)$, then $\mathrm{Reach}(\psi)$ *is dense in $\{\phi \in \mathcal{S} \mid \phi = \sum_{k\in\mathbb{Z}} p_k\phi_k,\ \phi_k \in \mathcal{S}_k \cap \mathcal{S},\ \phi_{-k} = \Phi(\phi_k)\}$.*

Proof. For every integer $j \geq |k|$, let $I_{j,k} := \{\rho(l, m) \mid l = j, j + 1,\ m = -l, \dots, l\}$, where $\rho : \{(l, m) \mid l \geq |k|,\ m = -l, \dots, l\} \to \mathbb{N}$ is the lexicographic ordering. Then the graph $\mathcal{G}_k$ with vertices $\{I_{j,k}\}_{j=|k|}^{\infty}$ and edges $\{(I_{j,k}, I_{j',k}) \mid I_{j,k} \cap I_{j',k} \neq \emptyset\}$ is linear.

In order to apply Theorem 3.1.21 to the restriction of (3.2.4) to $\mathcal{S}_k$, we should consider the projected dynamics onto $\mathcal{N}_{j,k} := \mathcal{L}_{j,k} \oplus \mathcal{L}_{j+1,k}$, where $\mathcal{L}_{l,k} := \mathrm{span}\{D^l_{k,m} \mid m = -l, \dots, l\}$. The only spectral gaps in S_k are $\sigma^j_k = |E^{j+1}_k - E^j_k| = \frac{j+1}{I_2}$, $j \geq |k|$. Notice that $(\sigma^j_k, l) \in \Xi^0_j$.

We write the electric potentials projected onto $\mathcal{N}_{j,k}$:

$$\begin{aligned}
\mathcal{E}_{\sigma^j_k}(\mathrm{i}B_1) &= \sum_{m=-j,\dots,j} a_{j,k,m}\delta_3 G_{(j,k,m),(j+1,k,m+1)} + a_{j,k,-m}\delta_3 G_{(j,k,m),(j+1,k,m-1)},\\
\mathcal{E}_{\sigma^j_k}(\mathrm{i}B_2) &= \sum_{m=-j,\dots,j} a_{j,k,m}\delta_3 F_{(j,k,m),(j+1,k,m+1)} - a_{j,k,-m}\delta_3 F_{(j,k,m),(j+1,k,m-1)},\\
\mathcal{E}_{\sigma^j_k}(\mathrm{i}B_3) &= \sum_{m=-j,\dots,j} -b_{j,k,m}\delta_3 F_{(j,k,m),(j+1,k,m)},
\end{aligned}$$

having used the explicit pairings (3.4.11), which can be found in Appendix 3.4.2, and which describe the transitions excited by the frequency σ^j. Note that here the sum does not run over k since we are considering the dynamics restricted to $\mathcal{S}_k$. We consider the family of excited modes

$$\mathcal{F}_{j,k} = \{\mathcal{E}_{\sigma^j_k}(\mathrm{i}B_l), W_{\mathrm{i}}(\mathcal{E}_{\sigma^j_k}(\mathrm{i}B_l)) \mid l = 1, 2, 3\} \subset \nu^0_j.$$

We claim that the Lie algebra generated by $\mathcal{F}_{j,k}$ is equal to $\mathfrak{su}((2j + 1) + (2(j + 1) + 1)) =: \mathfrak{su}(\mathcal{N}_{j,k})$. Such an identity has been proved in [28, Section 3.3] (with computations analogous to the ones we perform in the Appendix 3.4.1) since the projection to $\mathcal{N}_{j,k}$ is isomorphic to an analogous projection for the linear molecule. Hence, we conclude that system (3.2.4) is an m-tracker in $\mathcal{S}_k$, which concludes the proof of (i).

In order to prove (ii), we need the following result on the simultaneous control of left-invariant bilinear control systems on finite-dimensional connected compact simple Lie groups, here stated in the case of interest, that is the group $SU(n)$, and with multiple controls:

Lemma 3.2.4 ([18])**.** *Consider the finite direct sum bilinear control system on $\bigoplus_{k=1}^K \mathcal{H}^{(k)}$, where each $\mathcal{H}^{(k)}$ is a finite-dimensional Hilbert space, driven by m controls $u_1, \dots, u_m$, with $|u_j(t)| \leq 1$,*

$$\frac{d}{dt}\Psi(t) = \left(\bigoplus_{k=1}^K \mathrm{i}H^{(k)} + \sum_{j=1}^m u_j(t) \bigoplus_{k=1}^K \mathrm{i}H^{(k)}_j\right)\Psi(t), \quad \Psi(t) = \bigoplus_{k=1}^K \psi^{(k)}(t), \quad \psi^{(k)}(t) \in \mathcal{H}^{(k)},$$

where each $H^{(k)}_j$ is a hermitian matrix. Suppose that each single system is operator controllable, that is,

$$\mathrm{Lie}\{\mathrm{i}H^{(k)}, \dots, \mathrm{i}H^{(k)}_m\} = \mathfrak{su}(\mathcal{H}^{(k)}), \quad \forall k = 1, \dots, K.$$

Then the direct sum system is NOT simultaneously operator controllable if and only if there exist $k, k' \in \{1, \dots, K\}$, with $k \neq k'$, and an isomorphism of Lie algebras $f : \mathfrak{su}(\mathcal{H}^{(k)}) \to \mathfrak{su}(\mathcal{H}^{(k')})$ such that

$$f(\mathrm{i}H^{(k)}_j) = \mathrm{i}H^{(k')}_j, \quad j = 0, \dots, m. \tag{3.2.9}$$

In other words, given the finite direct sum of some finite-dimensional controllable systems, if we are able to prove that such an isomorphism cannot exist, then all the dynamics are independent and the last lemma implies simultaneous operator controllability, that is,

$$\mathrm{Lie}\left\{\bigoplus_{k=1}^K \mathrm{i}H^{(k)}, \dots, \bigoplus_{k=1}^K \mathrm{i}H^{(k)}_m\right\} = \bigoplus_{k=1}^K \mathfrak{su}(\mathcal{H}^{(k)}).$$

In our case, we are going to prove the non-existence of such isomorphism (except for k and $-k$) thanks to a dimension argument. Indeed, for any $j \in \mathbb{N}$, upon setting $K = 2j$, $m = 3$,

$$\mathcal{H}^{(k)} := \bigoplus_{l=0,\dots,j+1} \mathcal{L}_{l,k}, \quad H^{(k)} = H|_{\mathcal{H}^{(k)}}, \quad H_i^{(k)} = \sum_{l=0,\dots,j} \mathcal{E}_{\sigma_k^l}(\mathrm{i}B_i),\ i = 1,2,3$$

for $k = -j, \dots, j$, we obtain in particular from part (i) that each k component is operator controllable in $\mathcal{H}^{(k)}$, i.e., in any finite-dimensional truncation of $\mathcal{S}_k$. Moreover, we easily see that $\dim(\mathcal{H}^{(k)}) = \dim(\mathcal{H}^{(k')})$ if and only if $k' = \pm k$, and thus an isomorphism between $\mathfrak{su}(\mathcal{H}^{(k)})$ and $\mathfrak{su}(\mathcal{H}^{(k')})$ can exist only if $k' = \pm k$. On the other end, an isomorphism between $\mathfrak{su}(\mathcal{H}^{(k)})$ and $\mathfrak{su}(\mathcal{H}^{(-k)})$ that matches conditions (3.2.9) surely exists, and is given by the transformation of vectors $\Phi : \mathcal{S}_k \to \mathcal{S}_{-k}$ (defined in statement (ii)) lifted to a transformation of endomorphisms (indeed, this follows from the fact that $a_k = a_{-k}$ and $b_k = b_{-k}$, as one can see in (3.4.11)). So, we obtain that (3.2.4) is simultaneously controllable within the finite-dimensional truncation of $\bigoplus_k(\mathcal{S}_k \oplus \mathcal{S}_{-k})$, by means of spectral gaps (σ_k^j, l) that belong to Ξ_j^0. The application of Corollary 3.1.20 concludes the proof of (ii). □

3.2.3 Controllability of the quantum accidentally symmetric-top

So far we have studied the dynamics of a symmetric-top molecule with electric dipole moment along its symmetry axis and we have proven that its dynamics are trapped in the eigenspaces of P_3.

Nevertheless, for applications to molecules charged in the laboratory, or to particular molecules present in nature such as D_2S_2 (Figure 1.3.2) or H_2S_2, it is interesting to consider also the case in which the dipole is not along the symmetry axis: this case is called the *accidentally symmetric molecule*.

Under a non-resonance condition, we are going to prove that, if the dipole moment is not orthogonal to the symmetry axis of the molecule, the rotational dynamics of an accidentally symmetric-top are approximately controllable. To prove this statement, we are going to apply Theorem 3.1.21 to (3.2.4). Moreover, the following Theorem will be crucial in the next section for proving the controllability of an asymmetric-top.

Theorem 3.2.5. *Assume that $I_1 = I_2$ and $\frac{I_2}{I_3} \notin \mathbb{Q}$. If $\delta = (\delta_1, \delta_2, \delta_3)^T$ is such that $\delta \neq (0,0,\delta_3)^T$ and $\delta \neq (\delta_1, \delta_2, 0)^T$, then system (3.2.4) is an m-tracker, and in particular approximately controllable.*

Proof. First of all, one can check, for example in [68, Table 2.1], that the pairings induced by the interaction Hamiltonians satisfy

$$\langle D_{k,m}^j, \mathrm{i}B_l D_{k',m'}^{j'} \rangle = 0, \tag{3.2.10}$$

when $|j' - j| > 1$, or $|k' - k| > 1$ or $|m' - m| > 1$, for every $l = 1,2,3$. Equation (3.2.10) is the general form of the so-called selection rules.

We then define for every $j \in \mathbb{N}$ the set $I_j := \{\rho(l,k,m) \mid l = j, j+1,\ k,m = -l,\dots,l\} \subset \mathbb{N}$, where $\rho : \{(l,k,m) \mid l \in \mathbb{N}, k,m = -l,\dots,l\} \to \mathbb{N}$ is the lexicographic ordering. The graph $\mathcal{G}$ whose vertices are the sets I_j and whose edges are $\{(I_j, I_{j'}) \mid I_j \cap I_{j'} \neq \emptyset\} = \{(I_j, I_{j+1}) \mid j \in \mathbb{N}\}$ is linear. In order to apply Theorem 3.1.21 we shall consider the projection of (3.2.4) onto each space $\mathcal{M}_j := \mathcal{H}_j \oplus \mathcal{H}_{j+1}$, where $\mathcal{H}_l := \mathrm{span}\{D_{k,m}^l \mid k,m = -l,\dots,l\}$. The dimension of $\mathcal{M}_j$ is $(2j+1)^2 + (2(j+1)+1)^2$, and we identify $\mathfrak{su}(\mathcal{M}_j)$ with $\mathfrak{su}((2j+1)^2 + (2(j+1)+1)^2)$.

According to (3.2.10), the three types of spectral gaps in $\mathcal{M}_j$, $j \in \mathbb{N}$, which we should consider are

$$\lambda_k^j := |E_{k+1}^{j+1} - E_k^j| = \left|\frac{j+1}{I_2} + \left(\frac{1}{2I_3} - \frac{1}{2I_2}\right)(2k+1)\right|, \quad k = -j,\dots,j, \tag{3.2.11}$$

corresponding to pairings for which both j and k move (see Figure 3.1),

$$\eta_k := |E_{k+1}^j - E_k^j| = \left|\left(\frac{1}{2I_3} - \frac{1}{2I_2}\right)(2k+1)\right|, \quad k = -j,\dots,j, \tag{3.2.12}$$

and

$$\sigma^j := |E_k^{j+1} - E_k^j| = \frac{j+1}{I_2}, \quad k = -j,\dots,j, \tag{3.2.13}$$

for which, respectively, only k or j moves (see, Figures 3.5(a) and 3.5(b)).

We now classify the spectral gaps in terms of the sets Ξ_j^0 and Ξ_j^1 introduced in Section 3.1.

Lemma 3.2.6. *Let $I_2/I_3 \notin \mathbb{Q}$. Then $(\lambda_k^j, l), (\sigma^j, l) \in \Xi_j^0$, and $(\eta_k, l) \in \Xi_j^1$, for all $k = -j,\dots,j$, $l = 1,2,3$.*

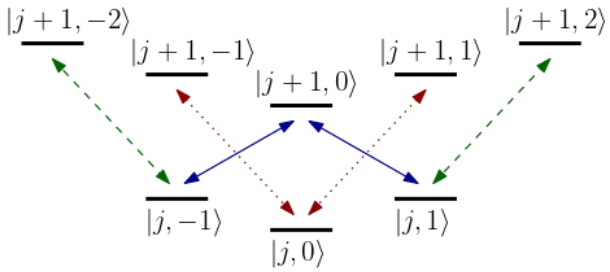


Figure 3.1: Graph of the transitions associated with the frequency λ_k^j between eigenstates $|j,k\rangle = |j,k,m\rangle := D^j_{k,m}$ (m fixed). Same-shaped arrows correspond to equal spectral gaps.

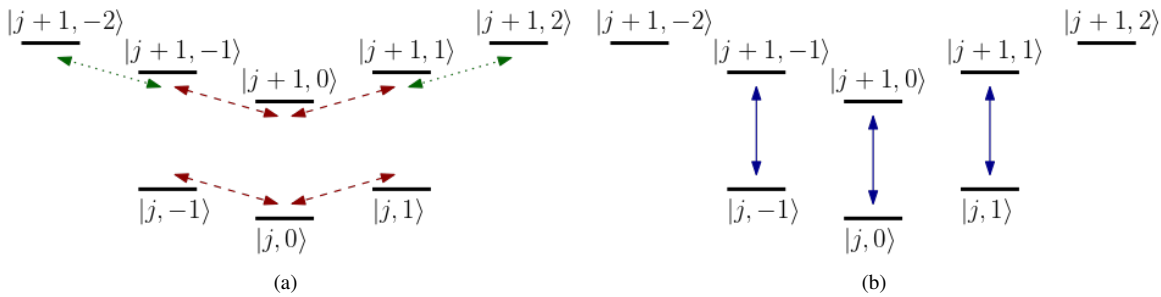


Figure 3.2: Transitions between states: (a) at frequency η_k; (b) at frequency σ^j. Same-shaped arrows correspond to equal spectral gaps.

Proof. Because of the selection rules (3.2.10), we only need to check if there are common spectral gaps in the spaces $\mathcal{M}_j$ and $\mathcal{M}_{j'}$ for $j' \neq j$.

We start by proving that $(\lambda_k^j, l), (\sigma^j, l) \in \Xi_j^0$ by showing that a spectral gap of the type λ_k^j (respectively, σ^j) is different from any spectral gap of the type $\lambda_{k'}^{j'}$, $\sigma^{j'}$, or $\eta_{k'}$ unless $\lambda_k^j = \lambda_{k'}^{j'}$ and $(k,j) = (k',j')$ (respectively, $\sigma^j = \sigma^{j'}$ and $j = j'$).

Using the explicit structure of the spectrum (3.2.7), any spectral gap of the type $\lambda_{k'}^{j'}$, $\sigma^{j'}$, or $\eta_{k'}$ can be written as

$$\left|\frac{q_1}{I_2} + q_2\left(\frac{1}{I_3} - \frac{1}{I_2}\right)\right|, \qquad q_1, q_2 \in \mathbb{Q}.$$

Since, moreover, $\frac{1}{I_2}$ and $\left(\frac{1}{I_3} - \frac{1}{I_2}\right)$ are $\mathbb{Q}$-linearly independent, one easily deduces that, indeed, $(\lambda_k^j, l), (\sigma^j, l) \in \Xi_j^0$.

Notice that the gaps of the type η_k correspond to internal pairings in the spaces $\mathcal{H}_j$. Henceforth, in order to prove that $(\eta_k, l) \in \Xi_j^1$ it is enough to check that η_k is different from any gap of the type $\lambda_{k'}^j, \sigma^j$. This fact has already been noticed in the proof of the first part of the statement. The proof of the lemma is then concluded. □

Next, we introduce the family of excited modes associated with the spectral gap λ_k^j, that is,

$$\mathcal{F}_j := \{\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_l), W_{\mathrm{i}}(\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_l)) \mid l = 1,2,3,\ k = -j,\dots,j\},$$

where the operators $\mathcal{E}_\mu$ and W_ξ are defined in Section 3.1, and where, with a slight abuse of notation, we write B_l instead of $\Pi_{\mathcal{M}_j} B_l \Pi_{\mathcal{M}_j}$. Notice that $\mathcal{F}_j \subset \nu_j^0$ as it follows from Lemma 3.2.6, where ν_j^0 is defined as in (3.1.13).

In order to write down the matrices in $\mathcal{F}_j$, we need to study the resonances between the spectral gaps inside $\mathcal{M}_j$. We claim that there are no internal resonances except those due to the degeneracy $E_k^j = E_{-k}^j$. Indeed, we already noticed in Lemma 3.2.6 that a spectral gap of the type λ_k^j is different from any spectral gap of the type $\lambda_{k'}^{j'}$, $\sigma^{j'}$, or $\eta_{k'}$ unless $\lambda_k^j = \lambda_{k'}^{j'}$ and $(k,j) = (k',j')$. We collect in the lemma below also the similar observations that σ^j is different from any spectral gap of the type $\lambda_{k'}^{j'}$, $\sigma^{j'}$, or $\eta_{k'}$ unless $\sigma^j = \sigma^{j'}$ and $j = j'$, and that $\eta_k \neq \eta_{k'}$ if $k \neq k'$.

Lemma 3.2.7. *Let $I_2/I_3 \notin \mathbb{Q}$. Then*

1. ***λ_k^j-resonances:*** *the equation*

$$|E_{k+1}^{j+1} - E_k^j| = |E_{s+h}^{j''} - E_s^{j'}|,\ j \le j' \le j'' \le j+1,\ -j' \le s \le j',\ h \in \{-1,0,1\},$$

implies that $j' = j$, $j'' = j+1$, $s = \pm k$, $s + h = \pm(k+1)$*;*

2. η_k***-resonances:*** *the equation*

$$|E^j_{k+1} - E^j_k| = |E^{j''}_{s+h} - E^{j'}_s|, \ j \le j' \le j'' \le j+1, \ -j' \le s \le j', \ h \in \{-1, 0, 1\},$$

implies that $j' = j'' = j$ *or* $j' = j'' = j+1$ *and* $s = \pm k$, $s + h = \pm(k+1)$*;*

3. σ^j***-resonances:*** *the equation*

$$|E^{j+1}_k - E^j_k| = |E^{j''}_{s+h} - E^{j'}_s|, \ j \le j' \le j'' \le j+1, \ -j' \le s \le j', \ h \in \{-1, 0, 1\},$$

implies that $j' = j$, $j'' = j+1$, $h = 0$, $s = \pm k$.

Denote by $\mathrm{L}_j := \mathrm{Lie}(\mathcal{F}_j)$ the Lie algebra generated by the matrices in $\mathcal{F}_j$. Let us introduce the generalized Pauli matrices

$$G_{j,k} = e_{j,k} - e_{k,j}, \quad F_{j,k} = \mathrm{i}e_{j,k} + \mathrm{i}e_{k,j}, \quad D_{j,k} = \mathrm{i}e_{j,j} - \mathrm{i}e_{k,k},$$

where $e_{j,k}$ denotes the $(2j+1)^2 + (2(j+1)+1)^2$-square matrix whose entries are all zero, except the one at row j and column k, which is equal to 1. Consider again the lexicographic ordering $\rho : \{(l,k,m) \mid l = j, j+1, \ k, m = -l, \dots, l\} \to \mathbb{N}$. By a slight abuse of notation, also set $e_{(l,k,m),(l',k',m')} = e_{\rho(l,k,m),\rho(l',k',m')}$. The analogous identification can be used to define $G_{(l,k,m),(l',k',m')}, F_{(l,k,m),(l',k',m')}, D_{(l,k,m),(l',k',m')}$. The next proposition tells us how the elements in L_j look like. For a proof, see Appendix 3.4.1.

Proposition 3.2.8. *Let* $m = -j, \dots, j$ *and* $k = -j, \dots, j$ *with* $k \neq 0$. *Then the matrices* $X_{(j,k,m),(j+1,k+1,m)} - X_{(j,-k,m),(j+1,-k-1,m)}$ *and* $X_{(j,k,m),(j+1,k+1,m\pm1)} - X_{(j,-k,m),(j+1,-k-1,m\pm1)}$ *are in* L_j*, where* $X \in \{G, F\}$.

To break the degeneracy between k and $-k$ which appears in the matrices that we found in Proposition 3.2.8, and obtain all the elementary matrices that one needs to generate $\mathfrak{su}(\mathcal{M}_j)$, we need to exploit the other two types of spectral gaps that we have introduced in (3.2.12) and (3.2.13) (see Figure 3.5).

Let us introduce the family of excited modes at the frequencies σ^j and η_k,

$$\mathcal{P}_j := \{\mathcal{E}_{\sigma^j}(\mathrm{i}B_l), W_{\mathrm{i}}(\mathcal{E}_{\sigma^j}(\mathrm{i}B_l)), \mathcal{E}_{\eta_k}(\mathrm{i}B_l), W_{\mathrm{i}}(\mathcal{E}_{\eta_k}(\mathrm{i}B_l)) \mid l = 1, 2, 3, \ k = -j, \dots, j\},$$

and notice that, by Lemma 3.2.6, $\mathcal{P}_j \subset \nu^1_j$ (cf. (3.1.13)). Therefore,

$$\widetilde{\mathcal{P}}_j := \{A, [B, C] \mid A, B \in \mathrm{L}_j, C \in \mathcal{P}_j\} \subset \mathcal{T}_j,$$

where we recall that $\mathcal{T}_j$ is the minimal ideal of $\mathrm{Lie}(\nu^1_j)$ containing ν^0_j.

The following proposition, whose proof is given in Appendix 3.4.2, concludes the proof of Theorem 3.2.5.

Proposition 3.2.9. $\mathrm{Lie}(\widetilde{\mathcal{P}}_j) = \mathfrak{su}(\mathcal{M}_j)$.

□

Remark 3.2.10.
- The assumption $I_2/I_3 \notin \mathbb{Q}$ on the moments of inertia appearing in Theorem 3.2.5 is technical, and prevents the system from having both external resonances (as we saw in Lemma 3.2.6) and internal ones (Lemma 3.2.7). Anyway, we have not proven that controllability fails if the ratio I_2/I_3 is rational.
- As a matter of fact, if $I_2/I_3 = 1$, the top is symmetric spherical (i.e., $I_1 = I_2 = I_3$) and any axis in the molecular frame is a symmetry axis. Then, Theorem 3.2.1 implies that (3.2.4) is not controllable for spherical symmetric tops.

3.2.4 Non-controllability and reachable sets of the quantum orthogonal accidentally symmetric-top

We now consider the case where $\delta = (\delta_1, \delta_2, 0)^T$, left out by Theorem 3.2.5. The situation in which the dipole lies in the plane orthogonal to the symmetry axis of the molecule (that we shall call the *orthogonal* accidentally symmetric-top) is interesting from the point of view of chemistry, since the accidentally symmetric-top molecules present in nature are usually of that kind (see Figure 1.3.2). In order to study this problem, let us introduce the Wang functions [68, Section 7.2]

$$S^j_{0,m,0} := D^j_{0,m}, \qquad S^j_{k,m,p} := \frac{1}{\sqrt{2}}(D^j_{k,m} + (-1)^p D^j_{-k,m}), \quad k = 1, \dots, j, \tag{3.2.14}$$

for $j \in \mathbb{N}$, $m = -j, \dots, j$, and $p = 0, 1$. Due to the k-degeneracy $E_k^j = E_{-k}^j$ in the spectrum of the rotational Hamiltonian H, the functions $S_{k,m,p}^j$ still form an orthogonal basis of eigenfunctions of H. Then we consider the change of basis $D_{k,m}^j \to e^{-\mathrm{i}k\theta} D_{k,m}^j$, and we choose $\theta \in [0, 2\pi)$ such that

$$\begin{cases} e^{-\mathrm{i}\theta}(\delta_2 + \mathrm{i}\delta_1) = \mathrm{i}\sqrt{\delta_1^2 + \delta_2^2}, \\ e^{\mathrm{i}\theta}(\delta_2 - \mathrm{i}\delta_1) = -\mathrm{i}\sqrt{\delta_1^2 + \delta_2^2}. \end{cases} \tag{3.2.15}$$

System (3.2.15) describes the rotation of angle $\mp\theta$ in the complex plane of the vector $\delta_2 \pm \mathrm{i}\delta_1$. The composition of these two changes of basis gives us the rotated Wang states $S_{k,m,p}^j(\theta) := \frac{1}{\sqrt{2}}(e^{-\mathrm{i}k\theta} D_{k,m}^j + (-1)^p e^{\mathrm{i}k\theta} D_{-k,m}^j)$, for $k \neq 0$, and $S_{0,m,0}^j = D_{0,m}^j$.

In the next theorem we express in this new basis a symmetry which prevents the system from being controllable. We define the spaces

$$\mathcal{L}_{e(o)} := \overline{\mathrm{span}}\{S_{k,m,p}^j \mid j \in \mathbb{N},\ k = 0, \dots, j,\ m = -j, \dots, j,\ p = 0, 1,\ j + k + p \text{ even (odd)}\}.$$

Theorem 3.2.11. *Let $I_1 = I_2$ and $\delta = (\delta_1, \delta_2, 0)^T$. Then the parity of $j + p + k$ is conserved, that is, the spaces $\mathcal{L}_e$ and $\mathcal{L}_o$ are invariant for the propagators of* (3.2.4).

Proof. We need to prove that the pairings allowed by the controlled vector fields B_1, B_2 and B_3 conserve the parity of $j + p + k$. To do so, let us compute

$$\begin{aligned} \langle S_{k,m,p}^j(\theta), \mathrm{i}B_1 S_{k+1,m+1,p}^{j+1}(\theta)\rangle &= -c_{j,k,m} e^{-\mathrm{i}\theta}(\delta_2 + \mathrm{i}\delta_1) + c_{j,k,m} e^{\mathrm{i}\theta}(\delta_2 - \mathrm{i}\delta_1) \\ &= -2\mathrm{i}c_{j,k,m}\sqrt{\delta_1^2 + \delta_2^2}, \\ \langle S_{k,m,p}^j(\theta), \mathrm{i}B_1 S_{k+1,m+1,p'}^{j+1}(\theta)\rangle &= -c_{j,k,m} e^{-\mathrm{i}\theta}(\delta_2 + \mathrm{i}\delta_1) - c_{j,k,m} e^{\mathrm{i}\theta}(\delta_2 - \mathrm{i}\delta_1) \\ &= 0, \qquad p \neq p', \end{aligned} \tag{3.2.16}$$

having used the expression of the Wang functions as linear combinations of Wigner functions, the explicit pairings (3.4.2) which can be found in Appendix 3.4.1, and the choice of θ made in (3.2.15). Then we also have

$$\begin{cases} \langle S_{k,m,p}^j(\theta), \mathrm{i}B_1 S_{k+1,m+1,p}^j(\theta)\rangle = 0, \\ \langle S_{k,m,p}^j(\theta), \mathrm{i}B_1 S_{k+1,m+1,p'}^j(\theta)\rangle = -2\mathrm{i}h_{j,k,m}\sqrt{\delta_1^2 + \delta_2^2}, \quad p \neq p', \end{cases} \tag{3.2.17}$$

having used this time the pairings (3.4.10), which can be found in Appendix 3.4.2. From (3.2.16) and (3.2.17) we can see that the allowed transitions only depend on the parity of $j + p$ and k; indeed, we have either transitions between states of the form

$$\begin{cases} j + p & \text{even} \\ k & \text{even} \end{cases} \longleftrightarrow \begin{cases} j' + p' & \text{odd} \\ k' & \text{odd,} \end{cases}$$

or transitions between states of the form

$$\begin{cases} j + p & \text{even} \\ k & \text{odd} \end{cases} \longleftrightarrow \begin{cases} j' + p' & \text{odd} \\ k' & \text{even.} \end{cases}$$

The same happens if we replace $m + 1$ with $m - 1$ and $k + 1$ with $k - 1$ in (3.2.16) and (3.2.17). Because of the selection rules (3.2.10), these are the only transitions allowed by the field B_1. One can easily check, in the same way, that every transition induced by B_2, B_3 also conserves the parity of $j + p + k$. □

Having established that $L^2(\mathrm{SO}(3)) = \mathcal{L}_e \oplus \mathcal{L}_o$ is a decomposition in orthogonal invariant subspaces for the motion of an orthogonal accidentally symmetric molecule, we next prove that it is also a decomposition in simultaneously approximately reachable sets:

Theorem 3.2.12. *Let $I_1 = I_2$, $\frac{I_1}{I_2} \notin \mathbb{Q}$. If $\delta = (\delta_1, \delta_2, 0)^T$ with $\delta_1 \neq 0$ or $\delta_2 \neq 0$, then*

(i) the Schrödinger equation (3.2.4) is an m-tracker in the Hilbert space $\mathcal{L}_e$, and in the Hilbert space $\mathcal{L}_o$. In particular, $\mathrm{Reach}(\psi)$ *is dense in $\mathcal{L}_{e(o)} \cap \mathcal{S}$ for all $\psi \in \mathcal{L}_{e(o)} \cap \mathcal{S}$.*

(ii) the Schrödinger equation (3.2.4) is simultaneously approximately controllable w.r.t. the orthogonal decomposition $L^2(\mathrm{SO}(3)) = \mathcal{L}_e \oplus \mathcal{L}_o$. That is, if $\psi \in \mathcal{S}$ decomposes as $\psi = p_e\psi_e + p_o\psi_o$, $\psi_{e(o)} \in \mathcal{L}_{e(o)} \cap \mathcal{S}$, $|p_e|^2 + |p_o|^2 = 1$, then $\mathrm{Reach}(\psi)$ *is dense in* $\{\phi \in \mathcal{S} \mid \phi = p_e\phi_e + p_o\phi_o,\ \phi_{e(o)} \in \mathcal{L}_{e(o)} \cap \mathcal{S}\}$.

Proof. The proof of part (i) goes through the same reasonings of Theorem 3.2.5's proof. The proof of part (ii) follows the arguments proposed in the proof of Theorem 3.2.3 part (ii), in particular it is again an application of Lemma 3.2.4 and Corollary 3.1.20

We outline the proof of (i) for $\mathcal{L}_e$, the computations for $\mathcal{L}_o$ being analogous. We already know that $\mathcal{L}_e$ is invariant; we shall then prove that (3.2.4) is an m-tracker in the Hilbert space $\mathcal{L}_e$. We then define for every $j \in \mathbb{N}$ the set $I_j := \{\rho(l,k,m,p) \mid l = j, j+1,\ k = 0,\dots,l,\ m = -l,\dots,l,\ p = 0,1,\ j+k+p \text{ even}\} \subset \mathbb{N}$, where $\rho : \{(l,k,m,p) \mid l = j, j+1,\ k = 0,\dots,l,\ m = -l,\dots,l,\ p = 0,1,\ j+k+p \text{ even}\} \to \mathbb{N}$ is the lexicographic ordering. The graph $\mathcal{G}_e$ whose vertices are the sets I_j and whose edges are $\{(I_j, I_{j'}) \mid I_j \cap I_{j'} \neq \emptyset\} = \{(I_j, I_{j+1}) \mid j \in \mathbb{N}\}$ is linear.

Let us project (3.2.4) onto the subspace of $\mathcal{L}_e$ given by $\mathcal{M}_{e,j} := \mathcal{H}_{e,j} \oplus \mathcal{H}_{e,j+1}$, where $\mathcal{H}_{e,l} := \mathrm{span}\{S^j_{k,m,p} \mid j+p+k \text{ even},\ j = l\}$, $l \in \mathbb{N}$. The dimension of $\mathcal{M}_{e,j}$ is $(2j+1)(j+1) + (2(j+1)+1)(j+1)$, if j is even, and $(2j+1)j + (2(j+1)+1)(j+2)$, if j is odd. Let us assume that j is even, being the computation in the case j odd analogous. We identify $\mathfrak{su}(\mathcal{M}_{e,j})$ with $\mathfrak{su}((2j+1)(j+1) + (2(j+1)+1)(j+1))$.

Referring to the notations introduced in Section 3.1, we shall consider the following spectral gaps in $\mathcal{M}_{e,j}$

$$
\begin{aligned}
\lambda^j_{\pm k} &:= |E^{j+1}_{k\pm1} - E^j_k| = \left|\frac{j+1}{I_2} + \left(\frac{1}{2I_3} - \frac{1}{2I_2}\right)(\pm 2k+1)\right| \in \Sigma_j, \quad k = 0,\dots,j,\\
\eta_{\pm k} &:= |E^{j+1}_{k\pm1} - E^{j+1}_k| = \left|\left(\frac{1}{2I_3} - \frac{1}{2I_2}\right)(\pm 2k+1)\right| \in \Sigma_j, \quad k = 0,\dots,j.
\end{aligned}
\tag{3.2.18}
$$

As in Lemma 3.2.6, the assumption $\frac{I_2}{I_3} \notin \mathbb{Q}$ guarantees that $(\lambda^j_{\pm k}, l) \in \Xi^0_j$, and $(\eta_{\pm k}, l) \in \Xi^1_j$, for all $k = 0,\dots,j$,

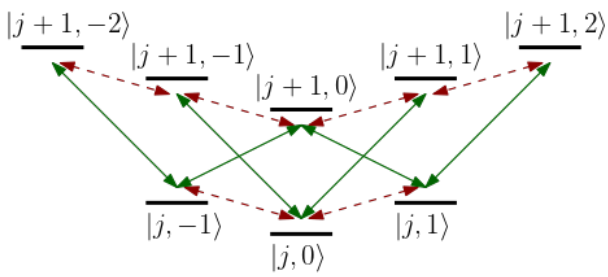


Figure 3.3: Graph of the transitions associated with the frequency $\lambda^j_{\pm k}$ (solid arrows) and the frequency $\eta_{\pm k}$ (dashed arrows) between eigenstates $|j,k\rangle = |j,k,m\rangle := D^j_{k,m}$ (m is fixed).

$l = 1,2,3$.

We drive the electric fields at the frequencies defined in (3.2.18) to excite the corresponding transitions between the rotational states of H. To be more precise, as in Lemma 3.2.7, the assumption $\frac{I_2}{I_3} \notin \mathbb{Q}$ guarantees that the frequencies (3.2.18) are not resonant between each other, and thus we can write that the three polarizations driven at frequency $\lambda^j_{\pm k}$, $k = 0,\dots,j$, are represented by

$$
\begin{aligned}
\mathcal{E}_{\lambda^j_{\pm k}}(\mathrm{i}B^e_1) &= \sum_{m=-j,\dots,j} -2c_{j,\pm k,m}\delta_1 F_{(j,k,m,p),(j+1,k\pm1,m+1,p)} - 2c_{j,\pm k,-m}\delta_1 F_{(j,k,m,p),(j+1,k\pm1,m-1,p)},\\
\mathcal{E}_{\lambda^j_{\pm k}}(\mathrm{i}B^e_2) &= \sum_{m=-j,\dots,j} -2c_{j,\pm k,m}\delta_1 G_{(j,k,m,p),(j+1,k\pm1,m+1,p)} + 2c_{j,\pm k,-m}\delta_1 G_{(j,k,m,p),(j+1,k\pm1,m-1,p)},\\
\mathcal{E}_{\lambda^j_{\pm k}}(\mathrm{i}B^e_3) &= \sum_{m=-j,\dots,j} -2d_{j,\pm k,m}\delta_1 G_{(j,k,m,p),(j+1,k\pm1,m,p)},
\end{aligned}
\tag{3.2.19}
$$

where $p = 0$ if k is even, and $p = 1$ if k is odd. The three fields in (3.2.19) are seen as skew-adjoint operators acting on the Hilbert space $\mathcal{M}_{e,j}$, and, with a slight abuse of notation, we write B^e_l instead of $B^{e,(j)}_l := \Pi_{\mathcal{M}_{e,j}} B_l \Pi_{\mathcal{M}_{e,j}}$, where $\Pi_{\mathcal{M}_{e,j}}$ is the orthogonal projection onto $\mathcal{M}_{e,j}$.

In (3.2.19), the matrices $G_{s,t}, F_{s,t} \in \mathfrak{su}(\mathcal{M}_j)$ are defined by $G_{s,t} = e_{s,t} - e_{t,s}$, $F_{s,t} = \mathrm{i}e_{s,t} + \mathrm{i}e_{t,s}$, where $e_{s,t}$ denotes the $(2j+1)(j+1) + (2(j+1)+1)(j+1)$-square matrix whose entries are all zero, except the one at row s

and column t, which is equal to 1. Moreover, we are implicitly using the lexicographic correspondance between the sets $\{(l,k,m,p) \mid l = j, j+1, k = 0, ..., l, m = -l, ..., l, p = 0, 1\}$ and $\{1, 2, ..., (2j+1)(j+1) + (2(j+1)+1)(j+1)\}$, to label the matrices in (3.2.19).

Finally, the coupling constants in (3.2.19) are given by the pairings (3.4.1), where we have already performed a rotation around the symmetry axis to get rid of the δ_2-component (see eq. (3.4.2)).

In the same way, one can represent the interaction operators $\mathcal{E}_{\eta_{\pm k}}(\mathrm{i}B_l^e)$, $l = 1, 2, 3$, $k = 0, ..., j$ relative to the spectral gaps $\eta_{\pm k}$. We have

(3.2.20)

$$\mathcal{E}_{\eta_{\pm k}}(\mathrm{i}B_1^e) = \sum_{l=j,j+1,m=-l,\dots,l-1} \mp 2h_{l,\pm k,m}\delta_1 F_{(l,k,m,p),(l,k\pm1,m+1,p')} + \sum_{l=j,j+1,m=-l+1,\dots,l} \pm 2h_{l,\pm k,-m}\delta_1 F_{(l,k,m,p),(l,k\pm1,m-1,p')},$$

$$\mathcal{E}_{\eta_{\pm k}}(\mathrm{i}B_2^e) = \sum_{l=j,j+1,m=-l,\dots,l-1} \pm 2h_{l,\pm k,m}\delta_1 G_{(l,k,m,p),(l,k\pm1,m+1,p')} + \sum_{l=j,j+1,m=-l+1,\dots,l} \pm 2h_{l,\pm k,-m}\delta_1 G_{(l,k,m,p),(l,k\pm1,m-1,p')},$$

$$\mathcal{E}_{\eta_{\pm k}}(\mathrm{i}B_3^e) = \sum_{l=j,j+1,m=-l,\dots,l} \pm 2q_{l,\pm k,m}\delta_1 G_{(l,k,m,p),(l,k\pm1,m,p')},$$

where $p = 0, p' = 1$ if k is even, and $p = 1, p' = 0$ if k is odd. The coupling constants in (3.2.20) are given by the pairings (3.4.10), and also here we get rid of the δ_2-component.

We now introduce the family

$$\mathcal{F}_j^0 := \{\mathcal{E}_{\lambda_{\pm k}^j}(\mathrm{i}B_l^e), W_{\mathrm{i}}(\mathcal{E}_{\lambda_{\pm k}^j}(\mathrm{i}B_l^e)), \mid l = 1, 2, 3, k = 0, ..., j\} \subset \nu_j^0$$

of the interaction operators excited at non-resonant frequencies, and we denote by $\mathrm{Lie}(\mathcal{F}_j^0)$ the Lie algebra generated by the matrices in $\mathcal{F}_j^0$; finally, let us introduce the new family

$$\mathcal{F}_j := \{A, \left[W_\xi(\mathcal{E}_{\eta_{\pm k}}(\mathrm{i}B_l^e)), B\right] \mid A, B \in \mathrm{Lie}(\mathcal{F}_j^0),\ l = 1, 2, 3, \xi = 1, \mathrm{i}, \quad k = 0, ..., j\} \subset \mathcal{T}_j,$$

the sets of operators ν_j^0 and $\mathcal{T}_j$ being defined in Section 3.1.

Then, direct Lie bracket computations, analogous to the ones performed in Appendix 3.4.1 and 3.4.2, prove that $\mathrm{Lie}(\mathcal{F}_j) = \mathfrak{su}(\mathcal{M}_{e,j})$, for every $j \in \mathbb{N}$, which concludes the proof of (i).

To proof part (ii), we apply Lemma 3.2.4 to the finite-dimensional truncations of $\mathcal{L}_e \oplus \mathcal{L}_o$: indeed, for any $j \in \mathbb{N}$, upon setting $K = 2$, $m = 6(j+1)$ and

$$\mathcal{H}^{(r)} := \bigoplus_{l=0,\dots,j+1} \mathcal{H}_{r,l}, \quad H^{(r)} = H|_{\mathcal{H}^{(r)}}, \quad H_i^{(r)} = \sum_{l=0,\dots,j} \mathcal{E}_{\lambda_{\pm k}^l}(\mathrm{i}B_i^r),\ i = 1, 2, 3,\ k = 0, \dots, j,$$
$$H_i^{(r)} = \sum_{l=0,\dots,j} \mathcal{E}_{\eta_{\pm k}^l}(\mathrm{i}B_i^r),\ i = 4, 5, 6,\ k = 0, \dots, j,$$

for $r = e, o$, we obtain in particular from part (i) that each r component is operator controllable in $\mathcal{H}^{(r)}$, i.e., in any finite-dimensional truncation of $\mathcal{L}_r$. We easily see that $\dim \mathcal{H}^{(e)} \neq \dim \mathcal{H}^{(o)}$, implying that there cannot be an isomorphism between $\mathfrak{su}(\mathcal{H}^{(e)})$ and $\mathfrak{su}(\mathcal{H}^{(o)})$. Then, Lemma 3.2.4 implies that (3.2.4) is simultaneously controllable in every finite-dimensional truncation of $\mathcal{L}_e \oplus \mathcal{L}_o$ be means of spectral gaps $(\lambda_{\pm k}^j, l), (\eta_{\pm k}^j, l)$ that belongs to Ξ_j^0 and Ξ_j^1. The application of Corollary 3.1.20 concludes the proof of (ii). □

3.3 Asymmetric molecule

3.3.1 Eigenfunctions of the asymmetric-top

It is convenient to adopt a slightly different notation to describe the asymmetry of the rigid body: we denote as $\{a, b, c\} = \{a_1, a_2, a_3\}$ the principal axes of inertia, such that the associated inertia moments satisfy $I_a < I_b < I_c$. We also introduce the rotational constants $A > B > C$, related to the inertia moments through the identities $2A = 1/I_a, 2B = 1/I_b, 2C = 1/I_c$. We then write the rotational Hamiltonian as a function of the rotational constants

$$H = H(A, B, C) = AP_a^2 + BP_b^2 + CP_c^2,$$

and we want to study the controllability of (3.2.4). We have to choose which principal axis corresponds to a_3 (which in the symmetric top case is the symmetry axis of the molecule): let us set $a = a_1, b = a_2, c = a_3$, and hence

$H = H(A, B, C) = AP_1^2 + BP_2^2 + CP_3^2$. As we have previously seen, the Wang functions $S^j_{k,m,p}$ defined in (3.2.14) (in terms of the Wigner functions $D^j_{k,m}$ (cf. (3.2.5)) which are the solution to the eigenvalue problem (3.2.6)) are the eigenfunctions of the symmetric top rotational Hamiltonian $H(B, B, C) = BP^2 + (C - B)P_3^2$. We also recall that

$$[H(B, B, C), J^2] = [H(B, B, C), J_3] = [H(B, B, C), P_3] = 0.$$

When $A > B > C$, the asymmetric rotational Hamiltonian $H(A, B, C)$ shares the first two symmetries with the symmetric one

$$[H(A, B, C), J^2] = [H(A, B, C), J_3] = 0,$$

while the third symmetry is broken

$$[H(A, B, C), P_3] \neq 0, \quad \text{if } A > B.$$

So, the eigenfunctions of $H(A, B, C)$ must be eigenfunctions of J^2 and J_3 too, and hence they are linear combinations in k of the same j and m. This fact is usually understood by saying that j and m are still good quantum numbers for an asymmetric molecule, while k is not. It means that the eigenfunctions $\{\Psi^j_{\tau,m} \mid j \in \mathbb{N}, m, \tau = -j, \dots, j\}$ of $H(A, B, C)$ must satisfy

$$\Psi^j_{\tau,m}(\alpha, \beta, \gamma) = \sum_{\substack{k=0,\dots,j \\ p=0,1}} c^j_{k,m,p}(\tau) S^j_{k,m,p}(\alpha, \beta, \gamma). \tag{3.3.1}$$

Other useful symmetries of these eigenfunctions are known, which allow to conclude that: the coefficients $c^j_{k,m,p}(\tau)$ in (3.3.1) can be taken in $\mathbb{R}$; the coefficients $c^j_{k,m,p}(\tau)$ in (3.3.1) do not depend on m; for any $\Psi^j_{\tau,m}$, the sum in (3.3.1) involves even or odd k only; for any $\Psi^j_{\tau,m}$, the sum in (3.3.1) involves $p = 0$ or $p = 1$ only (see, e.g., [68, Chapter 7]). That is, any eigenfunction $\Psi^j_{\tau,m}$ of $H(A, B, C)$ must satisfy the following additional requirement

$$\Psi^j_{\tau,m}(\alpha, \beta, \gamma) = \sum_{\substack{k=0,\dots,j, \\ k \text{ only even or only odd} \\ p=0 \text{ or } p=1}} c^j_{k,p}(\tau) S^j_{k,m,p}(\alpha, \beta, \gamma), \tag{3.3.2}$$

for certain $c^j_{k,p}(\tau) \in \mathbb{R}$. Moreover, it is also well-known that the eigenvalues of $H(A, B, C)$ are still $(2j + 1)$-degenerate w.r.t m, while the k-degeneracy is lifted (see, e.g., [68, Chapter 7]): the spectrum of $H(A, B, C)$ is the set of eigenvalues $\{E^j_\tau \mid j \in \mathbb{N}, \tau = -j, \dots, j\}$, and

$$H(A, B, C)\Psi^j_{\tau,m} = E^j_\tau \Psi^j_{\tau,m}, \quad m = -j, \dots, j$$

and each E^j_τ, is degenerate with associated eigenspace spanned by $\{\Psi^j_{\tau,m} \mid m = -j, \dots, j\}$. We also remark that, of course, a formula analogous to (3.3.2) holds w.r.t. the $D^j_{k,m}$ representation, that is,

$$\Psi^j_{\tau,m}(\alpha, \beta, \gamma) = \sum_{\substack{0 \le k \le j, \\ k \text{ only even or only odd}}} c^j_k(\tau) D^j_{k,m}(\alpha, \beta, \gamma). \tag{3.3.3}$$

3.3.2 Symmetries: non-controllability of critical dipole configurations

Thanks to the structure (3.3.2) of the eigenfunctions of the asymmetric-top, we can derive three consequences on the controllability properties of (3.2.4). Indeed, in Theorem 3.2.1 we proved that

$$\delta = (0, 0, \delta_3)^T \quad \Rightarrow \quad \langle S^j_{k,m,p}, B_i S^{j'}_{k',m',p'} \rangle = 0 \quad \text{if } k \neq k', \ i = 1, 2, 3, \tag{3.3.4}$$

moreover, analogously to the proof of Theorem 3.2.11, using the pairings (3.4.1) and (3.4.10) one sees that

$$\delta = (\delta_1, 0, 0)^T \ \Rightarrow \ \langle S^j_{k,m,p}, B_i S^{j'}_{k',m',p'} \rangle = 0 \quad \text{if } j + k + p \not\equiv j' + k' + p' \mod 2, \ i = 1, 2, 3, \tag{3.3.5}$$

and also that

$$\delta = (0, \delta_2, 0)^T \ \Rightarrow \ \langle S^j_{k,m,p}, B_i S^{j'}_{k',m',p'} \rangle = 0 \quad \text{if } j + p \not\equiv j' + p' \mod 2, \ i = 1, 2, 3. \tag{3.3.6}$$

We thus define

$$\mathcal{K}_{e(o)} := \overline{\text{span}}\{S^j_{k,m,p} \mid j \in \mathbb{N},\ m = -j, \dots, j,\ k = 0, \dots, j,\ p = 0, 1,\ \ k \text{ even(odd)}\},$$
$$\mathcal{L}_{e(o)} := \overline{\text{span}}\{S^j_{k,m,p} \mid j \in \mathbb{N},\ m = -j, \dots, j,\ k = 0, \dots, j,\ p = 0, 1,\ \ j + k + p \text{ even(odd)}\},$$
$$\mathcal{G}_{e(o)} := \overline{\text{span}}\{S^j_{k,m,p} \mid j \in \mathbb{N},\ m = -j, \dots, j,\ k = 0, \dots, j,\ p = 0, 1,\ \ j + p \text{ even(odd)}\}$$

that in particular give three different orthogonal decompositions of the ambient space

$$L^2(\text{SO}(3)) = \mathcal{K}_e \oplus \mathcal{K}_o = \mathcal{L}_e \oplus \mathcal{L}_o = \mathcal{G}_e \oplus \mathcal{G}_o.$$

Then, as the $\Psi^j_{\tau,m}$ are eigenfunctions of H, (3.3.2) implies that the decompositions are preserved by the rotational Hamiltonian:

$$H\mathcal{K}_{e(o)} \subset \mathcal{K}_{e(o)}\ ,\ \ H\mathcal{L}_{e(o)} \subset \mathcal{L}_{e(o)}\ ,\ \text{and}\ \ H\mathcal{G}_{e(o)} \subset \mathcal{G}_{e(o)}$$

while (3.3.2) plus (3.3.4) imply

$$\delta = (0, 0, \delta_3)^T \quad \Rightarrow B_i\mathcal{K}_{e(o)} \subset \mathcal{K}_{e(o)},\ \ i = 1, 2, 3,$$

(3.3.2) plus (3.3.5) imply

$$\delta = (\delta_1, 0, 0)^T \quad \Rightarrow B_i\mathcal{L}_{e(o)} \subset \mathcal{L}_{e(o)},\ \ i = 1, 2, 3,$$

and (3.3.2) plus (3.3.6) imply

$$\delta = (0, \delta_2, 0)^T \quad \Rightarrow B_i\mathcal{G}_{e(o)} \subset \mathcal{G}_{e(o)},\ \ i = 1, 2, 3.$$

We have thus proved the following

Theorem 3.3.1. *Let $A \geq B \geq C > 0$.*

(i) If $\delta = (0, 0, \delta_3)^T$, then the spaces $\mathcal{K}_e$ and $\mathcal{K}_o$ are invariant for the propagators of (3.2.4). *In particular,* (3.2.4) *is not controllable.*

(ii) If $\delta = (\delta_1, 0, 0)^T$, then the spaces $\mathcal{L}_e$ and $\mathcal{L}_o$ are invariant for the propagators of (3.2.4). *In particular,* (3.2.4) *is not controllable.*

(iii) If $\delta = (0, \delta_2, 0)^T$, then the spaces $\mathcal{G}_e$ and $\mathcal{G}_o$ are invariant for the propagators of (3.2.4). *In particular,* (3.2.4) *is not controllable.*

3.3.3 Controllability of the quantum asymmetric-top

In this section we prove that, except for the critical configurations (i),(ii), and (iii) of Theorem 3.3.1, the system (3.2.4) is almost always an m-tracker:

Theorem 3.3.2. *Let $A > B > C > 0$. If $\delta \neq (\delta_1, 0, 0)^T, (0, \delta_2, 0)^T, (0, 0, \delta_3)^T$,* (3.2.4) *is an m-tracker for almost every value of A, B, and C. In particular, it is approximately controllable for almost every value of A, B, and C.*

Proof. In what follows it will be crucial to express the asymmetric rotational Hamiltonian as a perturbation of a symmetric rotational Hamiltonian. Let us first consider the case $\delta \neq (\delta_1, \delta_2, 0)^T, (0, 0, \delta_3)^T$. The case $\delta = (\delta_1, \delta_2, 0)^T$ with $\delta_1 \neq 0$ and $\delta_2 \neq 0$ will be treated at the end.

We then express the asymmetric Hamiltonian as a perturbation of an oblate symmetric Hamiltonian, using a single asymmetry parameter:

$$\begin{aligned} H(A, B, C) &= AP_1^2 + BP_2^2 + CP_3^2 \\ &= \frac{1}{2}(A + B)P^2 + [C - \frac{1}{2}(A + B)]P_3^2 + \Big(\frac{A - B}{2C - B - A}\Big)[C - \frac{1}{2}(A + B)](P_1^2 - P_2^2) \\ &= H\Big(\frac{1}{2}(A + B), \frac{1}{2}(A + B), C\Big) + bV =: H(b), \end{aligned} \tag{3.3.7}$$

where $H\Big(\frac{1}{2}(A + B), \frac{1}{2}(A + B), C\Big)$ is the rotational Hamiltonian of an oblate symmetric top with rotational constants $\frac{1}{2}(A + B)$ and C, and we have defined the Wang oblate asymmetry parameter

$$b := \frac{A - B}{2C - B - A} \in [-1, 0], \tag{3.3.8}$$

and a perturbation operator

$$V := [C - \frac{1}{2}(A+B)](P_1^2 - P_2^2).$$

The proof is based on an application of Theorem 3.1.21 in combination with a perturbative approach from the construction given in the proof of Theorem 3.2.5. Define for every $j \in \mathbb{N}$ the set $I_j := \{\rho(l,\tau,m) \mid l = j, j+1,\ \tau, m = -l,\dots,l\} \subset \mathbb{N}$, where $\rho : \{(l,\tau,m) \mid l \in \mathbb{N}, \tau, m = -l,\dots,l\} \to \mathbb{N}$ is the lexicographic ordering. The graph $\mathcal{G}$ whose vertices are the sets I_j and whose edges are $\{(I_j, I_{j'}) \mid I_j \cap I_{j'} \neq \emptyset\} = \{(I_j, I_{j+1}) \mid j \in \mathbb{N}\}$ is linear. For every $j \in \mathbb{N}$, we consider

$$\mathcal{M}_j := \mathcal{H}_j \oplus \mathcal{H}_{j+1}, \quad \mathcal{H}_l := \operatorname{span}\{\Psi^l_{\tau,m} \mid \tau, m = -l,\dots,l\}.$$

The dimension of $\mathcal{M}_j$ is $(2j+1)^2 + (2(j+1)+1)^2$, and we identify $\mathfrak{su}(\mathcal{M}_j)$ with $\mathfrak{su}((2j+1)^2 + (2(j+1)+1)^2)$. Notice that as $\mathcal{M}_j$ is by definition invariant under the action of $H(b)$, we identify $H(b)$ with its matrix representation acting on $\mathcal{M}_j$ and its eigenvalues are the same as if it acted on $L^2(\mathrm{SO}(3))$. Set

$$\begin{aligned} E^j_{k,0} &:= E^j_k, \quad k = 0,\dots,j, \\ E^j_{k,1} &:= E^j_{-k}, \quad k = 1,\dots,j, \end{aligned}$$

being the E^j_k defined in (3.2.7), and let $E^j_{k,0} = E^j_{k,1}$, $k > 0$, be a degenerate eigenvalue of $H(0)$ with different eigenfunctions $S^j_{k,m,0}$ and $S^j_{k,m,1}$, $m = -j,\dots,j$, $k = 1,\dots,j$. We can then consider the eigenvalue $E^j_{k,p}(b)$ of $H(b)$ which converges to $E^j_{k,p}$ as b tends to 0, for $p = 0,1$. It is well known [68, Chapter 7] that $E^j_{k,p}(b)$ is still $(2j+1)$-degenerate w.r.t. m, but the 2-fold k-degeneracy is broken: $E^j_{k,0}(b) \neq E^j_{k,1}(b)$ if $b \neq 0$. Moreover, since $\mathcal{M}_j$ is finite-dimensional, the function $[-1,0] \ni b \mapsto E^j_{k,p}(b) \in \mathbb{R}$ is analytic.

Since for $b = 0$ the k-degeneracy appears, we need to choose the good basis of the eigenspace $\mathcal{E}^j_k := \operatorname{span}\{D^j_{k,m}, D^j_{-k,m} \mid m = -j,\dots,j\}$ corresponding to the unperturbed degenerate eigenvalue E^j_k in order to expand the eigenbasis with respect to b. Here, the good basis of the eigenspace means the basis to which the expanded eigenbasis converges as the perturbation goes to zero. This is equivalent to ask that the perturbation V is diagonal in the basis chosen for the degenerate eigenspace [101, Chapter 5]. Since [68, Chapter 7]

$$\langle D^j_{k,m}, V D^j_{\pm k,m'} \rangle = 0, \quad \text{if } m' \neq m,$$

and

$$\langle D^j_{k,m}, V D^j_{-k,m} \rangle = \begin{cases} 0, & \text{if } k \neq \pm 1, \\ [C - \frac{1}{2}(A+B)]\frac{j(j+1)}{2}, & \text{if } k = \pm 1, \end{cases} \tag{3.3.9}$$

we see that the perturbation is not diagonal in the Wigner basis $\{D^j_{k,m}, D^j_{-k,m} \mid m = -j,\dots,j\}$, but it is diagonal in the Wang basis $\{S^j_{k,m,0}, S^j_{k,m,1} \mid m = -j,\dots j\}$, as a basis of $\mathcal{E}^j_k$, for every $k = 0,\dots,j$. In other words, the asymmetric top eigenfunctions $\Psi^j_{\tau,m} = \Psi^j_{\tau,m}(b)$ tend to Wang functions as the asymmetry parameter b goes to zero, as it is well-known. So, to each asymmetric top eigenfunction $\Psi^j_{\tau,m}(b)$ is attached one and only one perturbed symmetric top eigenfunction $S^j_{k,m,p}(b)$, and we can write

$$\mathcal{H}_l = \operatorname{span}\{S^l_{k,m,p}(b) \mid m = -j,\dots,j,\ k = 0,\dots,j,\ p = 0,1\},$$

for any $b \in [-1,0]$. Notice that $[-1,0] \ni b \mapsto S^j_{k,m,p}(b)$ is analytic (being a family of eigenvectors of an analytic family of matrices $H(b)\Pi_{\mathcal{M}_j}$) and $S^j_{k,m,p}(b) \to S^j_{k,m,p}$ as $b \to 0$. We then express the matrices $\Pi_{\mathcal{M}_j} B_i \Pi_{\mathcal{M}_j}$ of the control problem (projected on $\mathcal{M}_j$, that with abuse of notation we still denote B_i in the same way as the operators on $L^2(\mathrm{SO}(3))$) in this basis that depends on the asymmetry parameter.

Remark 3.3.3. From (3.3.9) we can also evidence that the k-degeneracy for $k = 1$ is lifted even at first order, since:

$$\frac{d}{db}\Big|_{b=0} E^j_{1,p}(b) = \langle S^j_{1,m,p}, V S^j_{1,m,p} \rangle = \begin{cases} [C - \frac{1}{2}(A+B)]\frac{j(j+1)}{2}, & \text{if } p = 0, \\ -[C - \frac{1}{2}(A+B)]\frac{j(j+1)}{2}, & \text{if } p = 1, \end{cases}$$

while for $k > 1$ one has to expand at higher order to see this fact [68, Table 7.8].

The spectral gaps in $\mathcal{M}_j$ that we consider are perturbations of symmetric top spectral gaps (cf. figures 3.4 and 3.5). Indeed, we define:

$$\begin{aligned} &\lambda^j_{k,0}(b) := |E^{j+1}_{k+1,0}(b) - E^j_{k,0}(b)|, \quad k = 0, \dots, j, \\ &\lambda^j_{k,1}(b) := |E^{j+1}_{k-1,1}(b) - E^j_{k,1}(b)|, \quad k = 2, \dots, j, \quad \lambda^j_{1,1}(b) := |E^{j+1}_{0,0}(b) - E^j_{1,1}(b)| \end{aligned} \tag{3.3.10}$$

$$\begin{aligned} &\rho^j_{k,0}(b) := |E^{j+1}_{k-1,0}(b) - E^j_{k,0}(b)|, \quad k = 1, \dots, j, \quad \rho^j_{0,0}(b) := |E^{j+1}_{1,1}(b) - E^j_{0,0}(b)| \\ &\rho^j_{k,1}(b) := |E^{j+1}_{k+1,1}(b) - E^j_{k,1}(b)|, \quad k = 1, \dots, j, \end{aligned} \tag{3.3.11}$$

then

$$\begin{aligned} &\eta^j_{k,0}(b) := |E^j_{k+1,0}(b) - E^j_{k,0}(b)|, \quad k = 0, \dots, j-1, \\ &\eta^j_{k,1}(b) := |E^j_{k-1,1}(b) - E^j_{k,1}(b)|, \quad k = 2, \dots, j, \quad \eta^j_{1,1}(b) := |E^j_{0,0}(b) - E^j_{1,1}(b)| \end{aligned} \tag{3.3.12}$$

and finally

$$\sigma^j_{k,p}(b) := |E^{j+1}_{k,p}(b) - E^j_{k,p}(b)|, \quad k = 1, \dots, j, \ p = 0, 1, \qquad \sigma^j_{0,0}(b) := |E^{j+1}_{0,0}(b) - E^j_{0,0}(b)|. \tag{3.3.13}$$

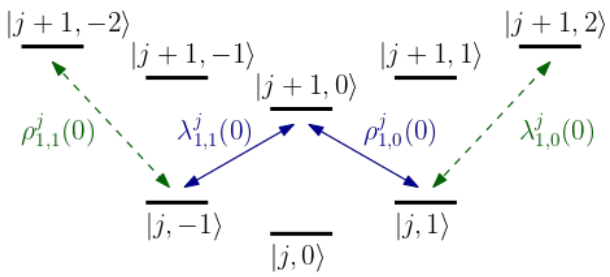
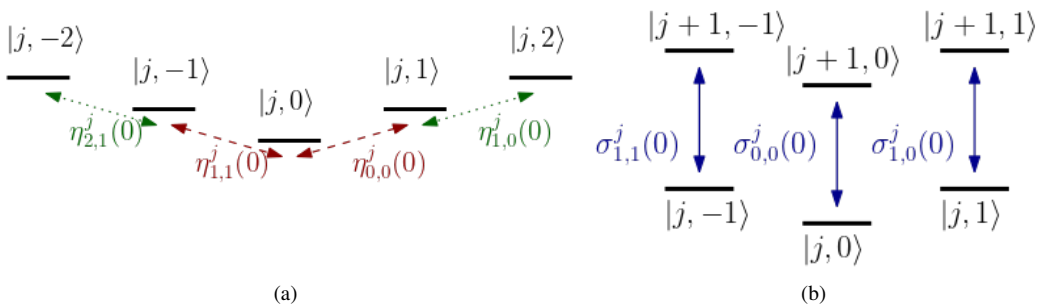


Figure 3.4: Graph of the transitions associated with the unperturbed frequencies $\lambda^j_{k,p}(0)$ and $\rho^j_{k,p}(0)$ between unperturbed eigenstates $|j,k\rangle = |j,k,m\rangle := D^j_{k,m}$ (m fixed). Same-shaped arrows correspond to equal spectral gaps.



(a) (b)

Figure 3.5: Transitions between unperturbed eigenstates $|j,k\rangle = |j,k,m\rangle := D^j_{k,m}$ (m fixed): (a) at unperturbed frequency $\eta^j_{k,p}(0)$; (b) at unperturbed frequency $\sigma^j_{k,p}(0)$. Same-shaped arrows correspond to equal spectral gaps.

Remark 3.3.4. The spectral gaps listed above exhibit several symmetries at $b = 0$, due to the fact that $E^j_{k,0}(0) = E^j_{k,1}(0)$: indeed, we have (compare also with figures 3.4 and 3.5)

$$\begin{aligned} &\lambda^j_{0,0}(0) = \rho^j_{0,0}(0)\,, \quad \lambda^j_{k,0}(0) = \rho^j_{k,1}(0)\,, \quad \lambda^j_{k,1}(0) = \rho^j_{k,0}(0)\,, \quad k = 1, \dots, j, \\ &\eta^j_{k,0}(0) = \eta^j_{k+1,1}(0)\,, k = 0, \dots, j-1, \quad \sigma^j_{k,0}(0) = \sigma^j_{k,1}(0)\,, \quad k = 1, \dots, j. \end{aligned} \tag{3.3.14}$$

Lemma 3.3.5. *Let $(A+B)/C \notin \mathbb{Q}$. Then, for almost every $b \in [-1,0]$, $(\omega^j_{k,p}(b), l) \in \Xi^0_j$, for all $\omega \in \{\lambda, \rho, \sigma\}$ for all $k = 0, \dots, j$, if $p = 0$, and for all $k = 1, \dots, j$, if $p = 1$, with $l = 1, 2, 3$. Moreover, $(\eta^j_{k,p}(b), l) \in \Xi^1_j$, for all $k = 0, \dots, j-1$, if $p = 0$ and for all $k = 1, \dots, j$, if $p = 1$, with $l = 1, 2, 3$.*

Proof. In order to prove that, for almost every b, $(\omega^j_{k,p}(b), l)$ belongs to Ξ^1_j for all $\omega \in \{\lambda, \rho, \eta, \sigma\}$, we have to prove that the spectral gaps $\omega^j_{k,p}(b)$ do not couple transitions between two states that are, respectively, in $\mathcal{H}_{j-1}$ and $\mathcal{H}_j$ or in $\mathcal{H}_{j+1}$ and $\mathcal{H}_{j+2}$, for almost every b. We are thus concerned with the condition

$$\omega^j_{k,p}(b) \neq \omega, \quad \forall \omega \in \Sigma_{j-1,j} \cup \Sigma_{j+1,j+2}, \tag{3.3.15}$$

where $\Sigma_{t,u} := \{|E^t_{k,p}(b) - E^u_{k',p'}(b)| \mid k, k' = 0, \dots, j,\ p, p' = 0, 1\}$ is the set of spectral gaps of $H(b)$ between eigenstates in $\mathcal{H}_m$ and $\mathcal{H}_n$. Since every spectral gap ω of $H(b)$ can be seen as an analytic function $\omega(b)$ where $\omega(0)$ is a spectral gap of $H(0)$, and since the zeros of an analytic function (in this case, the function $\omega^j_{k,p}(b) - \omega(b)$) on $[-1,0]$ are finite, condition (3.3.15) is implied for all but a finite number of $b \in [-1,0]$ if it is true at $b = 0$. At $b = 0$, (3.3.15) is true if $(A+B)/C \notin \mathbb{Q}$ after Lemma 3.2.6.

The additional requirement $(\omega^j_{k,p}(b), l) \in \Xi^0_j$ $\forall \omega \in \{\lambda, \rho, \sigma\}$, is proved in an analogous way: for each $m, n \in \mathbb{N} \setminus \{j, j+1\}$, we are concerned with the condition

$$\omega^j_{k,p}(b) \neq \omega, \quad \forall \omega \in \Sigma_{m,n} \tag{3.3.16}$$

that holds true at $b = 0$, if $(A+B)/C \notin \mathbb{Q}$, after Lemma 3.2.6. So, by analyticity, (3.3.16) holds true for all but a finite number of $b \in [-1,0]$. Hence, the set Λ defined as the set of b such that condition (3.3.16) holds true for all $m, n \in \mathbb{N} \setminus \{j, j+1\}$ is given by a countable intersection of sets of full measure 1[2], which has measure 1. This concludes the proof. □

Following the proof of Theorem 3.2.5, we consider first the family of decoupled control operators

$$\begin{aligned}\mathcal{F}_j(b) := \Big\{ &\frac{1}{2}\Big(W_\xi \mathcal{E}_{\lambda^j_{0,0}(b)}(\mathrm{i}B_l) + W_\xi \mathcal{E}_{\rho^j_{0,0}(b)}(\mathrm{i}B_l)\Big), \frac{1}{2}\Big(W_\xi \mathcal{E}_{\lambda^j_{k,0}(b)}(\mathrm{i}B_l) + W_\xi \mathcal{E}_{\rho^j_{k,1}(b)}(\mathrm{i}B_l)\Big), \\ &\frac{1}{2}\Big(W_\xi \mathcal{E}_{\lambda^j_{k,1}(b)}(\mathrm{i}B_l) + W_\xi \mathcal{E}_{\rho^j_{k,0}(b)}(\mathrm{i}B_l)\Big) \,\Big|\, l = 1,2,3,\ k = 1, \dots, j,\ \xi = 1, \mathrm{i}\Big\}.\end{aligned} \tag{3.3.17}$$

We denote by $\mathrm{L}_j(b) := \mathrm{Lie}(\mathcal{F}_j(b))$ and notice that, thanks to Lemma 3.3.5, $\mathrm{L}_j(b) \subset \mathrm{Lie}(\nu^0_j)$ (cf. (3.1.13)) for almost every b. Then we define the family of matrices

(3.3.18)

$$\begin{aligned}\mathcal{P}_j(b) := &\Big\{\frac{1}{2}\Big(W_\xi \mathcal{E}_{\eta^j_{k,0}(b)}(\mathrm{i}B_l) + W_\xi \mathcal{E}_{\eta^j_{k+1,1}(b)}(\mathrm{i}B_l)\Big) \Big|\, l = 1,2,3,\ k = 0, \dots, j,\ \xi = 1, \mathrm{i}\Big\} \\ &\cup \Big\{W_\xi \mathcal{E}_{\sigma^j_{0,0}(b)}(\mathrm{i}B_l), \frac{1}{2}\Big(W_\xi \mathcal{E}_{\sigma^j_{k,0}(b)}(\mathrm{i}B_l) + W_\xi \mathcal{E}_{\sigma^j_{k,1}(b)}(\mathrm{i}B_l)\Big) \,\Big|\, l = 1,2,3,\ k = 1, \dots, j,\ \xi = 1, \mathrm{i}\Big\},\end{aligned}$$

and notice that, by Lemma 3.3.5, $\mathcal{P}_j(b) \subset \mathrm{Lie}(\nu^1_j)$ (cf. (3.1.13)), for almost every b. Therefore,

$$\widetilde{\mathcal{P}}_j(b) := \{A, [B, C] \mid A, B \in \mathrm{L}_j(b), C \in \mathcal{P}_j(b)\} \subset \mathcal{T}_j, \text{ for almost every } b \in [-1,0],$$

where we recall that $\mathcal{T}_j$ is the minimal ideal of $\mathrm{Lie}(\nu^1_j)$ containing ν^0_j.

The next proposition concludes the proof of Theorem 3.3.2 with the additional hypothesis $\delta \neq (\delta_1, \delta_2, 0)$:

Proposition 3.3.6. *For almost every $b \in [-1,0]$, $\mathrm{Lie}(\widetilde{\mathcal{P}}_j(b)) = \mathfrak{su}(\mathcal{M}_j)$.*

Proof. We first claim that, for all but a finite number of $b \in [-1,0]$, one can write

$$\begin{aligned}\mathcal{E}_{\lambda^j_{k,0}(b)}(\mathrm{i}B_3) + \mathcal{E}_{\rho^j_{k,1}(b)}(\mathrm{i}B_3) = \ &\sum_{\substack{m=-j,\dots,j \\ p=0,1}} \langle S^j_{k,m,p}(b), \mathrm{i}B_3 S^{j+1}_{k+1,m,p}(b)\rangle\ |S^j_{k,m,p}(b)\rangle\langle S^{j+1}_{k+1,m,p}(b)| \\ &+ \langle S^{j+1}_{k+1,m,p}(b), \mathrm{i}B_3 S^j_{k,m,p}(b)\rangle\ |S^{j+1}_{k+1,m,p}(b)\rangle\langle S^j_{k,m,p}(b)|,\end{aligned} \tag{3.3.19}$$

where the operator $|\psi\rangle\langle\phi|$ is the rank-one projector defined by $|\psi\rangle\langle\phi|\varphi := \langle\varphi, \psi\rangle\phi$, for all $\psi, \phi, \varphi \in L^2(\mathrm{SO}(3))$. Indeed, (3.3.19) holds when there are no internal resonances, that is, for all $b \in [-1,0]$ such that

$$\lambda^j_{k,0}(b), \rho^j_{k,1}(b) \neq \omega, \quad \forall \omega \in \Sigma_{j,j+1} \setminus \{\lambda^j_{k,0}(b), \rho^j_{k,1}(b)\}. \tag{3.3.20}$$

[2]Indeed, $\Lambda = \bigcap_{m,n \in \mathbb{N}\setminus\{j,j+1\}} \Lambda_{m,n}$ where $\Lambda_{m,n}$ is defined as the set of $b \in [-1,0]$ such that (3.3.16) holds true.

Since there exists a finite number of gaps, and every gap ω can be written as the analytic perturbation $\omega(b)$ of a gap at $b = 0$, and since (3.3.20) holds if $(A + B)/C \notin \mathbb{Q}$ at $b = 0$ (cf. Lemma 3.2.7), by analyticity (3.3.20) holds for all but a finite number of $b \in [-1, 0]$, and the claim is proved. In particular, when $(A + B)/C \notin \mathbb{Q}$, (3.3.19) holds at $b = 0$ and gives an analytic expression (that is, the RHS) for $\mathcal{E}_{\lambda^j_{k,0}(b)}(\mathrm{i}B_3) + \mathcal{E}_{\rho^j_{k,1}(b)}(\mathrm{i}B_3)$, for a.e. b. Analogous formulas to (3.3.19) hold for the other matrices, corresponding to $\xi = 1$, of (3.3.17) and (3.3.18). Noticing that

$$\lambda^j_{k,0}(b)\, W_{\mathrm{i}} \mathcal{E}_{\lambda^j_{k,0}(b)}(\mathrm{i}B_3) = \Big[\mathrm{i}H(b), \mathcal{E}_{\lambda^j_{k,0}(b)}(\mathrm{i}B_3)\Big],$$

we see that also the matrices corresponding to $\xi = \mathrm{i}$ in (3.3.17) and (3.3.18) coincide with analytic curves of matrices for all but a finite number of b. To conclude, since the statement holds at $b = 0$ when $(A + B)/C \notin \mathbb{Q}$ and $\delta \neq (0, 0, \delta_3)^T, (\delta_1, \delta_2, 0)^T$ (cf. Proposition 3.2.9), by analyticity it holds for all but a finite number of $b \in [-1, 0]$. □

We now turn to the case $\delta = (\delta_1, \delta_2, 0)^T$, with $\delta_1 \neq 0$ and $\delta_2 \neq 0$. Recalling the choice we made at the beginning of section 3.3.1 for the principal axis of inertia (that is, $a = a_1, b = a_2, c = a_3$), we have that δ_1 is the dipole component along the principal axis a. Let us then change convention and set $a = a_3, b = a_2, c = a_1$, so that the rotational Hamiltonian reads $H(A, B, C) = CP_1^2 + BP_2^2 + AP_3^2$, and the dipole reads $(0, \delta_2, \delta_1)^T$ in the new a_1, a_2, a_3 molecular frame. We then write $H(A, B, C)$ as in (3.3.7), exchanging the role of A and C in the formula, and obtaining thus the perturbation of an associated prolate symmetric top: that is,

$$\begin{aligned} H(A, B, C) &= CP_1^2 + BP_2^2 + AP_3^2 \\ &= \frac{1}{2}(C + B)P^2 + [A - \frac{1}{2}(C + B)]P_3^2 + \Big(\frac{C - B}{2A - B - C}\Big)[A - \frac{1}{2}(C + B)](P_1^2 - P_2^2) \\ &= H\Big(A, \frac{1}{2}(C + B), \frac{1}{2}(C + B)\Big) + \widetilde{b}\widetilde{V} =: H(\widetilde{b}), \end{aligned} \tag{3.3.21}$$

where $H\Big(A, \frac{1}{2}(C + B), \frac{1}{2}(C + B)\Big)$ is the rotational Hamiltonian of a prolate symmetric top with rotational constants A and $\frac{1}{2}(C + B)$, and we have defined the new asymmetry parameter

$$\widetilde{b} := \frac{C - B}{2A - B - C} \in [-1, 0], \tag{3.3.22}$$

and a perturbation operator

$$\widetilde{V} := [A - \frac{1}{2}(C + B)](P_1^2 - P_2^2).$$

We can then apply the same proof and conclude that in the case left (which is $\delta = (\delta_1, \delta_2, 0)^T$ with $\delta_1 \neq 0$ and $\delta_2 \neq 0$, w.r.t. the choice $a = a_1, b = a_2, c = a_3$) the system (3.2.4) is an m-tracker. □

3.4 Appendix

Sections 3.4.1 and 3.4.2 of this Appendix aim at providing the proofs of two important original propositions, that were stated in the proof of Theorem 3.2.5.

3.4.1 Proof of Proposition 3.2.8

As a consequence of Lemma 3.2.7, part 1, if $I_2/I_3 \notin \mathbb{Q}$, the only transitions driven by the fields $\mathrm{i}B_l$, $l = 1, 2, 3$, excited at frequency λ^j_k, are the ones corresponding to the following matrix elements (written in the basis of $\mathcal{M}_j$ given by the Wigner functions) and can be computed using, e.g., [68, Table 2.1]:

$$\begin{cases} \langle D^j_{k,m}, \mathrm{i}B_1 D^{j+1}_{k+1,m\pm1}\rangle = -c_{j,k,\pm m}(\delta_2 + \mathrm{i}\delta_1), \\ \langle D^j_{k,m}, \mathrm{i}B_1 D^{j+1}_{k-1,m\pm1}\rangle = c_{j,-k,\pm m}(\delta_2 - \mathrm{i}\delta_1), \\ \langle D^j_{k,m}, \mathrm{i}B_2 D^{j+1}_{k+1,m\pm1}\rangle = \mp\mathrm{i}c_{j,k,\pm m}(\delta_2 + \mathrm{i}\delta_1), \\ \langle D^j_{k,m}, \mathrm{i}B_2 D^{j+1}_{k-1,m\pm1}\rangle = \pm\mathrm{i}c_{j,-k,\pm m}(\delta_2 - \mathrm{i}\delta_1), \\ \langle D^j_{k,m}, \mathrm{i}B_3 D^{j+1}_{k\pm1,m}\rangle = \pm\mathrm{i}d_{j,\pm k,m}(\delta_2 \pm \mathrm{i}\delta_1), \end{cases} \tag{3.4.1}$$

where

$$c_{j,k,m} := \frac{[(j + k + 1)(j + k + 2)]^{1/2}[(j + m + 1)(j + m + 2)]^{1/2}}{4(j + 1)[(2j + 1)(2j + 3)]^{1/2}},$$

and

$$d_{j,k,m} := \frac{[(j+k+1)(j+k+2)]^{1/2}[(j+1)^2 - m^2]^{1/2}}{2(j+1)[(2j+1)(2j+3)]^{1/2}}.$$

Now, using a symmetry argument, we explain how to get rid of one electric dipole component between δ_1 and δ_2.

By the very definition of the Euler angles, one has that the rotation of angle θ around the symmetry axis a_3 is given by $\gamma \mapsto \gamma + \theta$. This rotation acts on the Wigner functions in the following way

$$D^j_{k,m}(\alpha,\beta,\gamma) \mapsto D^j_{k,m}(\alpha,\beta,\gamma+\theta) = e^{\mathrm{i}k\theta} D^j_{k,m}(\alpha,\beta,\gamma) =: D^j_{k,m}(\theta)(\alpha,\beta,\gamma),$$

having used the explicit expression of the symmetric states (3.2.5). Note that these rotated Wigner functions form again an orthogonal basis for $L^2(\mathrm{SO}(3))$ of eigenfunctions of the rotational Hamiltonian H, so we can also analyze the controllability problem in this new basis. In this new basis the matrix elements (corresponding to the frequency λ^j_k) of the controlled fields are

$$\begin{cases} \langle D^j_{k,m}(\theta), \mathrm{i}B_1 D^{j+1}_{k+1,m+1}(\theta)\rangle &= -c_{j,k,m} e^{-\mathrm{i}\theta}(\delta_2 + \mathrm{i}\delta_1), \\ \langle D^j_{k,m}(\theta), \mathrm{i}B_1 D^{j+1}_{k-1,m+1}(\theta)\rangle &= c_{j,-k,m} e^{\mathrm{i}\theta}(\delta_2 - \mathrm{i}\delta_1), \end{cases} \tag{3.4.2}$$

and the same happens for all the other transitions described in (3.4.1). So, the effect of this change of basis is that we are actually rotating the first two components of the dipole moment, by the angle θ. We can now choose $\theta \in [0, 2\pi)$ such that

$$e^{-\mathrm{i}\theta}(\delta_2 + \mathrm{i}\delta_1) = \sqrt{\delta_1^2 + \delta_2^2} = e^{\mathrm{i}\theta}(\delta_2 - \mathrm{i}\delta_1).$$

In other words, thanks to this change of basis, we can assume without loss of generality that $\delta_1 = 0$, since we can rotate the vector $\delta_2 \pm \mathrm{i}\delta_1$ and get rid of its imaginary part (note that in (3.2.15) and in the proof of Theorem 3.2.11 we are rotating the vector $\delta_2 \pm \mathrm{i}\delta_1$ in the other sense, i.e., to get rid of its real part). This will simplify the expression of the controlled fields. Note that

$$\begin{aligned} W_{\mathrm{i}}(G_{(j,k,m),(j+1,k+1,n)}) &= -F_{(j,k,m),(j+1,k+1,n)}, \\ W_{\mathrm{i}}(F_{(j,k,m),(j+1,k+1,n)}) &= G_{(j,k,m),(j+1,k+1,n)}. \end{aligned} \tag{3.4.3}$$

Finally, we can conveniently represent the matrices corresponding to the controlled vector field (projected onto $\mathcal{M}_j$) in the rotated basis found with the symmetry argument. So, for each $k = -j, \dots, j$, because of Lemma 3.2.7, part 1, and (3.4.1), we have

$$\begin{aligned} \mathcal{E}_{\lambda^j_k}(\mathrm{i}B_1) = \sum_{m=-j,\dots,j} & -c_{j,k,m}\delta_2 G_{(j,k,m),(j+1,k+1,m+1)} - c_{j,k,-m}\delta_2 G_{(j,k,m),(j+1,k+1,m-1)} \\ & + c_{j,k,m}\delta_2 G_{(j,-k,m),(j+1,-k-1,m+1)} + c_{j,k,-m}\delta_2 G_{(j,-k,m),(j+1,-k-1,m-1)}, \end{aligned} \tag{3.4.4}$$

$$\begin{aligned} \mathcal{E}_{\lambda^j_k}(\mathrm{i}B_2) = \sum_{m=-j,\dots,j} & -c_{j,k,m}\delta_2 F_{(j,k,m),(j+1,k+1,m+1)} + c_{j,k,-m}\delta_2 F_{(j,k,m),(j+1,k+1,m-1)} \\ & + c_{j,k,m}\delta_2 F_{(j,-k,m),(j+1,-k-1,m+1)} - c_{j,k,-m}\delta_2 F_{(j,-k,m),(j+1,-k-1,m-1)}, \end{aligned} \tag{3.4.5}$$

$$\mathcal{E}_{\lambda^j_k}(\mathrm{i}B_3) = \sum_{m=-j,\dots,j} d_{j,k,m}\delta_2 F_{(j,k,m),(j+1,k+1,m)} - d_{j,k,m}\delta_2 F_{(j,-k,m),(j+1,-k-1,m)}, \tag{3.4.6}$$

where, with a slight abuse of notation, we write B_l instead of $\Pi_{\mathcal{M}_j} B_l \Pi_{\mathcal{M}_j}$.

Now we show how the sum over m in (3.4.4), (3.4.5) and (3.4.6) can be decomposed, in order to obtain that the matrices $X_{(j,k,m),(j+1,k+1,m\pm1)} + X_{(j,-k,m),(j+1,-k-1,m\pm1)}$ and $X_{(j,k,m),(j+1,k+1,m)} - X_{(j,-k,m),(j+1,-k-1,m)}$ are in L_j, for any $m, k = -j, \dots, j$, where $X \in \{G, F\}$. Recall the laws of the Lie algebra $\mathfrak{su}$ described in (3.1.9),(3.1.10),(3.1.11). Let us first fix $k \neq 0$ and consider

$$\begin{aligned} & W_{\mathrm{i}}(\mathcal{E}_{\lambda^j_k}(\mathrm{i}B_3)) \\ & \quad = \sum_{m=-j,\dots,j} d_{j,k,m}\delta_2 G_{(j,k,m),(j+1,k+1,m)} - d_{j,k,m}\delta_2 G_{(j,-k,m),(j+1,-k-1,m)}, \end{aligned}$$

and the brackets

$$\begin{aligned}\mathrm{ad}^{2s}_{\mathcal{E}_{\lambda^j_k}(\mathrm{i}B_3)}(W_{\mathrm{i}}(\mathcal{E}_{\lambda^j_k}(\mathrm{i}B_3))) = &\sum_{m=-j,\dots,j}(-1)^s 2^{2s} d^{2s+1}_{j,k,m}\delta_2^{2s+1} G_{(j,k,m),(j+1,k+1,m)}\\ &+(-1)^s 2^{2s}(-d_{j,k,m})^{2s+1}\delta_2^{2s+1}G_{(j,-k,m),(j+1,-k-1,m)},\end{aligned}$$

for $s \in \mathbb{N}$, where $\mathrm{ad}_A(B) = [A, B]$ and $\mathrm{ad}^{n+1}_A(B) = [A, \mathrm{ad}^n_A(B)]$. Since $d_{j,k,m} = d_{j,k,-m}$, the invertibility of the Vandermonde matrix gives that

$$\begin{aligned}&G_{(j,k,m),(j+1,k+1,m)} + G_{(j,k,-m),(j+1,k+1,-m)}\\ &-G_{(j,-k,m),(j+1,-k-1,m)} - G_{(j,-k,-m),(j+1,-k-1,-m)} \in \mathrm{L}_j,\end{aligned} \tag{3.4.7}$$

for $m = 0, \dots, j$. In particular, $G_{(j,k,0),(j+1,k+1,0)} - G_{(j,-k,0),(j+1,-k-1,0)}$ is in L_j. Hence,

$$\begin{aligned}&\Big[\Big[\frac{\mathcal{E}_{\lambda_k}(\mathrm{i}B_1) - W_{\mathrm{i}}(\mathcal{E}_{\lambda_k}(\mathrm{i}B_2))}{2}, G_{(j,k,0),(j+1,k+1,0)} - G_{(j,-k,0),(j+1,-k-1,0)}\Big],\\ &G_{(j,k,0),(j+1,k+1,0)} - G_{(j,-k,0),(j+1,-k-1,0)}\Big] = c_{j,k,0}\delta_2 G_{(j,k,0),(j+1,k+1,-1)}\\ &+ c_{j,k,-1}\delta_2 G_{(j,k,1),(j+1,k+1,0)} - c_{j,k,0}\delta_2 G_{(j,-k,0),(j+1,-k-1,-1)}\\ &- c_{j,k,-1}\delta_2 G_{(j,-k,1),(j+1,-k-1,0)}\end{aligned} \tag{3.4.8}$$

is also in L_j. Define

$$\begin{aligned}Q_0 =& c_{j,k,0}\delta_2 G_{(j,k,0),(j+1,k+1,-1)} + c_{j,k,-1}\delta_2 G_{(j,k,1),(j+1,k+1,0)}\\ &- c_{j,k,0}\delta_2 G_{(j,-k,0),(j+1,-k-1,-1)} - c_{j,k,-1}\delta_2 G_{(j,-k,1),(j+1,-k-1,0)},\\ Q_m =& c_{j,k,-m}\delta_2 G_{(j,k,-m),(j+1,k+1,-m-1)} + c_{j,k,-m-1}\delta_2 G_{(j,k,m+1),(j+1,k+1,m)}\\ &- c_{j,k,-m}\delta_2 G_{(j,-k,-m),(j+1,-k-1,-m-1)} - c_{j,k,-m-1}\delta_2 G_{(j,-k,m+1),(j+1,-k-1,m)},\end{aligned}$$

if $0 < m < j$, and

$$Q_j = c_{j,k,-j}\delta_2 G_{(j,k,-j),(j+1,k+1,-j-1)} - c_{j,k,-j}\delta_2 G_{(j,-k,-j),(j+1,-k-1,-j-1)}.$$

We have

$$\begin{aligned}&\Big[\Big[\sum_{m=s,\dots,j} Q_m, G_{(j,k,s),(j+1,k+1,s)} + G_{(j,k,-s),(j+1,k+1,-s)} - G_{(j,-k,s),(j+1,-k-1,s)}\\ &- G_{(j,-k,-s),(j+1,-k-1,-s)}\Big], G_{(j,k,s),(j+1,k+1,s)} + G_{(j,k,-s),(j+1,k+1,-s)}\\ &- G_{(j,-k,s),(j+1,-k-1,s)} - G_{(j,-k,-s),(j+1,-k-1,-s)}\Big] = Q_s,\end{aligned}$$

for $s = 1, \dots, j$. By iteration on s and because of (3.4.7), it follows that $Q_s \in \mathrm{L}_j$ for every $s = 0, \dots, j$. Now, since

$$\frac{Q_j}{c_{j,k,-j}\delta_2} = G_{(j,k,-j),(j+1,k+1,-j-1)} - G_{(j,-k,-j),(j+1,-k-1,-j-1)} \in \mathrm{L}_j,$$

then

$$\begin{aligned}&\mathrm{ad}^2_{G_{(j,k,-j),(j+1,k+1,-j-1)} - G_{(j,-k,-j),(j+1,-k-1,-j-1)}}(G_{(j,k,j),(j+1,k+1,j)}\\ &+ G_{(j,k,-j),(j+1,k+1,-j)} - G_{(j,-k,j),(j+1,-k-1,j)} - G_{(j,-k,-j),(j+1,-k-1,-j)})\\ &= G_{(j,k,-j),(j+1,k+1,-j)} - G_{(j,-k,-j),(j+1,-k-1,-j)} \in \mathrm{L}_j,\end{aligned}$$

which, in turns, implies that

$$\begin{aligned}&\mathrm{ad}^2_{G_{(j,k,-j),(j+1,k+1,-j)} - G_{(j,-k,-j),(j+1,-k-1,-j)}}(Q_{j-1})\\ &= c_{j,k,-j+1}G_{(j,k,-j+1),(j+1,k+1,-j)} - c_{j,k,-j+1}G_{(j,-k,-j+1),(j+1,-k-1,-j)} \in \mathrm{L}_j.\end{aligned}$$

Iterating the argument,

$$G_{(j,k,m),(j+1,k+1,m)} - G_{(j,-k,m),(j+1,-k-1,m)} \in \mathrm{L}_j, \quad m = -j, \dots, j \tag{3.4.9}$$

and $G_{(j,k,m),(j+1,k+1,m-1)} - G_{(j,-k,m),(j+1,-k-1,m-1)}$ are in L_j for $m = -j, \dots, j$.

By the same argument as above, with $\frac{\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_1) - W_{\mathrm{i}}(\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_2))}{2}$ replaced by

$$\begin{aligned}\frac{\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_1) + W_{\mathrm{i}}(\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_2))}{2} = \sum_{m=-j,\dots,j} & -c_{j,k,m} G_{(j,k,m),(j+1,k+1,m+1)} \\ & + c_{j,k,m} G_{(j,-k,m),(j+1,-k-1,m+1)}\end{aligned}$$

in (3.4.8) we also have that $G_{(j,k,m),(j+1,k+1,m+1)} - G_{(j,-k,m),(j+1,-k-1,m+1)}$ is in L_j for all $m = -j, \dots, j$.

If we now replace $\frac{\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_1) - W_{\mathrm{i}}(\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_2))}{2}$ with

$$\begin{aligned}\frac{\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_2) + W_{\mathrm{i}}(\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_1))}{2} = \sum_{m=-j,\dots,j} & -c_{j,k,-m} F_{(j,k,m),(j+1,k+1,m-1)} \\ & + c_{j,k,-m} F_{(j,-k,m),(j+1,-k-1,m-1)}\end{aligned}$$

or

$$\begin{aligned}\frac{\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_2) - W_{\mathrm{i}}(\mathcal{E}_{\lambda_k^j}(\mathrm{i}B_1))}{2} = \sum_{m=-j,\dots,j} & -c_{j,k,m} F_{(j,k,m),(j+1,k+1,m+1)} \\ & + c_{j,k,m} F_{(j,-k,m),(j+1,-k-1,m+1)},\end{aligned}$$

the arguments above prove that both $F_{(j,k,m),(j+1,k+1,m)} - F_{(j,-k,m),(j+1,-k-1,m)}$ and $F_{(j,k,m),(j+1,k+1,m\pm1)} - F_{(j,-k,m),(j+1,-k-1,m\pm1)}$ are in L_j for all $m = -j, \dots, j$.

3.4.2 Proof of Proposition 3.2.9

Using again [68, Table 2.1] we write the pairings

$$\begin{cases} \langle D^j_{k,m}, \mathrm{i}B_1 D^j_{k+1,m\pm1}\rangle = \mp h_{j,k,\pm m}(\delta_2 + \mathrm{i}\delta_1), \\ \langle D^j_{k,m}, \mathrm{i}B_1 D^j_{k-1,m\pm1}\rangle = \mp h_{j,-k,\pm m}(\delta_2 - \mathrm{i}\delta_1), \\ \langle D^j_{k,m}, \mathrm{i}B_2 D^j_{k+1,m\pm1}\rangle = -\mathrm{i}h_{j,k,\pm m}(\delta_2 + \mathrm{i}\delta_1), \\ \langle D^j_{k,m}, \mathrm{i}B_2 D^j_{k-1,m\pm1}\rangle = -\mathrm{i}h_{j,-k,\pm m}(\delta_2 - \mathrm{i}\delta_1), \\ \langle D^j_{k,m}, \mathrm{i}B_3 D^j_{k\pm1,m}\rangle = -\mathrm{i}q_{j,\pm k,m}(\delta_2 \pm \mathrm{i}\delta_1), \end{cases} \tag{3.4.10}$$

where

$$\begin{aligned} h_{j,k,m} &:= \frac{[j(j+1) - k(k+1)]^{1/2}[j(j+1) - m(m+1)]^{1/2}}{4j(j+1)}, \\ q_{j,k,m} &:= \frac{[j(j+1) - k(k+1)]^{1/2} m}{2j(j+1)}. \end{aligned}$$

Moreover,

$$\begin{cases} \langle D^j_{k,m}, \mathrm{i}B_1 D^{j+1}_{k,m\pm1}\rangle = a_{j,k,\pm m}\delta_3, \\ \langle D^j_{k,m}, \mathrm{i}B_2 D^{j+1}_{k,m\pm1}\rangle = \pm\mathrm{i}a_{j,k,\pm m}\delta_3, \\ \langle D^j_{k,m}, \mathrm{i}B_3 D^{j+1}_{k,m}\rangle = -\mathrm{i}b_{j,k,m}\delta_3, \end{cases} \tag{3.4.11}$$

where

$$\begin{aligned} a_{j,k,m} &:= \frac{[(j+1)^2 - k^2]^{1/2}[(j+m+1)(j+m+2)]^{1/2}}{2(j+1)[(2j+1)(2j+3)]^{1/2}}, \\ b_{j,k,m} &:= \frac{[(j+1)^2 - k^2]^{1/2}[(j+1)^2 - m^2]^{1/2}}{(j+1)[(2j+1)(2j+3)]^{1/2}}. \end{aligned}$$

Note that the $k \to k$ transitions are driven by δ_3. Recall that, up to a rotation, we can assume that $\delta_1 = 0$. Because of Lemma 3.2.7, parts 2 and 3, the expression of the controlled fields excited at the frequencies η_k and σ^j are

$$\begin{aligned}\mathcal{E}_{\eta_k}(\mathrm{i}B_1) = &\sum_{\substack{l=j,j+1,\\ m=-l,\dots,l-1}} -h_{l,k,m}\delta_2 G_{(l,k,m),(l,k+1,m+1)} - h_{l,k,m}\delta_2 G_{(l,-k,m),(l,-k-1,m+1)} \\ &+ \sum_{\substack{l=j,j+1,\\ m=-l+1,\dots,l}} h_{l,k,-m}\delta_2 G_{(l,k,m),(l,k+1,m-1)} + h_{l,k,-m}\delta_2 G_{(l,-k,m),(l,-k-1,m-1)},\end{aligned} \tag{3.4.12}$$

$$\begin{aligned}\mathcal{E}_{\eta_k}(\mathrm{i}B_2) = &\sum_{\substack{l=j,j+1,\\ m=-l,\dots,l-1}} -h_{l,k,m}\delta_2 F_{(l,k,m),(l,k+1,m+1)} - h_{l,k,m}\delta_2 F_{(l,-k,m),(l,-k-1,m+1)} \\ &+ \sum_{\substack{l=j,j+1,\\ m=-l+1,\dots,l}} -h_{l,k,-m}\delta_2 F_{(l,k,m),(l,k+1,m-1)} - h_{l,k,-m}\delta_2 F_{(l,-k,m),(l,-k-1,m-1)},\end{aligned} \tag{3.4.13}$$

$$\mathcal{E}_{\eta_k}(\mathrm{i}B_3) = \sum_{\substack{l=j,j+1,\\ m=-l,\dots,l}} -q_{l,k,m}\delta_2 F_{(l,k,m),(l,k+1,m)} - q_{l,k,m}\delta_2 F_{(l,-k,m),(l,-k-1,m)}, \tag{3.4.14}$$

and

$$\begin{aligned}\mathcal{E}_{\sigma^j}(\mathrm{i}B_1) &= \sum_{m,k=-j,\dots,j} a_{j,k,m}\delta_3 G_{(j,k,m),(j+1,k,m+1)} + a_{j,k,-m}\delta_3 G_{(j,k,m),(j+1,k,m-1)}, \\ \mathcal{E}_{\sigma^j}(\mathrm{i}B_2) &= \sum_{m,k=-j,\dots,j} a_{j,k,m}\delta_3 F_{(j,k,m),(j+1,k,m+1)} - a_{j,k,-m}\delta_3 F_{(j,k,m),(j+1,k,m-1)}, \\ \mathcal{E}_{\sigma^j}(\mathrm{i}B_3) &= \sum_{m,k=-j,\dots,j} -b_{j,k,m}\delta_3 F_{(j,k,m),(j+1,k,m)}.\end{aligned} \tag{3.4.15}$$

Note that in $\mathcal{E}_{\eta_k}(-iB_3)$ the term for $m = 0$ vanishes, since $q_{j,k,0} = 0$ for every j, k.

To decouple all the m-degeneracies in the excited modes, we just consider double brackets with the elementary matrices that we have obtained above. As an example, using (3.4.9) we can decouple the $m \to m$ transitions corresponding to the frequency σ^j by considering

$$\begin{aligned}&[[W_{\mathrm{i}}(\mathcal{E}_{\sigma^j}(\mathrm{i}B_3)), G_{(j,k,m),(j+1,k+1,m)} - G_{(j,-k,m),(j+1,-k-1,m)}], \\ &G_{(j,k,m),(j+1,k+1,m)} - G_{(j,-k,m),(j+1,-k-1,m)}] \\ &= G_{(j,k,m),(j+1,k,m)} + G_{(j,-k,m),(j+1,-k,m)} \in \mathrm{Lie}(\widetilde{\mathcal{P}}_j).\end{aligned}$$

Considering every possible double brackets as above, we obtain, for $X \in \{G, F\}$, that

$$X_{(j,k,m),(j+1,k,m)} + X_{(j,-k,m),(j+1,-k,m)} \in \mathrm{Lie}(\widetilde{\mathcal{P}}_j), \quad k \neq 0, \tag{3.4.16}$$

when we start from the matrices in (3.4.15), and that

$$X_{(l,k,m),(l,k+1,m)} + X_{(l,-k,m),(l,-k-1,m)}, X_{(l,k,m),(l,k+1,m\pm1)} + X_{(l,-k,m),(j,-k-1,m\pm1)}$$

are in $\mathrm{Lie}(\widetilde{\mathcal{P}}_j)$, $l = j, j+1$, $m, k \neq 0$, when we start from the matrices in (3.4.12), (3.4.13), (3.4.14). Now we can also generate the missing $k = 0$ elements of (3.4.9) by taking double brackets with $X_{(j+1,1,m),(j+1,2,m)} + X_{(j+1,-1,m),(j+1,-2,m)} \in \mathrm{Lie}(\widetilde{\mathcal{P}}_j)$. As an example, we have that

$$\begin{aligned}&[[\mathcal{E}_{\lambda_0^j}(\mathrm{i}B_3), F_{(j+1,1,m),(j+1,2,m)} + F_{(j+1,-1,m),(j+1,-2,m)}], \\ &F_{(j+1,1,m),(j+1,2,m)} + F_{(j+1,-1,m),(j+1,-2,m)}] \\ &= F_{(j,0,m),(j+1,1,m)} - F_{(j,0,m),(j+1,-1,m)} \in \mathrm{Lie}(\widetilde{\mathcal{P}}_j).\end{aligned}$$

Moreover, also the $m = 0$ elements in the transitions (3.4.14) are in $\mathrm{Lie}(\widetilde{\mathcal{P}}_j)$, as one can check by considering a bracket between two transitions obtained in (3.4.9) and (3.4.16). For example,

$$\begin{aligned}&[G_{(j,k,0),(j+1,k+1,0)} - G_{(j,-k,0),(j+1,-k-1,0)}, G_{(j+1,k+1,0),(j,k+1,0)} \\ &+ G_{(j+1,-k-1,0),(j,-k-1,0)}] = G_{(j,k,0),(j,k+1,0)} - G_{(j,-k,0),(j,-k-1,0)} \in \mathrm{Lie}(\widetilde{\mathcal{P}}_j).\end{aligned}$$

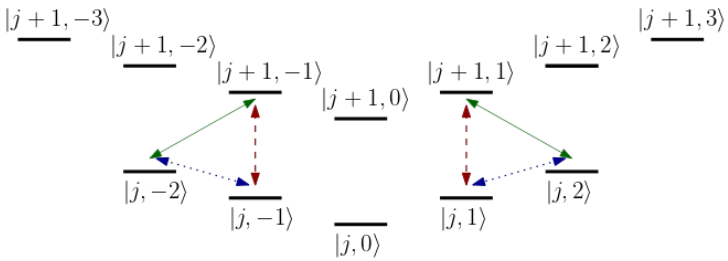


Figure 3.6: Three-wave mixing around $k = 1, -1$. The same-shaped arrows correspond to equal spectral gaps, and thus, coupled transitions. The goal of the three-wave mixing is to decouple those arrows.

Finally, we apply a three-wave mixing argument (Figure 3.4.2) in order to decouple the sum over k and $-k$ in every elementary matrices: consider the bracket between the following elements in $\mathrm{Lie}(\widetilde{\mathcal{P}}_j)$

$$\begin{aligned}&[G_{(j,k+1,m),(j,k,m)} + G_{(j,-k-1,m),(j,-k,m)}, G_{(j,k,m),(j+1,k,m)} + G_{(j,-k,m),(j+1,-k,m)}]\\ &= G_{(j,k+1,m),(j+1,k,m)} + G_{(j,-k-1,m),(j+1,-k,m)} \in \mathrm{Lie}(\widetilde{\mathcal{P}}_j), \quad k \neq 0,\end{aligned}$$

and notice that from (3.4.9) we already have that $G_{(j,k+1,m),(j+1,k,m)} - G_{(j,-k-1,m),(j+1,-k,m)}$ is in $\mathrm{Lie}(\widetilde{\mathcal{P}}_j)$, and hence $G_{(j,k+1,m),(j+1,k,m)}$ and $G_{(j,-k-1,m),(j+1,-k,m)}$ are in $\mathrm{Lie}(\widetilde{\mathcal{P}}_j)$. In this way we can break every k-degeneracy, and finally obtain that $\mathrm{Lie}(\widetilde{\mathcal{P}}_j) = \mathfrak{su}(\mathcal{M}_j)$, which concludes the proof.

Chapter 4

Enantiomer-selective transfer of rotational population in chiral asymmetric molecules

4.1 The physical model

In this chapter we consider a molecule made of two *identical*, *mirrored*, asymmetric-tops, whose rotations are controlled with three orthogonal electric fields. Identical means that the two tops have same inertia constants A, B, C and hence same rotational spectra. Mirrored means that the two tops have resp. electric dipoles $\delta^{(+)}$ and $\delta^{(-)}$ such that two components are equal, and and third differs only in sign. The two tops composing the molecule are also called *enantiomers*: the left-handed top is called S-enantiomer, and the right-handed is the R-enantiomer. The two enantiomers are *chiral* objects, meaning that they are not superimposable with their mirrored images: such a two-body system is also called a chiral asymmetric molecule.

We interpret the problem of enantiomer-selective transfer of population as the following control problem: assuming that the initial state of the Schrödinger equation (3.2.4) is supported on the same finite-dimensional combination of rotational eigenfunctions on both the enantiomers, and assuming that there is no conversion between the two enantiomers, we want to steer the system to a state that is supported on different finite-dimensional linear combinations of rotational eigenfunctions, on the two enantiomers. The interpretation is that, at the end of the controlled evolution, the enantiomers are selected because their rotational populations are on different states. This is surely possible if the two enantiomers are simultaneously controllable (Section 4.2), but it is also possible under weaker controllability properties on the reachable sets of the direct sum system (Section 4.3).

Given the nature of the problem, we focus on a finite-dimensional quantum system, under a generic non-resonant assumption (specified below in (4.1.2) and (4.1.3)) between the spectral gaps involved and the ones connecting states inside and outside the finite-dimensional subspace, that ensures an arbitrary precision of transfer despite the negligence of the infinite-dimensional complement. In general, for experimental set up, it is possible to prepare at low temperature a state that is supported in a finite-dimensional portion of the rotational spectrum, but we need to take into account an average over the orientational quantum number m. Moreover, we also want the transitions to couple with the three dipole components, to exploit the sign inversion.

The bilinear multi-input finite-dimensional Schrödinger equation which models this system reads as the direct sum system

$$\mathrm{i}\frac{d}{dt}\left(\psi^{(+)}(t)\oplus\psi^{(-)}(t)\right)=\left[\left(H^{(+)}\oplus H^{(-)}\right)+\sum_{l=1}^{3}u_l(t)\left(B_l^{(+)}\oplus B_l^{(-)}\right)\right]\left(\psi^{(+)}(t)\oplus\psi^{(-)}(t)\right) \tag{4.1.1}$$

where $\psi(t)^{(\pm)}\in\mathcal{H}:=\mathcal{H}_{j,\tau}\oplus\mathcal{H}_{j+1,\tau'}\oplus\mathcal{H}_{j+1,\tau''}$, $\tau\in\{-j,\dots,j\}$, $\tau',\tau''\in\{-j-1,\dots,j+1\}$,

$$\mathcal{H}_{l,r}:=\mathrm{span}\{\Psi^l_{r,m}\mid m=-l,\dots,l\},$$

$H^{(\pm)}=H|_{\mathcal{H}}$, $H=AP_1^2+BP_2^2+CP_3^2$, with rotational constants $A>B>C>0$ and $B_l^{(\pm)}=\Pi_{\mathcal{H}}\left(-\langle R^{(\pm)}\delta^{(\pm)},e_l\rangle\right)\Pi_{\mathcal{H}}$, where $\Pi_{\mathcal{H}}:L^2(\mathrm{SO}(3))\to\mathcal{H}$ denotes the orthogonal projection, and $\delta^{(\pm)}=(\delta_1^{(\pm)},\delta_2^{(\pm)},\delta_3^{(\pm)})^T$, with

$$|\delta_i^{(+)}|=|\delta_i^{(-)}|,\ i=1,2,3\quad\text{and}\quad\delta_1^{(+)}\delta_2^{(+)}\delta_3^{(+)}=-\delta_1^{(-)}\delta_2^{(-)}\delta_3^{(-)},$$

and $u(t)\in U$, for some neighborhood U of 0 in $\mathbb{R}^3$. Finally, $R^{(\pm)}\in\mathrm{SO}(3)$ describe the orientations of the two enantiomers in the space. The angular momentum operators P_i and the asymmetric-top eigenfunctions $\Psi^j_{\tau,m}$ have been introduced, resp., in Sections 3.2.1 and 3.3.1.

We are thus interested in the following control problem: given an initial and final state $\psi_i \oplus \psi_i, \psi_f \oplus \phi_f \in \mathcal{H} \oplus \mathcal{H}$, with $\psi_f \neq \phi_f$, we want to find a piecewise constant control $u = (u_1, u_2, u_3) : [0, T] \to U$ such that the solution of (4.1.1) satisfies

$$\psi(0)^{(+)} \oplus \psi(0)^{(-)} = \psi_i \oplus \psi_i \quad \text{and} \quad \psi(T)^{(+)} \oplus \psi(T)^{(-)} = \psi_f \oplus \phi_f.$$

A simplified version of (4.1.1) was studied in [82], where the authors considered a $3 \oplus 3$-level quantum system, to deduce some important properties that are confirmed in our more general analysis which takes into account also the m-degeneracies. For example, in [82] the authors proved that three polarizations and three dipole components are necessary for an enantio-selective transfer of rotational population. Detection of chirality through three orthogonal polarizations in dipole approximation has been observed in experiments of microwave spectroscopy [95].

We denote the spectral gaps of H in $\mathcal{H}$ as

$$\omega_1 := |E^{j+1}_{\tau'} - E^j_\tau|, \quad \omega_2 := |E^{j+1}_{\tau''} - E^{j+1}_{\tau'}|, \quad \omega_2 := |E^{j+1}_{\tau''} - E^j_\tau|.$$

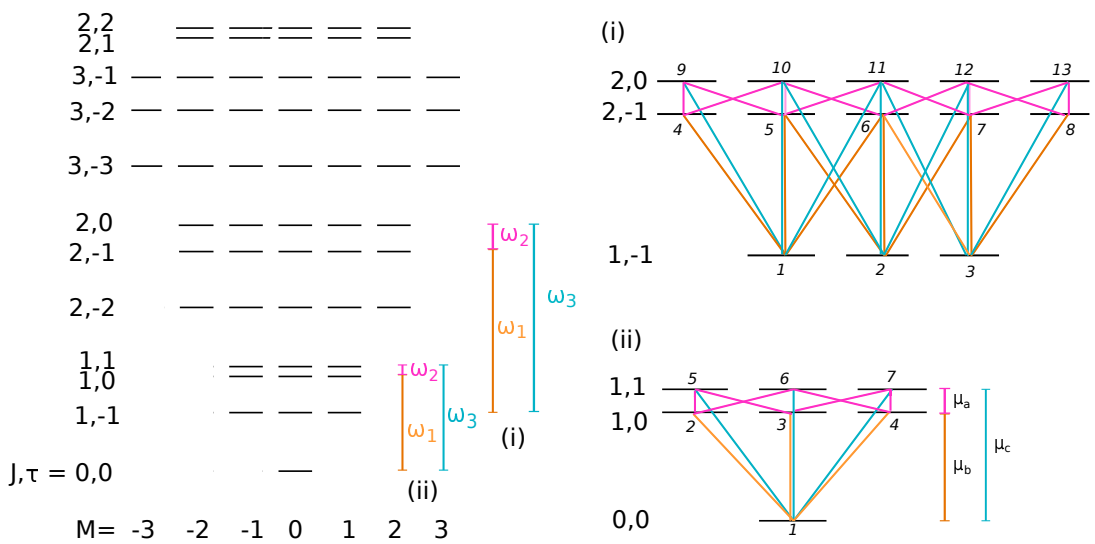


Figure 4.1: 2D spectral graphs of a near prolate asymmetric-top. In (i): transitions at frequencies $\omega_1 = |E^2_{-1} - E^1_{-1}|$, $\omega_2 = |E^2_0 - E^2_{-1}|$ and $\omega_3 = |E^2_0 - E^1_{-1}|$. In (ii): transitions at frequencies $\omega_1 = |E^1_0 - E^0_0|$, $\omega_2 = |E^1_1 - E^1_0|$ and $\omega_3 = |E^1_1 - E^0_0|$. Here the dipole components are labeled as: $\mu_b = \delta_1$, $\mu_a = \delta_2$, and $\mu_c = \delta_3$.

We remark here that there is an additional assumption on the space $\mathcal{H}$: the choice of τ, τ', τ'' has to be such that the spectral gaps $\omega_1, \omega_2, \omega_3$ couple with all dipole components, say resp. $\delta_1, \delta_2, \delta_3$; this is not always the case, as it may happen that the gaps are all coupled with δ_3 only, but in that case we only need to choose a different τ, which is always possible.

We denote as $I := \cup_{l \in \mathbb{N}} \{(l, r) \mid r = -l, \dots, l\}$ the set of spectral indices and $I_{\text{int}} = \{(j, \tau), (j+1, \tau'), (j+1, \tau'')\}$ the set of spectral indices involved in the space $\mathcal{H} \subset L^2(\text{SO}(3))$. Throughout the chapter we assume the following non-resonant assumptions

$$\omega_i \neq \omega_j \quad \text{if } i \neq j,\ i, j = 1, 2, 3, \tag{4.1.2}$$

$$\omega_i \neq \omega \quad \forall \omega \in \{|E^l_r - E^{l'}_{r'}| \mid (l, r) \in I_{\text{int}}, (l', r') \in I \setminus I_{\text{int}}\}. \tag{4.1.3}$$

(4.1.2) guarantees that there are no internal resonances, and (4.1.3) guarantees that there are no resonances that couple a state in $\mathcal{H}$ and a state outside $\mathcal{H}$. Then, Lemma 3.1.12 ensures that the transfer of population inside $\mathcal{H}$ is achievable with arbitrary small error, w.r.t. the infinite-dimensional system. Moreover, assumptions (4.1.2) and (4.1.3) are satisfied for almost every value of A, B, C, as proved resp. in (3.3.20) and Lemma 3.3.5.

The chapter is organized as follows: in Sections 4.2 and 4.3 we find combinations of polarizations B_l, $l = 1, 2, 3$, and frequencies ω_i, $i = 1, 2, 3$, such that the reduced operators $\mathcal{E}_{\omega_i}(B^{(+)}_l) \oplus \mathcal{E}_{\omega_i}(B^{(-)}_l)$ yields simultaneous

controllability of (4.1.1); based of these insights, in Section 4.4 we confirm the controllability results by numerically simulating the rotational dynamics for $j = 0, 1, 1$ and $j = 1, 2, 2$ systems, thus producing pulse sequences that numerically achieve enantiomer-selective transfer of population.

The results of this chapter are in the paper [83].

4.2 Controllability

In what follows, we identify $\mathfrak{su}(\mathcal{H})$ with $\mathfrak{su}(6j+7)$, where $\dim \mathcal{H} = 6j+7$. For brevity, we write $H^{\chi} = H^{(+)} \oplus H^{(-)}$ and $B_l^{\chi} = B_l^{(+)} \oplus B_l^{(-)}$. Recall that, for any $\sigma > 0$, the operator $\mathcal{E}_\sigma(B_l)$ is defined on the basis $\{\Psi^l_{\tau,m} \mid l = j, j+1,\ \tau, m = -l, \dots, l\}$ as

$$\langle \Psi^j_{\tau,m}, \mathcal{E}_\sigma(B_l)\Psi^{j'}_{\tau',m'}\rangle = \begin{cases} \langle \Psi^j_{\tau,m}, B_l \Psi^{j'}_{\tau',m'}\rangle, & \text{if } |E^j_\tau - E^{j'}_{\tau'}| = \sigma \\ 0, & \text{otherwise.} \end{cases}$$

The main result of this section is that with five combinations of polarizations and frequencies (that involve three polarizations and three dipole components) we are able to control (4.1.1).

Proposition 4.2.1. *Let $j \geq 1$, and assume that $\delta_1^{(+)} = \delta_1^{(-)}, \delta_2^{(+)} = -\delta_2^{(-)}$, and $\delta_3^{(+)} = \delta_3^{(-)}$. Then,*

(i) $\mathrm{Lie}\left\{\mathrm{i}H, \mathcal{E}_{\omega_1}(\mathrm{i}B_1), \mathcal{E}_{\omega_1}(\mathrm{i}B_2), \mathcal{E}_{\omega_3}(\mathrm{i}B_2), \mathcal{E}_{\omega_3}(\mathrm{i}B_3)\right\} = \mathfrak{su}(\mathcal{H})$*;*

(ii) $\mathrm{Lie}\left\{\mathrm{i}H^{\chi}, \mathcal{E}_{\omega_1}(\mathrm{i}B_1^{\chi}), \mathcal{E}_{\omega_1}(\mathrm{i}B_2^{\chi}), \mathcal{E}_{\omega_3}(\mathrm{i}B_2^{\chi}), \mathcal{E}_{\omega_3}(\mathrm{i}B_3^{\chi}), \mathcal{E}_{\omega_2}(B_l^{\chi})\right\} = \mathfrak{su}(\mathcal{H}) \oplus \mathfrak{su}(\mathcal{H})$, *for any $l = 1, 2, 3$.*

The proof of Proposition 4.2.1 is postponed to the Appendix 4.5, but we make several remarks here:

Remark 4.2.2. .

- By applying Corollary 3.1.17, we see that part (ii) of Proposition 4.2.1 in particular states that (4.1.1) is operator controllable. It actually states a stronger result: indeed, denoting $\psi^{\chi} = \psi^{(+)} \oplus \psi^{(-)}$, it says that

  $$\mathrm{i}\frac{d}{dt}\psi^{\chi}(t) = \left[H^{\chi} + u_1(t)\mathcal{E}_{\omega_1}(\mathrm{i}B_1^{\chi}) + u_2(t)\mathcal{E}_{\omega_1}(\mathrm{i}B_2^{\chi}) + u_3(t)\mathcal{E}_{\omega_3}(\mathrm{i}B_2^{\chi}) + u_4(t)\mathcal{E}_{\omega_3}(\mathrm{i}B_3^{\chi}) + u_5(t)\mathcal{E}_{\omega_2}(B_l^{\chi})\right]\psi^{\chi}(t)$$

  is operator controllable.

- Part (i) of Proposition 4.2.1 states that four combinations of polarizations and frequencies which involve three polarizations and two frequencies are sufficient to control one top. Part (ii) of Proposition 4.2.1 states that five combinations of polarizations and frequencies which involve three polarizations and three frequencies are sufficient to simultaneously control two tops. By numerically compute the dimension of the associated Lie algebra for small values of j, one can also see that it is the minimal number, that is, three (four) combinations cannot control (simultaneously) one (two) top(s).

- By numerically computing the Lie algebra for small values of j, one sees that there are many choices of combinations of five pulses that lead to simultaneous control. Of course one needs to consider three polarizations and three frequencies/dipole components (as it was already proved in [82]). Among the combinations that involve three polarizations and three frequencies, we realized that the only ones which *do not* lead to simultaneous control have the forms:

  $$(A): \quad \{\mathcal{E}_{\omega_{\pi(1)}}(\mathrm{i}B^{\chi}_{\sigma(1)}), \mathcal{E}_{\omega_{\pi(1)}}(\mathrm{i}B^{\chi}_{\sigma(2)}), \mathcal{E}_{\omega_{\pi(2)}}(\mathrm{i}B^{\chi}_{\sigma(1)}), \mathcal{E}_{\omega_{\pi(2)}}(\mathrm{i}B^{\chi}_{\sigma(2)}), \mathcal{E}_{\omega_{\pi(3)}}(B^{\chi}_{\sigma(3)})\},$$

  with π, σ permutations of $\{1, 2, 3\}$, or the form of five combinations where three of them are

  $$(B): \quad \{\mathcal{E}_{\omega_a}(\mathrm{i}B_1^{\chi}), \mathcal{E}_{\omega_a}(\mathrm{i}B_2^{\chi}), \mathcal{E}_{\omega_a}(\mathrm{i}B_3^{\chi})\}, \quad a \in \{1, 3\}.$$

  As we shall see in the next section, family of combinations like in (A) are still very useful to obtain enantiomer-selection within the simultaneously reachable sets.

For $j = 0$, we prove in the next example a controllability result for the specific subsystem whose dynamics will be numerically investigated in Sections 4.4.1 and 4.4.2.

Example 4. The scope of this example is proving that, for

$$\mathcal{H} = \mathcal{H}_{0,0} \oplus \mathcal{H}_{1,0} \oplus \mathcal{H}_{1,1} = \mathbb{C}^7$$

(which corresponds to Figure 4.1(ii)) and dipole components $\delta_1^{(+)} = \delta_1^{(-)}, \delta_2^{(+)} = \delta_2^{(-)}$, and $\delta_3^{(+)} = -\delta_3^{(-)}$ one has that

$$\text{Lie}\{\mathrm{i}H, \mathcal{E}_{\omega_1}(\mathrm{i}B_1), \mathcal{E}_{\omega_1}(\mathrm{i}B_3), \mathcal{E}_{\omega_2}(\mathrm{i}B_2), \mathcal{E}_{\omega_2}(\mathrm{i}B_3)\} = \mathfrak{su}(7), \tag{4.2.1}$$

$$\text{Lie}\{\mathrm{i}H^{\chi}, \mathcal{E}_{\omega_1}(\mathrm{i}B_1^{\chi}), \mathcal{E}_{\omega_1}(\mathrm{i}B_3^{\chi}), \mathcal{E}_{\omega_2}(\mathrm{i}B_2^{\chi}), \mathcal{E}_{\omega_2}(\mathrm{i}B_3^{\chi}), \mathcal{E}_{\omega_3}(\mathrm{i}B_1^{\chi})\} = \mathfrak{su}(7) \oplus \mathfrak{su}(7). \tag{4.2.2}$$

Of course, this can also be checked by computing numerically the dimension of the Lie algebra, but we give here an explicit proof for completeness. In this example we diagonalize the rotational Hamiltonian H of an asymmetric-top in $\mathcal{H}$ starting from its representation w.r.t. the symmetric-top representation $S^j_{k,m,p}$, to find eigenvalues and eigenvectors, and we express the control problem w.r.t. the representation $\Psi^j_{\tau,m}$ is which H is diagonal. We have

$$H = \text{diag}\left(E_0^0, E_0^1, E_0^1, E_0^1, E_1^1, E_1^1, E_1^1\right)$$

and using the pairings (3.4.1),(3.4.10),(3.4.11) we write

$$\begin{aligned}
\mathcal{E}_{\omega_1}(\mathrm{i}B_1) &= \frac{\delta_1}{\sqrt{6}}(G_{1,4} - G_{1,2}), \\
\mathcal{E}_{\omega_1}(\mathrm{i}B_3) &= -\frac{\delta_1}{\sqrt{3}}G_{1,3}, \\
\mathcal{E}_{\omega_2}(\mathrm{i}B_2) &= \frac{\delta_2}{2\sqrt{2}}(G_{3,5} + G_{4,6} - G_{2,6} - G_{3,7}), \\
\mathcal{E}_{\omega_2}(\mathrm{i}B_3) &= \frac{\delta_2}{2}(-F_{2,5} + F_{4,7}),
\end{aligned} \tag{4.2.3}$$

where the matrix elements are labeled according to Fig. 4.1(ii). We recall that, instead of using $\mathrm{i}H$ we may use the operator W_{i} thanks to the relation (3.1.3). Recalling the action of the operator W_{i} given in (3.4.3), and the laws of the Lie algebra $\mathfrak{su}$ described in (3.1.9),(3.1.10),(3.1.11), we compute (where $\propto$ means proportional by a non-zero number)

$$\begin{aligned}
\left[\mathcal{E}_{\omega_1}(\mathrm{i}B_1), W_{\mathrm{i}}(\mathcal{E}_{\omega_2}(\mathrm{i}B_3))\right] &\propto G_{1,5} + G_{1,7}, \\
\left[\mathcal{E}_{\omega_1}(\mathrm{i}B_3), \mathcal{E}_{\omega_2}(\mathrm{i}B_2)\right] &\propto G_{1,5} - G_{1,7}.
\end{aligned} \tag{4.2.4}$$

Taking the sum and the difference, we obtain

$$\begin{aligned}
\left[\mathcal{E}_{\omega_1}(\mathrm{i}B_1), W_{\mathrm{i}}(\mathcal{E}_{\omega_2}(\mathrm{i}B_3))\right] + \left[\mathcal{E}_{\omega_1}(\mathrm{i}B_3), \mathcal{E}_{\omega_2}(\mathrm{i}B_2)\right] &\propto G_{1,5} \\
\left[\mathcal{E}_{\omega_1}(\mathrm{i}B_1), W_{\mathrm{i}}(\mathcal{E}_{\omega_2}(\mathrm{i}B_3))\right] - \left[\mathcal{E}_{\omega_1}(\mathrm{i}B_3), \mathcal{E}_{\omega_2}(\mathrm{i}B_2)\right] &\propto G_{1,7}.
\end{aligned} \tag{4.2.5}$$

Moreover, we find

$$\begin{aligned}
\left[G_{1,7}, W_{\mathrm{i}}(\mathcal{E}_{\omega_2}(\mathrm{i}B_3))\right] &\propto G_{1,4} \\
\left[G_{1,5}, W_{\mathrm{i}}(\mathcal{E}_{\omega_2}(\mathrm{i}B_3))\right] &\propto G_{1,2} \\
\left[G_{1,2}, \mathcal{E}_{\omega_2}(\mathrm{i}B_2)\right] &\propto G_{1,6}.
\end{aligned} \tag{4.2.6}$$

So far, we have obtained all elements $G_{j,k}$ with $j = 1$. Using the laws of $\mathfrak{su}$ is now easy to get every element $G_{j,k}, F_{j,k}, D_{j,k}$, that is a basis of $\mathfrak{su}(7)$. We have proven (4.2.1). In order to prove (4.2.2), since

$$(\delta_1^{(+)}, \delta_2^{(+)}, \delta_3^{(+)}) = (\delta_1^{(-)}, \delta_2^{(-)}, -\delta_3^{(-)}) = (\delta_1, \delta_2, \delta_3),$$

it follows that

$$\text{Lie}\{\mathrm{i}H^{\chi}, \mathcal{E}_{\omega_1}(\mathrm{i}B_1^{\chi}), \mathcal{E}_{\omega_1}(\mathrm{i}B_3^{\chi}), \mathcal{E}_{\omega_2}(\mathrm{i}B_2^{\chi}), \mathcal{E}_{\omega_2}(\mathrm{i}B_3^{\chi})\} = \left\{\begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} \mid A \in \mathfrak{su}(7)\right\}. \tag{4.2.7}$$

We then consider

$$\mathcal{E}_{\omega_3}(\mathrm{i}B_1)^{\chi} = \begin{pmatrix} \mathcal{E}_{\omega_3}(\mathrm{i}B_1) & 0 \\ 0 & -\mathcal{E}_{\omega_3}(\mathrm{i}B_1) \end{pmatrix} \tag{4.2.8}$$

with $\mathcal{E}_{\omega_3}(\mathrm{i}B_1) = \frac{\delta_3}{\sqrt{6}}(F_{1,5} - F_{1,7})$ and the minus sign in the lower block occuring because we are assuming that $\delta_3^{(+)} = -\delta_3^{(-)}$. We also consider

$$M := \begin{pmatrix} G_{1,5} - G_{1,7} & 0 \\ 0 & G_{1,5} - G_{1,7} \end{pmatrix}$$

which is an element of the Lie algebra generated in (4.2.7). Moreover,

$$W_{\mathrm{i}}(\mathcal{E}_{\omega_3}(\mathrm{i}B_1^{\chi})) := \begin{pmatrix} G_{1,5} - G_{1,7} & 0 \\ 0 & -G_{1,5} + G_{1,7} \end{pmatrix}.$$

Taking the sum and difference of the two matrices, we obtain

$$\frac{1}{2}\left(W_{\mathrm{i}}(\mathcal{E}_{\omega_3}(\mathrm{i}B_1^{\chi})) + M\right) = \begin{pmatrix} G_{1,5} - G_{1,7} & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$\frac{1}{2}\left(W_{\mathrm{i}}(\mathcal{E}_{\omega_3}(\mathrm{i}B_1^{\chi})) - M\right) = \begin{pmatrix} 0 & 0 \\ 0 & -G_{1,5} + G_{1,7} \end{pmatrix}.$$

From here, we can apply Lemma 3.2.4 to conclude: in this case, $K = 2$ is the number of tops, which we denote by $(+)$ and $(-)$, the two Hilbert spaces are $\mathbb{C}^7$, $m = 5$ is the number of interaction Hamiltonians, and

$$\begin{aligned} H^{(+)} &= H^{(-)} = H, \qquad H_1^{(+)} = H_1^{(-)} = \mathcal{E}_{\omega_1}(\mathrm{i}B_1), \\ H_2^{(+)} &= H_2^{(-)} = \mathcal{E}_{\omega_1}(\mathrm{i}B_3), \quad H_3^{(+)} = H_3^{(-)} = \mathcal{E}_{\omega_2}(\mathrm{i}B_2), \\ H_4^{(+)} &= H_4^{(-)} = \mathcal{E}_{\omega_2}(\mathrm{i}B_3), \quad H_5^{(+)} = -H_5^{(-)} = \mathcal{E}_{\omega_3}(\mathrm{i}B_1). \end{aligned}$$

Indeed, we have proven that the LHS of (4.2.2) contains element of the form $A \oplus 0$, with $A \neq 0$, and this in particular implies that there cannot be an automorphism f of $\mathfrak{su}(7)$ which matches the conditions described in Lemma 3.2.4, otherwise such isomorphism should satisfies $f(A) = 0$, that is impossible.

We will show how to exploit these (minimal) sets of fields for the example of the propanediol molecule in Sec. 4.4.2.

4.3 Enantiomer-selection

In order to distinguish the two enantiomers via their final rotational population, it is not crucial that (4.1.1) is simultaneously controllable: it suffices that simultaneous controllability holds in smaller invariant subspaces of $\mathcal{H}$. Imagine that the initial population is averaged over the eigenstates corresponding to the eigenvalues E_τ^j, on both enantiomers. Using interactions of the form

$$\frac{1}{2}\left(\mathcal{E}_{\omega_1}(\mathrm{i}B_1) + W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_2)\right) =: \mathcal{E}_{\omega_1}(\mathrm{i}B_+) \tag{4.3.1}$$

$$\frac{1}{2}\left(\mathcal{E}_{\omega_2}(\mathrm{i}B_1) - W_{\mathrm{i}}\mathcal{E}_{\omega_2}(\mathrm{i}B_2)\right) =: \mathcal{E}_{\omega_2}(\mathrm{i}B_-) \tag{4.3.2}$$

and $\mathcal{E}_{\omega_3}(\mathrm{i}B_3)$, we see that $(2j + 1)$ 3-level systems are composed and invariant for (4.1.1) (see Figure 4.2 for an example with $j = 1$). The operators defined in (4.3.1) and (4.3.2) are usually called right- and left-circular polarizations, at frequencies ω_1 and ω_2.

We denote this new smaller Hilbert subspaces of $\mathcal{H}$ made by sums of 3-level systems as

$$\mathfrak{h} := \bigoplus_{l=-j,\dots,j} \mathfrak{h}_l, \quad \mathfrak{h}_l := \mathrm{span}\{\Psi_{\tau,l}^j, \Psi_{\tau',l+1}^{j+1}, \Psi_{\tau'',l}^{j+1}\}, \tag{4.3.3}$$

and we notice that each $\mathfrak{h}_l$ is invariant for $\mathcal{E}_{\omega_1}(\mathrm{i}B_+)$, $\mathcal{E}_{\omega_2}(\mathrm{i}B_-)$ and $\mathcal{E}_{\omega_3}(\mathrm{i}B_3)$ which allows to write (4.1.1) projected in $\mathfrak{h}$ as a direct sum control systems on each top. The main result is that, on each top, the 3-level systems are simultaneously controllable, and each 3-level system is simultaneously controllable w.r.t. the two tops, as stated in the following:

Proposition 4.3.1. *Let $j \geq 1$ and assume that $\delta_1^{(+)} = \delta_1^{(-)}, \delta_2^{(+)} = \delta_2^{(-)}$, and $\delta_3^{(+)} = -\delta_3^{(-)}$. Consider* (4.1.1) *projected onto $\mathfrak{h}$. Then,*

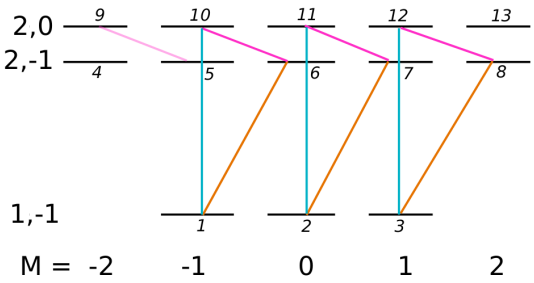


Figure 4.2: Spectral graph for eigenstates corresponding to the eigenvalues $E^1_{-1}, E^2_{-1}, E^2_0$ with transitions moved by $\mathcal{E}_{\omega_1}(\mathrm{i}B_+)$ (orange), $\mathcal{E}_{\omega_2}(\mathrm{i}B_-)$ (violet) and $\mathcal{E}_{\omega_2}(\mathrm{i}B_-)$ (blue). We can see the splitting given in (4.3.3) as follows: $\mathfrak{h}$ is spanned by states $1, 6, 10, 2, 7, 11, 3, 8, 12$; $\mathfrak{h}_{-1}$ is spanned by states $1, 6, 10$; $\mathfrak{h}_0$ is spanned by states $2, 7, 11$;$\mathfrak{h}_1$ is spanned by states $3, 8, 12$.

- $\mathrm{Lie}\{\mathrm{i}H, \mathcal{E}_{\omega_1}(\mathrm{i}B_+), \mathcal{E}_{\omega_2}(\mathrm{i}B_-)\} = \underbrace{\mathfrak{su}(3) \oplus \cdots \oplus \mathfrak{su}(3)}_{(2j+1)\text{-}times};$
- $\mathrm{Lie}\{\mathrm{i}H^\chi, \mathcal{E}_{\omega_1}(\mathrm{i}B^\chi_+), \mathcal{E}_{\omega_2}(\mathrm{i}B^\chi_-), \mathcal{E}_{\omega_3}(\mathrm{i}B^\chi_3)\} = (\underbrace{\mathfrak{su}(3) \oplus \cdots \oplus \mathfrak{su}(3)}_{(2j+1)\text{-}times}) \oplus (\underbrace{\mathfrak{su}(3) \oplus \cdots \oplus \mathfrak{su}(3)}_{(2j+1)\text{-}times});$

The proof of this result is basically contained in the following example, whose dynamics is numerically investigated in Section 4.4.3.

Example 5. The scope of this example is proving Proposition 4.3.1 for the example described in Figure 4.2.

In order to determine the Lie algebra for a single enantiomer, we first consider the interaction Hamiltonians

$$\mathcal{E}_{\omega_1}(\mathrm{i}B_+) \propto \delta_1\Big(G_{1,6} + \sqrt{3}G_{2,7} + \sqrt{6}G_{3,8}\Big), \tag{4.3.4}$$

$$\mathcal{E}_{\omega_2}(\mathrm{i}B_-) \propto \delta_2\Big(G_{8,12} + \sqrt{\frac{3}{2}}\Big(G_{6,10} + G_{7,11}\Big)\Big) \tag{4.3.5}$$

and show that, together with $\mathrm{i}H$, they generate $\mathfrak{su}(3) \oplus \mathfrak{su}(3) \oplus \mathfrak{su}(3)$. Recall that, instead of using $\mathrm{i}H$ we may use the operator W_{i}, whose action is given in (3.4.3) and whose relation with $\mathrm{i}H$ is given in (3.1.3). Recall moreover the rules of the Lie algebra $\mathfrak{su}$ given in (3.1.9),(3.1.10),(3.1.11). We have

$$W_{\mathrm{i}}(\mathcal{E}_{\omega_1}(\mathrm{i}B_+)) \propto F_{1,6} + \sqrt{3}F_{2,7} + \sqrt{6}F_{3,8}\,.$$

Moreover, abbreviating commutators as $\mathrm{ad}^{n+1}_A B = [A, \mathrm{ad}^n_A B]$ with $\mathrm{ad}^0_A B = B$, we note that

$$\mathrm{ad}^{2s}_{W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)}\mathcal{E}_{\omega_1}(\mathrm{i}B_+) \propto G_{1,6} + \sqrt{3}^{2s+1}G_{2,7} + \sqrt{6}^{2s+1}G_{3,8}$$

with $s = 0, 1, 2, \ldots$ Thus,

$$\begin{pmatrix} \mathrm{ad}^0_{W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)}\mathcal{E}_{\omega_1}(\mathrm{i}B_+) \\ \mathrm{ad}^2_{W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)}\mathcal{E}_{\omega_1}(\mathrm{i}B_+) \\ \mathrm{ad}^4_{W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)}\mathcal{E}_{\omega_1}(\mathrm{i}B_+) \end{pmatrix} = V \begin{pmatrix} G_{1,6} \\ G_{2,7} \\ G_{3,8} \end{pmatrix}$$

with

$$V = \begin{pmatrix} 1 & \sqrt{3} & \sqrt{6} \\ 1 & \sqrt{3}^3 & \sqrt{6}^3 \\ 1 & \sqrt{3}^5 & \sqrt{6}^5 \end{pmatrix}. \tag{4.3.6}$$

The matrix V, being a Vandermonde matrix, is invertible since the entries $1, \sqrt{3}, \sqrt{6}$ are all different which implies that $G_{1,6}, G_{2,7}, G_{3,8} \in \mathrm{Lie}\{\mathrm{i}H, \mathcal{E}_{\omega_1}(\mathrm{i}B_+)\}$. It then follows that

$$X_{1,6}, X_{2,7}, X_{3,8} \in \mathrm{Lie}\{\mathrm{i}H, \mathcal{E}_{\omega_1}(\mathrm{i}B_+)\},\ X \in \{G, F, D\}.$$

We then calculate the commutators

$$[[\mathcal{E}_{\omega_2}(\mathrm{i}B_-), G_{1,6}], G_{1,6}] \propto G_{6,10},$$
$$[[\mathcal{E}_{\omega_2}(\mathrm{i}B_-), G_{2,7}], G_{2,7}] \propto G_{7,11},$$
$$[[\mathcal{E}_{\omega_2}(\mathrm{i}B_-), G_{3,8}], G_{3,8}] \propto G_{8,12},$$

finding that

$$X_{6,10}, X_{7,11}, X_{8,12} \in \mathrm{Lie}\{\mathrm{i}H, \mathcal{E}_{\omega_1}(\mathrm{i}B_+), \mathcal{E}_{\omega_2}(\mathrm{i}B_-)\}, \quad X \in \{G, F, D\}. \tag{4.3.7}$$

Since

$$\mathrm{Lie}\Big\{X_{1,6}, X_{2,7}, X_{3,8}, X_{6,10}, X_{7,11}, X_{8,12} \mid X \in \{G, F, D\}\Big\} \cong \mathfrak{su}(3) \oplus \mathfrak{su}(3) \oplus \mathfrak{su}(3),$$

we have proven the first part of the statement.

To obtain the simultaneous control of each of these three cycles w.r.t. the two enantiomers, we consider the interaction with the third field, namely

$$\mathcal{E}_{\omega_3}(\mathrm{i}B_3) \propto \delta_3\Big(G_{2,11} + \frac{\sqrt{3}}{2}\Big(G_{3,12} + G_{1,10}\Big)\Big),$$

or, for the composite system consisting of the two enantiomers,

$$\mathcal{E}_{\omega_3}(\mathrm{i}B_3^{\chi}) = (\mathcal{E}_{\omega_3}(\mathrm{i}B_3)) \oplus (-\mathcal{E}_{\omega_3}(\mathrm{i}B_3)),$$

where we are assuming that the sign inversion is in the dipole components δ_3. From (4.3.7) we get the operators $G_{1,6} \oplus G_{1,6}$ and $G_{1,10} \oplus G_{1,10}$. We compute the double bracket

$$[[\mathcal{E}_{\omega_3}(\mathrm{i}B_3)^{\chi}, G_{1,6} \oplus G_{1,6}], G_{1,6} \oplus G_{1,6}] \propto G_{1,10} \oplus (-G_{1,10}),$$

and taking the sum and difference with $G_{1,10} \oplus G_{1,10}$, the operators $G_{1,10} \oplus \mathbf{0}$ and $\mathbf{0} \oplus G_{1,10}$ are generated. Form here, the proof is easily concluded.

Proof of Proposition 4.3.1. In order to generalize the previous example to any $E_{\tau}^{j}, E_{\tau'}^{j+1}, E_{\tau''}^{j+1}$, we follow the same construction and notice that the matrix V (cf. (4.3.6)) is again in Vandermonde form, with $2j + 1$ different entries in the first row and thus is invertible (this fact is also proved in the Appendix 4.5, see equation (4.5.8)). □

As we shall see for the example of carvone in Sec. 4.4.3, those isolated three-level systems are particularly suited for enantio-selective excitation in real molecules.

4.4 Application: Derivation of pulse sequences for asymmetric top molecules

We now show how to use the controllability results of the previous section to derive actual pulse sequences in order to control the rotational dynamics in asymmetric top molecules. In all examples presented below, the control target is to energetically separate an initially incoherent mixture of degenerate rotational states, as encountered in gas phase experiments with randomly oriented molecules.

We simulate the rotational dynamics for the R- and S-enantiomers of propanediol and of carvone by numerically solving the Schrödinger equation (4.1.1). For propanediol, the rotational constants are $A = 7644.7\,\mathrm{MHz}$, $B = 3927.3\,\mathrm{MHz}$, and $C = 2878.0\,\mathrm{MHz}$, and the dipole moments $\delta_1 = 1.2\,\mathrm{D}$, $\delta_2 = 1.9\,\mathrm{D}$ and $\delta_3 = 0.36\,\mathrm{D}$ [95]. For carvone, $A = 2237.21\,\mathrm{MHz}$, $B = 656.28\,\mathrm{MHz}$, and $C = 579.64\,\mathrm{MHz}$, and $\delta_1 = 2.0\,\mathrm{D}$ $\delta_2 = 3.0\,\mathrm{D}$, and $\delta_3 = 0.5\,\mathrm{D}$ [90].

Our choice of examples is motivated by experiments with propanediol [53] and carvone [96], on enantiomer-selective population transfer. Here, we address the problem of solving the degeneracy with respect to the orientational quantum number M, relevant whenever the initial state is chosen with $j > 0$. Our pulse sequences will induce the maximal degree of orientational- and enantiomer-selectivity.

We present two different control strategies to energetically separate population initially distributed over m-degenerate states. For the first strategy, we exploit evolution operator-controllability of the complete rotational subsystem, as shown in Sec. 4.2: We use the insight into which fields are required, for orientational, respectively enantiomer-specific, state transfer in Sec. 4.4.1 and 4.4.2. More in detail, Sec. 4.4.1 illustrates controllability of a single enantiomer, showing how to drive population initially in degenerate rotational states into levels separated in energy. In this case, the rotational dynamics of the two enantiomers is identical. Enantiomer-selective controllability is exemplified in Sec. 4.4.2, where we show how to energetically separate the two enantiomers. For the

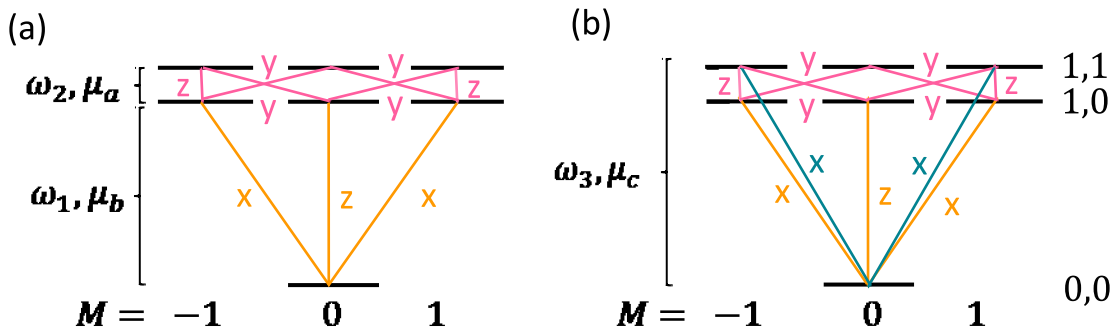


Figure 4.3: Choice of four, respectively five, microwave fields, which are sufficient to ensure evolution operator-controllability (a) and enantiomer-selective evolution operator-controllability (b) in the rotational subsystem consisting of the states $|0,0,0\rangle$, $|1,0,m\rangle$, and $|1,1,m\rangle$. The orange and pink lines in panel (a) indicate the four fields which yield complete controllability of this subsystem for a single enantiomer. The polarization of the fields is denoted by x, y, and z. The additional field which is required for enantiomer-selective control is indicated in panel (b) by turquoise lines. For propanediol, the frequencies are $\omega_1 = 11363$ MHz, $\omega_2 = 849.1$ MHz, $\omega_3 = 12212$ MHz.

second strategy, we use the simultaneous controllability of "parallel" three-level cycles, introduced in Sec. 4.3, for enantiomer-specific state transfer in Sec. 4.4.3. The working principle of both strategies is to combine enantiomer-selectivity (due to the sign difference in one of the dipole moments) with an energetic separation of population residing initially in degenerate states.

In Sec. 4.4.1 and 4.4.2, the pulses drive transitions within the $E_0^0/E_0^1/E_1^1$ rotational submanifold, cf. Fig. 4.3, for the example of propanediol molecules. Even in this comparatively small manifold, the pulse sequence for enantiomer-selective population transfer consists of 12 pulses sampled from five different fields, i.e., five different combinations of polarization directions and frequencies. In order to obtain a simpler sequence, we forego full evolution operator-controllability in Sec. 4.4.3 and use a sequence of three pulses which partitions the rotational submanifold into isolated subsystems and drives simultaneously several three-wave mixing cycles. For this strategy to succeed, the initial rotational submanifold needs to have the smallest degeneracy factor $g_j = 2j+1$. We therefore consider transitions within the $E_{-1}^1, E_{-1}^2, E_0^2$ rotational submanifold in Sec. 4.4.3, this time using carvone molecules as an example. In the following Sections we use the quantum mechanical notation to denote the eigenstates of the rotational Hamiltonian: $\Psi_{\tau,m}^j = |j,\tau,m\rangle$.

4.4.1 Orientation-selective excitation exploiting complete controllability

The simplest rotational subsystem that allows for enantiomer-selective population transfer using three-wave mixing spectroscopy consists of the rotational states $|j,\tau,m\rangle = |0,0,0\rangle$, $|1,0,m\rangle$, and $|1,1,m\rangle$ with $m = -1,0,1$, and rotational energies $E_\tau^j = E_0^0$, E_0^1, and E_1^1, cf. Fig. 4.3. In the following, an x-,y- or z-polarization field denotes, resp., the control field $B_1 =: B_x$, $B_2 =: B_y$ or $B_3 =: B_z$. An asymmetric top molecule is completely controllable with four fields, as we have shown in Sec. 4.2 (Proposition 4.2.1 (i)). In the Example 4, we proved it for the investigated rotational system using two fields with frequency $\omega_1 = (E_0^1 - E_0^0)$ and x-, respectively z-polarization, and two fields with frequency $\omega_2 = (E_1^1 - E_0^1)$ and y-, respectively z-polarization. The transitions induced by these fields are indicated by orange and pink lines in Fig. 4.3(a); they form closed loops connecting the four states $|0,0,0\rangle$, $|1,0,1\rangle$, $|1,1,1\rangle$, and $|1,0,0\rangle$. Complete controllability implies that population in any initial state within the rotational manifold can be driven into any other initial state within that manifold (with both enantiomers undergoing the same dynamics). This means in particular that population in degenerate states, for example $|1,0,\pm1\rangle$, can be driven into states with different energy. Such an energetic separation can serve as precursor for complete enantiomer-selective excitation, as we show below. It also has further applications and could, for example, be used towards purifying an incoherent ensemble with electric fields only or distilling a specific molecular orientation.

We consider the following control problem: Given that the initial state is an incoherent ensemble of the two degenerate $|1,0,m=\pm1\rangle$ states, that as a density matrix is expressed as

$$\rho(0) = \frac{1}{2}|1,0,-1\rangle\langle 1,0,-1| + \frac{1}{2}|1,0,1\rangle\langle 1,0,1|, \tag{4.4.1}$$

find a pulse sequence that drives the population with $m = +1$ into a final state with different rotational energy than the $m = -1$ component. As an example, we have chosen $|0,0,0\rangle$ and $1/\sqrt{2}(|1,1,-1\rangle + |1,1,1\rangle)$ as target states.

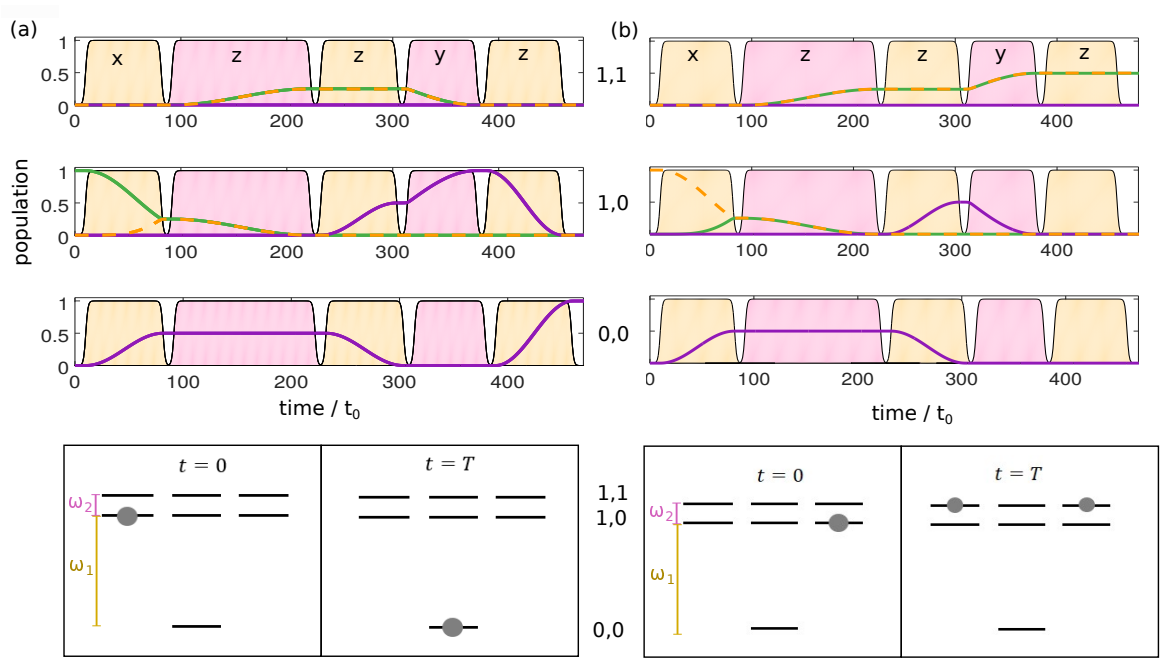


Figure 4.4: Control of the rotational dynamics for propanediol molecules to energetically separate the degenerate initial states $|1,0,-1\rangle$ (a) and$|1,0,1\rangle$ (b). Both enantiomers undergo the same dynamics. Top: Population of the rotational states $|0,0,0\rangle$ (lowest panels), $|1,0,m\rangle$ (middle panels), and $|1,1,m\rangle$ (upper panels). The population dynamics of the degenerate states are depicted by green ($m=-1$), purple ($m=0$), and orange ($m=1$) lines. The envelope of the pulses is indicated by the orange ($\omega=\omega_1$) and pink ($\omega=\omega_2$) shapes, and the polarization of the corresponding fields by x, y, and z. Time is given in units of $t_0 = 1/B$. Bottom: Sketch of the initial ($t=0$) and final ($t=T$) states, marked by gray dots.

The initial and desired final states are sketched as gray dots in the bottom panels of Fig. 4.4, the upper panel of which shows the pulse sequence that drives the corresponding rotational dynamics. In detail, starting from the initial states $|1,0,-1\rangle$ (see Fig. 4.4(a)) and $|1,0,1\rangle$ (see Fig. 4.4(b)), the state $|1,0,0\rangle$ (purple line in the middle panel) can be reached by two different excitation pathways: *via* the states $|1,1,\pm1\rangle$ and *via* $|0,0,0\rangle$. The 1st, 2nd, and 4th pulse transfer 50% of the population to state $|1,0,0\rangle$ *via* the first pathway, while pulses 1 and 3 transfer the other half of the initial population along the second pathway. Interference between the two pathways in $|1,0,0\rangle$ is constructive for the initial state $|1,0,-1\rangle$ and destructive for the initial state $|1,0,1\rangle$.

Therefore, the initial state $|1,0,-1\rangle$ is transferred to $|1,0,0\rangle$ while the initial state $|1,0,1\rangle$ is transferred to $1/\sqrt{2}(|1,1,-1\rangle + |1,1,1\rangle)$ at the end of pulse 4. Finally, the 5th pulse transfers the population from $|1,0,0\rangle$ to the desired final state $|0,0,0\rangle$ in Fig. 4.4(a) while not affecting the population in $|1,1,\pm1\rangle$ Fig. 4.4(b). The two initially degenerate states thus become energetically separated using four fields, with two different frequencies and two polarization components.

4.4.2 Enantiomer-selective control exploiting complete controllability

For enantiomer-selective control, an additional field with frequency $\omega_3 = \omega_1 + \omega_2$ is required to allow for three-wave mixing. In our example, we choose x-polarization for ω_3 such that we have three mutually orthogonal fields with $\mathcal{E}_{\omega_1}(B_z)$ (central orange line in Fig. 4.3 (b)), $\mathcal{E}_{\omega_2}(B_y)$ (pink lines), and $\mathcal{E}_{\omega_3}(B_x)$ (turquoise lines). If the initial state is the ground rotational state, three-wave mixing results in complete separation of the enantiomers into energetically separated levels [82]. This requires, however, preparation of the molecules close to zero temperature. For typical experimental conditions, the initial state has to be chosen with $j > 0$ [53, 96] and thus contains degenerate rotational states. Then, three fields are not sufficient to obtain complete enantiomer-selectivity. We illustrate this in Fig. 4.5, considering the initial ensemble with

$$\rho^{(\pm)}(0) = \frac{1}{2}\left(|1,0,-1\rangle\langle 1,0,-1| + |1,0,1\rangle\langle 1,0,1|\right). \tag{4.4.2}$$

The initial states $|1,0,-1\rangle$ and $|1,0,1\rangle$ are depicted in Fig. 4.5(e) and (f) with the gray circles indicating that both enantiomers occupy the same states. The control aim is to drive the two enantiomers into rotational states

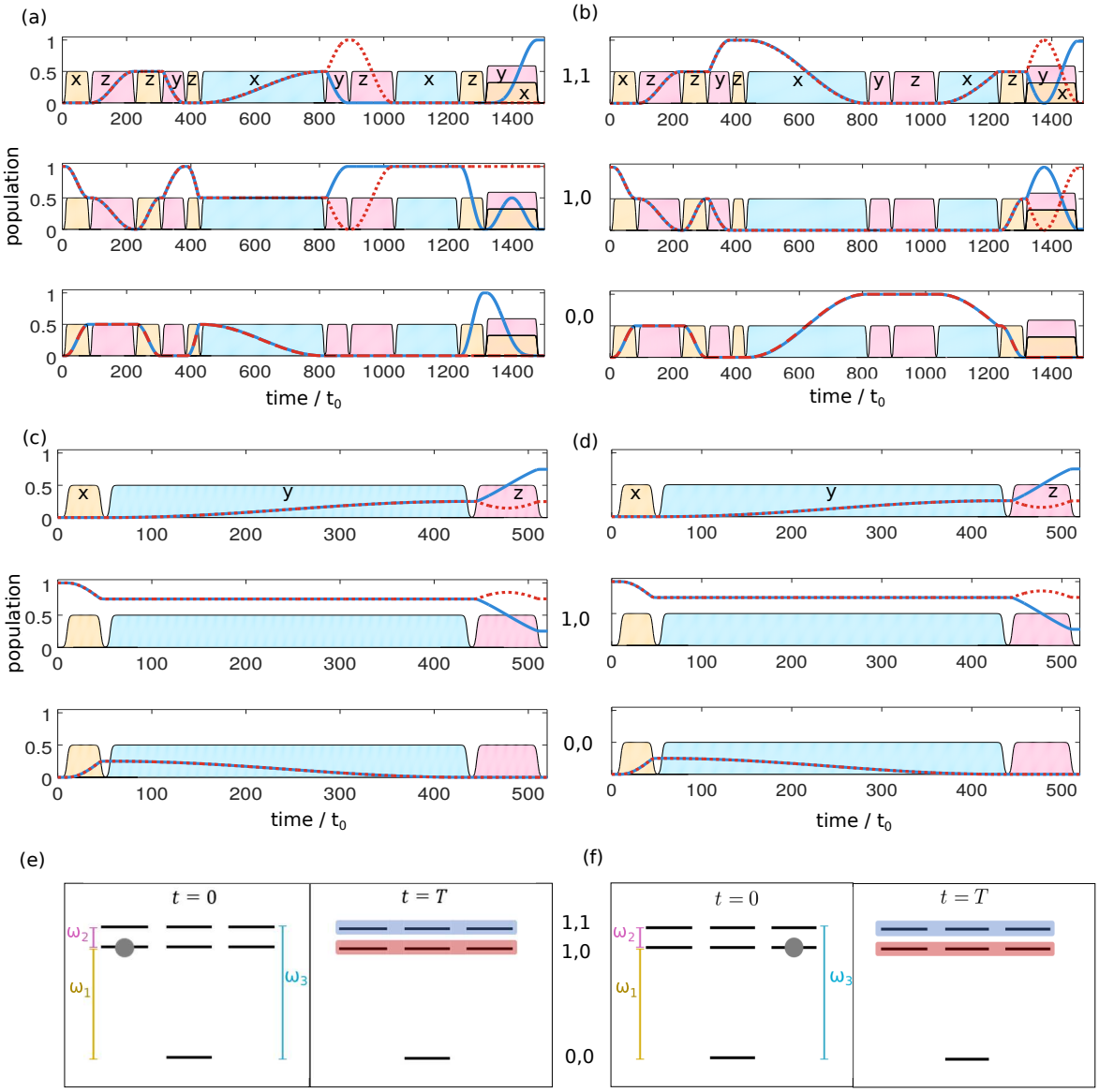


Figure 4.5: Full control of enantiomer-selective state transfer despite m-degeneracy using five different fields in panels (a,b) with the two enantiomers denoted by solid blue and dashed red lines. The complete pulse sequence reads: (1) $\mathcal{E}_{\omega_1}(B_x)$; (2) $\mathcal{E}_{\omega_2}(B_z)$; (3) $\mathcal{E}_{\omega_1}(B_z)$; (4) $\mathcal{E}_{\omega_2}(B_y)$; (5) $\mathcal{E}_{\omega_1}(B_z)$; (6) $\mathcal{E}_{\omega_3}(B_x)$; (7) $\mathcal{E}_{\omega_2}(B_y)$; (8) $\mathcal{E}_{\omega_2}(B_z)$; (9) $\mathcal{E}_{\omega_3}(B_x)$; (10) $\mathcal{E}_{\omega_1}(B_z)$; (11) $\mathcal{E}_{\omega_2}(B_y)$; (12) $\mathcal{E}_{\omega_1}(B_x)$. Panels (c,d) show for comparison enantiomer-selective state transfer in standard three-wave mixing cycles that is incomplete due to the m-degeneracy (using $\mathcal{E}_{\omega_1}(B_x)$; $\mathcal{E}_{\omega_2}(B_z)$; $\mathcal{E}_{\omega_3}(B_y)$). Panels (a,c) depict the rotational dynamics for the initial state $|1,0,-1\rangle$ and (b), (d) those for the initial state $|1,0,1\rangle$ with the sup-panels showing the accumulated population of the rotational states $|0,0,0\rangle$ (lowest panels), $|1,0,M\rangle$ (middle panels), and $|1,1,M\rangle$ (top panels). The pulse envelopes are indicated by orange ($\omega = \omega_1$), pink ($\omega = \omega_2$), and turquoise ($\omega = \omega_3$) shapes. The height of these shapes corresponds to the maximal electric field strength and the polarization is denoted by x, y and z. Time is given in units of $t_0 = 1/B$. Panels (e) and (f) illustrate the initial ($t = 0$) and final ($t = T$) populations with gray indicating both enantiomers in the same state and blue and red representing the two separated enantiomers.

with different energies, cf. the red and blue shades in Fig. 4.5(e) and (f). The combination of fields $\mathcal{E}_{\omega_1}(B_z)$, $\mathcal{E}_{\omega_2}(B_y)$, and $\mathcal{E}_{\omega_3}(B_x)$, indicated in Fig. 4.3(b), which works if the initial state is $|0,0,0\rangle$, obviously fails for the initial density matrix (4.4.2) since it does not create three-wave mixing cycles for the $|1,0,m\rangle$ states. This can be remedied by choosing instead a sequence containing the fields $\mathcal{E}_{\omega_1}(B_x)$, $\mathcal{E}_{\omega_2}(B_z)$, and $\mathcal{E}_{\omega_3}(B_y)$. However, due to insufficient controllability with three fields in the presence of m-degeneracy, the population transfer is only partially enantiomer-selective, cf. the corresponding rotational dynamics in Fig. 4.5(c) and (d), where the solid blue and dashed red lines present the two enantiomers. For complete enantio-selective excitation, all five fields depicted in Fig. 4.3(b) are required, as is illustrated by Fig. 4.5(a) and (b). We use the five fields that yield simultaneous control, as proved in the Example 4.

The pulse sequence, which leads to complete separation of the enantiomers into energetically separated levels, consists of 12 pulses: the first four pulses are the same as the pulse sequence shown in Fig. 4.4. Transferring the initial states $|1,0,-1\rangle$ and $|1,0,1\rangle$ into $|1,0,0\rangle$, respectively $1/\sqrt{2}(|1,1,-1\rangle + |1,1,1\rangle)$, they lead to an energetic separation of the two initially degenerate m-states, but are not yet enantiomer-selective. Two more pulse sequences realize enantiomer-selective three-wave mixing cycles for the two initial states separately. First, enantiomer-selective transfer for the initial state $|1,0,-1\rangle$ is obtained by three-wave mixing with the fields $\mathcal{E}_{\omega_1}(B_z)$, $\mathcal{E}_{\omega_3}(B_x)$, and $\mathcal{E}_{\omega_2}(B_y)$ (pulses 5, 6, and 7). Analogously, pulses 9, 10, and 11 form a three-wave mixing cycle for the initial state $|1,0,1\rangle$. After pulse 11 the enantiomers of both initial states are separated in energy. The two cycles for the different m-states are synchronized by applying pulse 12 (at the same time as pulse 11), such that all population of one enantiomer is collected in the highest rotational state (blue lines) while all population of the other enantiomer is excited to the intermediate level (dashed red lines). Figure 4.5(a) and (b) thus confirms complete enantio-selective state transfer in a racemic mixture of initially degenerate m-states for a set of microwave fields for which simultaneous controllability is proved in Example 4.

The Lie algebraic analysis of simultaneous controllability of Sec. 4.2 yields the control Hamiltonians which are required for enantiomer-selective population transfer, but does not make any predictions about the temporal shape of the electric field. In particular, it does not predict the number of individual pulses. The control sequence shown in Fig. 4.5(a) and (b) contains 12 individual pulses applied either sequentially or overlapping. Here, complete enantio-selectivity is obtained by constructing an individual three-wave mixing cycle for every initial state. This implies that population initially in the degenerate m-states first has to be separated in energy so that they can be addressed individually. If the degeneracies become larger (for higher j), the pulse sequences become more and more complicated, because more degenerate states have to be separated in energy and three-wave mixing cycles for each of these states have to be constructed. Such pulse sequences may experimentally not be feasible or at least technically very challenging to implement. This is true in particular for rotational subsystems with higher rotational quantum numbers as in earlier microwave three-wave mixing experiments [96], where cycles with $j = 1/2/2$ or $j = 2/3/3$ have been addressed because of their better frequency match and higher Boltzmann factors. For these cases, circularly polarized fields B_+ and B_- (cf. (4.3.1) and (4.3.2)) resulting in simpler pulse sequences may be better suited. This will be discussed in the next section.

4.4.3 Complete enantiomer-selective population transfer using synchronized three-wave mixing

Another route to enantiomer-selective state transfer is provided by partitioning the relevant rotational manifold into subsystems that form individual three-wave mixing cycles, as discussed in Sec. 4.3. Provided that the initial state contains population only within the various three-level cycles, the lack of complete controllability does not preclude enantiomer-selective population transfer: one needs to consider rotational systems $|j,\tau,m\rangle$, $|j+1,\tau',m\rangle$, $|j+1,\tau'',m\rangle$ and choose the transitions realizing the three-wave mixing such that the initial state resides in the states with lower j. An advantage of this approach is that three different fields, if properly chosen, are sufficient to simultaneously control the reachable states (as proved in Proposition 4.3.1).

As an experimentally relevant example, we consider the rotational subsystem made up of $|1,-1,m\rangle$, $|2,-1,m\rangle$, and $|2,0,m\rangle$ and construct a pulse sequence that achieves complete enantiomer-selective population transfer despite m-degeneracy. This is proved to be possible in the Example 5. We assume that, initially, only the lowest rotational levels, those with $j = 1$, are populated. From a physical point of view, this initial condition can be realized if all or at least the upper two rotational levels are chosen in an excited vibrational level where the thermal population of the higher rotational levels is negligible [82]. The initial state is then given in terms of the density matrix

$$\rho^{(\pm)}(0) = \frac{1}{3}\big(|1,-1,-1\rangle\langle 1,-1,-1| + |1,-1,0\rangle\langle 1,-1,0| + |1,-1,1\rangle\langle 1,-1,1|\big)\,. \tag{4.4.3}$$

Applying a standard three-wave mixing pulse sequence with linearly polarized fields with orthogonal polarization directions results at most in about 80% enantio-selectivity (data not shown). In contrast, the circularly polarized

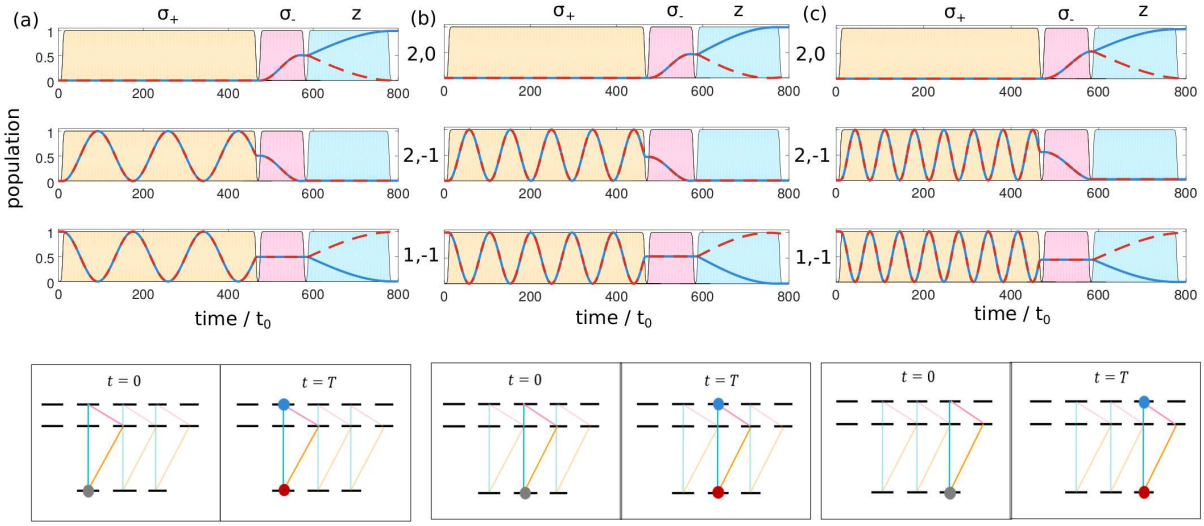


Figure 4.6: Full control of enantiomer-selective state transfer, based on synchronized three-wave mixing with $\mathcal{E}_{\omega_1}(B_+)$, $\mathcal{E}_{\omega_2}(B_-)$, $\mathcal{E}_{\omega_3}(B_z)$. Panels (a), (b), and (c) depict the rotational dynamics for the initial states with $m = -1$, $m = 0$, and $m = 1$, respectively, with the overall population in $|1, -1, m\rangle$, $|2, -1, m\rangle$, and $|2, 0, m\rangle$ shown in the upper, middle, and lower sub-panels. The two enantiomers are denoted by solid blue and dashed red lines. The envelope of the pulses is indicated by the orange ($\omega = \omega_1$), pink ($\omega = \omega_2$), and turquoise ($\omega = \omega_3$) shapes. Time is given in units of $t_0 = 1/B$. Bottom: Sketch of the initial ($t = 0$) and final ($t = T$) states with gray circles indicating both enantiomers in the same state, blue and red circles representing the two (separated) enantiomers. The transitions induced by the three fields are indicated by the orange, pink, and turquoise lines with the transition affecting the respective initial state highlighted. For carvone, the frequencies are $\omega_1 = 3976.1$ MHz, $\omega_2 = 229.9$ MHz and $\omega_3 = 4206,0$ MHz.

fields discussed in Sec. 4.3 allow for a complete separation of the enantiomers. This can be seen in Fig. 4.6. The three subsystems, which are isolated by applying left- and right-circularly polarized light are indicated in the bottom panels of Fig. 4.6: The field with +-polarization (orange line) induces transitions between $|1, -1, m\rangle$ and $|2, -1, m+1\rangle$, while the −-polarized field (pink line) drives transitions between $|2, -1, m\rangle$ and $|2, 0, m-1\rangle$, and the linearly z-polarized field (turquoise line) closes the cycles. For all the initially populated, degenerate m-states, the population is thus trapped into a three-level subsystem and cannot spread over the whole manifold, as it would happen when using three linearly polarized fields with orthogonal polarization directions.

The corresponding rotational dynamics is depicted in the upper panels of Fig. 4.6(a)–(c). The pulse sequence that leads to complete enantio-selective excitation is essentially a three-wave mixing cycle: The first pulse creates a 50/50 coherence between the ground and first excited rotational level of each three-level system. The second pulse transfers the population from the intermediate state to the highest state and the third, z-polarized pulse induces the enantiomer-specific interference between the ground state and highest excited state. There is, however, an important difference to the standard three-wave mixing cycles used so far — the pulses are chosen such that they synchronize the three subsystems, allowing to reach a 50/50 coherence between the ground and first excited state for each of the subsystems. As can be seen in Fig. 4.6, the Rabi frequencies of each subsystem are different, since they correspond to different m-transitions. This exactly corresponds to the fact that the Clebsch-Gordon coefficients (which are the coefficients $c_{j,k,m}$ in (3.4.1)) are different, and hence the matrix V in (4.3.6) is invertible. A 50/50 coherence for all three subsystems occurs after three Rabi oscillations for the subsystem depicted in (a), 5 oscillations for (b), and 7 oscillations for (c). The synchronized three-level cycles then lead to complete separation of the enantiomers into energetically separated levels, by applying a sequence of only three pulses, cf. Fig. 4.6. When choosing the pulse amplitude and duration, it is important to realize that the subsystems undergo either all an even or all an odd number of Rabi oscillations, so that they accumulate the same phase. Otherwise, the interference effects induced by the third pulse will cancel each other.

In the present example, synchronized three-wave mixing with circularly polarized pulses improves the enantio-selectivity from 80% for standard three-wave mixing with linearly polarized pulses to almost 100%, assuming no thermal population in the two upper levels.

Our excitation scheme can easily be extended to rotational manifolds with larger j, since the manifolds can always be broken up into isolated subsystems where three pulses are sufficient to energetically separate the enantiomers.

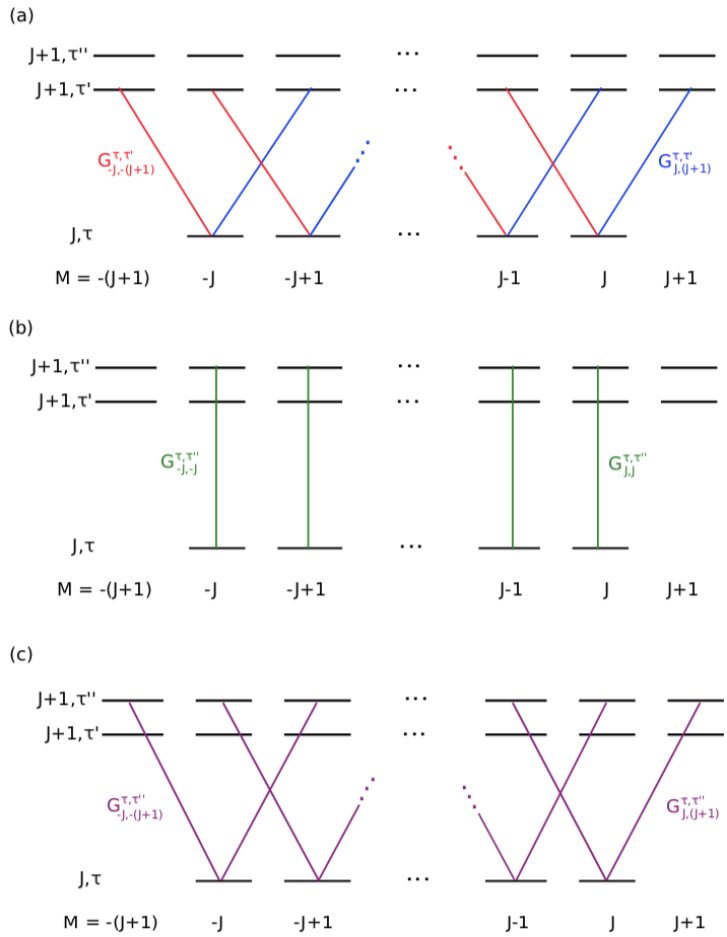


Figure 4.7: Four (five) fields with frequencies ω_1, ω_2, and ω_3 are sufficient to ensure (enantiomer-selective) evolution-operator-controllability for any rotational subsystem consisting of the levels with quantum numbers (j, τ), $(j+1, \tau')$, and $(j+1, \tau'')$. (a) The red and blue lines indicate the transitions induced by the interaction Hamiltonians $\mathcal{E}_{\omega_1}(\mathrm{i}B_1)$ and $\mathcal{E}_{\omega_1}(\mathrm{i}B_2)$. The blue (red) lines alone represent the interaction Hamiltonians $\mathcal{E}_{\omega_1}(\mathrm{i}B_+)$ ($\mathcal{E}_{\omega_1}(\mathrm{i}B_-)$). The green and purple lines present $\mathcal{E}_{\omega_3}(\mathrm{i}B_3)$ (b) and $\mathcal{E}_{\omega_3}(\mathrm{i}B_2)$ (c). Each of these lines represents one of the matrices $G^{\tau,\tau'}_{m,m'}$.

The number of pulses and fields is thus independent of the number of degenerate states in the initial ensemble. The duration of the first pulse may have to be longer (or its amplitude larger), since, for larger j, this pulse needs to synchronize Rabi oscillations of more three-level cycles. However, this does not pose a fundamental difficulty.

4.5 Appendix: proof of Proposition 4.2.1

We write the control problem w.r.t. the asymmetric-top representation $\Psi^j_{\tau,m}$. Thanks to the fact that the coefficients $c^j_k(\tau)$ in (3.3.3) do not depend on m, when one writes the control operators B_l w.r.t. the $\Psi^j_{\tau,m}$, the summation over these coefficients only results in a common prefactor, which is not relevant for the generated Lie algebra, as it can be factored out. Note further that the m-dependence of the control operators is solely determined by the m-dependence in (3.4.1), (3.4.10), (3.4.11). This means that we do not need to compute explicitly the eigenvalues E^j_τ, nor to express the eigenfunctions $\Psi^j_{\tau,m}$ of H as linear combination of symmetric-top eigenfunctions $S^j_{k,m,p}$ (as we actually did in the examples 4 and 5) in order to express the control problem in the asymmetric-top representation. This fact is quite remarkable and relies on the algebraic structure of angular momentum theory. Let us explicitly show this for the representation of $\mathrm{i}B_3$ (decoupled at frequency ω_3) in the $\Psi^j_{\tau,m}$ basis (the other operators are computed analogously): we have

$$\mathcal{E}_{\omega_3}(\mathrm{i}B_3) = \sum_{m=-j,\dots,j} \langle \Psi^j_{\tau,m}, \mathrm{i}B_3 \Psi^{j+1}_{\tau'',m} \rangle \, |\Psi^j_{\tau,m}\rangle\langle \Psi^{j+1}_{\tau'',m}| + \langle \Psi^{j+1}_{\tau'',m}, \mathrm{i}B_3 \Psi^j_{\tau,m} \rangle \, |\Psi^{j+1}_{\tau'',m}\rangle\langle \Psi^j_{\tau,m}|,$$

where the operator $|\psi\rangle\langle\phi|$ is the rank-one projector defined by $|\psi\rangle\langle\phi|\varphi := \langle\varphi,\psi\rangle\phi$, for all $\psi,\phi,\varphi \in L^2(\mathrm{SO}(3))$. Computing the matrix elements

$$\begin{aligned}
\langle \Psi^j_{\tau,m}, \mathrm{i}B_3 \Psi^{j+1}_{\tau'',m}\rangle &= \left\langle \sum_{-j\le k\le j} c^{j+1}_k(\tau) D^j_{k,m}, \mathrm{i}B_3 \sum_{-j-1\le k\le j+1} c^j_k(\tau'') D^{j+1}_{k,m}\right\rangle \\
&= [(j+1)^2 - m^2]^{1/2} \\
&\times \sum_{-j\le k\le j} \Big(-\mathrm{i}c^j_k(\tau)c^{j+1}_{k-1}(\tau'')d_{j,-k}(\delta_2 - \mathrm{i}\delta_1) - \mathrm{i}c^j_k(\tau)c^{j+1}_k(\tau'')b_{j,k}\delta_3 + \mathrm{i}c^j_k(\tau)c^{j+1}_{k+1}(\tau'')d_{j,k}(\delta_2 + \mathrm{i}\delta_1)\Big) \\
&:= [(j+1)^2 - m^2]^{1/2} C^j(\tau,\tau''),
\end{aligned}$$

where we have used (3.4.1) and (3.4.11), and defined

$$b_{j,k} := \frac{[(j+1)^2 - k^2]^{1/2}}{(j+1)[(2j+1)(2j+3)]^{1/2}}, \quad d_{j,k} := \frac{[(j+k+1)(j+k+2)]^{1/2}}{2(j+1)[(2j+1)(2j+3)]^{1/2}},$$

we see that $C^j(\tau,\tau'')$ is a common factor that does not depend on m. Moreover, plugging the information that k is even or odd only (cf. (3.3.3)), in the definition of $C^j(\tau,\tau'')$, we find that either $c^{j+1}_{k-1} = c^{j+1}_{k+1} = 0$ or $c^{j+1}_k = 0$, implying that $C^j(\tau,\tau'')$ depends on δ_3 or $\delta_2 \pm \mathrm{i}\delta_1$ only. Furthermore, when $C^j(\tau,\tau'')$ depends on $\delta_2 \pm \mathrm{i}\delta_1$, using the representation (3.3.2) (where there is the additional information that $p = 0$ or 1 only), one sees that $C^j(\tau,\tau'')$ actually depends on δ_1 or δ_2 only. In this sense, we need to choose eigenstates $\Psi^j_{\tau,m}$, $\Psi^{j+1}_{\tau',m}$, and $\Psi^{j+1}_{\tau'',m}$ such that the spectral gaps $\omega_1,\omega_2,\omega_3$ couple with all dipole components, say resp. $\delta_1,\delta_2,\delta_3$ (and not only with δ_3, as it may happen), but this assumption is always true, by possibly choosing a different τ. Summarizing, we have $C^j(\tau,\tau'') = -\mathrm{i}\delta_3 \sum_{-j\le k\le j} c^j_k(\tau)c^{j+1}_k(\tau)$, and we remark that, as the dependence of the coefficients $c^j_{k,\tau}(\beta) := c^j_k(\tau)$ and $c^{j+1}_{k,\tau''}(\beta) := c^{j+1}_k(\tau'')$ is analytic in the Wang asymmetry parameter $b \in [-1,0]$ (cf. (3.3.8)), the coefficients $C^j(\tau,\tau'')$ is also analytic in b and non-zero for a.e. $b \in [-1,0]$ as long as $c^j_{k,\tau}(b=0) \neq 0$ and $c^{j+1}_{k,\tau''}(b=0) \neq 0$ and thus

$$\mathcal{E}_{\omega_3}(\mathrm{i}B_3) \propto \delta_3 \sum_{m=-j,\dots,j} \mathrm{i}[(j+1)^2 - m^2]^{1/2} |\Psi^j_{\tau,m}\rangle\langle\Psi^{j+1}_{\tau'',m}| + \mathrm{i}[(j+1)^2 - m^2]^{1/2} |\Psi^{j+1}_{\tau'',m}\rangle\langle\Psi^j_{\tau,m}|.$$

With similar arguments, we can express all the control fields as proportional to the following operators:

$$\begin{aligned}
\mathcal{E}_{\omega_1}(\mathrm{i}B_1) &= \delta_1\Big(\sqrt{(j+1)(2j+1)}(G^{\tau,\tau'}_{-j,-j-1} + G^{\tau,\tau'}_{j,j+1}) + \sqrt{j(2j+1)}(G^{\tau,\tau'}_{-j+1,-j} + G^{\tau,\tau'}_{j-1,j}) \\
&+ \dots + \sqrt{3}(G^{\tau,\tau'}_{j-1,j-2} + G^{\tau,\tau'}_{-j+1,-j+2}) + (G^{\tau,\tau'}_{j,j-1} + G^{\tau,\tau'}_{-j,-j+1})\Big),
\end{aligned} \tag{4.5.1}$$

$$\begin{aligned}
\mathcal{E}_{\omega_1}(\mathrm{i}B_2) &= \delta_1\Big(\sqrt{(j+1)(2j+1)}(-F^{\tau,\tau'}_{-j,-(j+1)} + F^{\tau,\tau'}_{j,j+1}) + \sqrt{j(2j+1)}(-F^{\tau,\tau'}_{-j+1,-j} + F^{\tau,\tau'}_{j-1,j}) \\
&+ \dots + \sqrt{3}(-F^{\tau,\tau'}_{j-1,j-2} + F^{\tau,\tau'}_{-j+1,-j+2}) + (-F^{\tau,\tau'}_{j,j-1} + F^{\tau,\tau'}_{-j,-j+1})\Big),
\end{aligned} \tag{4.5.2}$$

$$\begin{aligned}
\mathcal{E}_{\omega_3}(\mathrm{i}B_2) &= \delta_3\Big(\sqrt{(j+1)(2j+1)}(-G^{\tau,\tau''}_{-j,-(j+1)} + G^{\tau,\tau''}_{j,j+1}) + \sqrt{j(2j+1)}(-G^{\tau,\tau''}_{-j+1,-j} + G^{\tau,\tau''}_{j-1,j}) \\
&+ \dots + \sqrt{3}(-G^{\tau,\tau''}_{j-1,j-2} + G^{\tau,\tau''}_{-j+1,-j+2}) + (-G^{\tau,\tau''}_{j,j-1} + G^{\tau,\tau''}_{-j,-j+1})\Big),
\end{aligned} \tag{4.5.3}$$

$$\begin{aligned}
\mathcal{E}_{\omega_3}(\mathrm{i}B_3) &= \delta_3\Big(\sqrt{2j+1}(F^{\tau,\tau''}_{-j,-j} + F^{\tau,\tau''}_{j,j}) + \sqrt{4j}(F^{\tau,\tau''}_{-j+1,-j+1} + F^{\tau,\tau''}_{j-1,j-1}) \\
&+ \dots + (j+1)F^{\tau,\tau''}_{0,0}\Big).
\end{aligned} \tag{4.5.4}$$

Labeling the three rotational levels by τ, τ' and τ'', we denote the matrices that describe the interaction between the states $\Psi^j_{\tau,m}$ and $\Psi^{j+1}_{\tau',m'}$ as $G^{\tau,\tau'}_{m,m'}$ and $F^{\tau,\tau'}_{m,m'}$, and the interaction between the states $\Psi^j_{\tau,m}$ and $\Psi^{j+1}_{\tau'',m'}$ as $G^{\tau,\tau''}_{m,m'}$ and $F^{\tau,\tau''}_{m,m'}$. The colored lines in Fig. 4.7 indicate which of the rotational states are connected.

We denote

$$\mathrm{L} := \mathrm{Lie}\left\{\mathrm{i}H, \mathcal{E}_{\omega_1}(\mathrm{i}B_1), \mathcal{E}_{\omega_1}(\mathrm{i}B_2), \mathcal{E}_{\omega_3}(\mathrm{i}B_2), \mathcal{E}_{\omega_3}(\mathrm{i}B_3)\right\}$$

and we prove part (i) in several steps.

Step 1: Isolating the basis elements occurring in $\mathcal{E}_{\omega_1}(\mathrm{i}B_1)$ and $\mathcal{E}_{\omega_1}(\mathrm{i}B_2)$

Recalling the action of the operator W_{i} (cf. (3.4.3)), we consider

$$\begin{aligned}\mathcal{E}_{\omega_1}(\mathrm{i}B_+) &:= \frac{1}{2}\left(\mathcal{E}_{\omega_1}(\mathrm{i}B_1) + W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_2)\right)\\ &= \delta_1\left(\sqrt{(j+1)(2j+1)}G^{\tau,\tau'}_{j,j+1} + \sqrt{j(2j+1)}G^{\tau,\tau'}_{j-1,j} + \ldots + \sqrt{3}G^{\tau,\tau'}_{-j+1,-j+2} + G^{\tau,\tau'}_{-j,-j+1}\right)\end{aligned} \tag{4.5.5}$$

and

$$\begin{aligned}\mathcal{E}_{\omega_1}(\mathrm{i}B_-) &:= \frac{1}{2}\left(\mathcal{E}_{\omega_1}(\mathrm{i}B_1) - W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_2)\right)\\ &= \delta_1\left(\sqrt{(j+1)(2j+1)}G^{\tau,\tau'}_{-j,-(j+1)} + \sqrt{j(2j+1)}G^{\tau,\tau'}_{-j+1,-j} + \ldots + \sqrt{3}G^{\tau,\tau'}_{j-1,j-2} + G^{\tau,\tau'}_{j,j-1}\right),\end{aligned} \tag{4.5.6}$$

Operators in Eqs. (4.5.5) and (4.5.6) contain only those matrices which correspond to the blue and red lines in Fig. 4.7 (a). Using the abbreviations $\mathrm{ad}_A^{n+1}B = [A, \mathrm{ad}_A^n B]$ and $\mathrm{ad}_A^0 B = B$, we find

$$\mathrm{ad}^{2s}_{W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)}\mathcal{E}_{\omega_1}(\mathrm{i}B_+) \propto \left(\sqrt{(j+1)(2j+1)}^{2s+1}G^{\tau,\tau'}_{j,j+1} + \sqrt{j(2j+1)}^{2s+1}G^{\tau,\tau'}_{j-1,j} + \ldots + \sqrt{3}^{2s+1}G^{\tau,\tau'}_{-j+1,-j+2} + G^{\tau,\tau'}_{-j,-j+1}\right)$$

for $s = 0, \ldots, 2j$. We can thus write

$$\begin{pmatrix}\mathrm{ad}^0_{W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)\\ \mathrm{ad}^2_{W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)\\ \vdots\\ \mathrm{ad}^{4j-2}_{W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)\\ \mathrm{ad}^{4j}_{W_{\mathrm{i}}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)}\mathcal{E}_{\omega_1}(\mathrm{i}B_+)\end{pmatrix} = V\begin{pmatrix}G^{\tau,\tau'}_{j,j+1}\\ G^{\tau,\tau'}_{j-1,j}\\ \vdots\\ G^{\tau,\tau'}_{-j+1,-j+2}\\ G^{\tau,\tau'}_{-j,-j+1}\end{pmatrix} \tag{4.5.7}$$

with

$$V = \begin{pmatrix}\sqrt{(j+1)(2j+1)} & \sqrt{j(2j+1)} & \cdots & \sqrt{3} & 1\\ \sqrt{(j+1)(2j+1)}^3 & \sqrt{j(2j+1)}^3 & \cdots & \sqrt{3}^3 & 1\\ \sqrt{(j+1)(2j+1)}^5 & \sqrt{j(2j+1)}^5 & & \sqrt{3}^5 & 1\\ \vdots & & & & \\ \sqrt{(j+1)(2j+1)}^{4j-1} & \sqrt{j(2j+1)}^{4j-1} & & \sqrt{3}^{4j-1} & 1\\ \sqrt{(j+1)(2j+1)}^{4j+1} & \sqrt{j(2j+1)}^{4j+1} & & \sqrt{3}^{4j+1} & 1\end{pmatrix}. \tag{4.5.8}$$

Since V is a Vandermonde matrix, its determinant is given by the product of the sum and the difference of every pair of the coefficients in the first row. Noticing that those coefficients form a positive, strictly increasing sequence, we see that they are all different. Thus V is invertible, and we find that

$$G^{\tau,\tau'}_{j,j+1}, G^{\tau,\tau'}_{j-1,j}, \ldots, G^{\tau,\tau'}_{-j+1,-j+2}, G^{\tau,\tau'}_{-j,-j+1} \in \mathrm{L}, \tag{4.5.9}$$

Replacing $\mathcal{E}_{\omega_1}(\mathrm{i}B_+)$ by $\mathcal{E}_{\omega_1}(\mathrm{i}B_-)$ in Eq. (4.5.7), we find analogously that

$$G^{\tau,\tau'}_{-j,-(j+1)}, G^{\tau,\tau'}_{-j+1,-j}, \ldots, G^{\tau,\tau'}_{j-1,j-2}, G^{\tau,\tau'}_{j,j-1} \in \mathrm{L}. \tag{4.5.10}$$

We have thus shown that each of the basis elements indicated by the blue and red lines in Fig. 4.7 is an element of L.

Step 2: Isolating the basis elements occurring in $\mathcal{E}_{\omega_3}(\mathrm{i}B_3)$

We now reproduce the previous argument for the operator $\mathcal{E}_{\omega_3}(\mathrm{i}B_3)$. Replacing $\mathcal{E}_{\omega_1}(\mathrm{i}B_+)$ by $\mathcal{E}_{\omega_3}(\mathrm{i}B_3)$ in Eq. (4.5.7), and noticing that in this case the sequence of coefficients in the first row of the corresponding matrix V is positive and strictly decreasing, we find that

$$\begin{aligned}&F^{\tau,\tau''}_{-j,-j} + F^{\tau,\tau''}_{j,j}, F^{\tau,\tau''}_{-j+1,-j+1} + F^{\tau,\tau''}_{j-1,j-1},\\ &\qquad\qquad \ldots, F^{\tau,\tau''}_{0,0} \in \mathrm{L},\end{aligned} \tag{4.5.11}$$

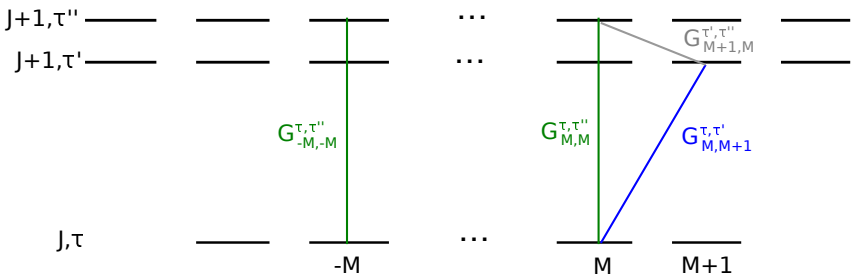


Figure 4.8: Illustration of the double commutator Eq. (4.5.14): The commutator between $G^{\tau,\tau''}_{-M,-M} + G^{\tau,\tau''}_{M,M}$ (green lines) and $G^{\tau,\tau'}_{M,M+1}$ (blue line) results in the basis element indicated by the gray line. The commutator between the basis elements represented by the gray and blue lines then results in $G^{\tau,\tau''}_{M,M}$ (right green line) alone.

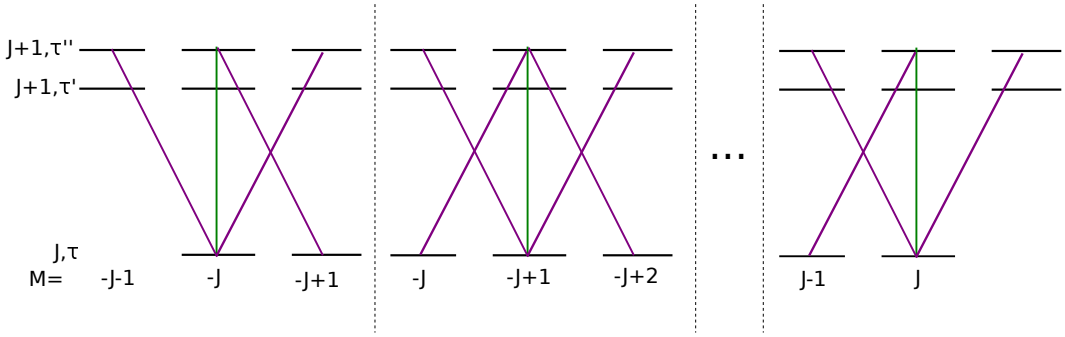


Figure 4.9: Illustration of the double commutator between $\mathcal{E}_{\omega_3}(\mathrm{i}B_2)$ and the basis elements (4.5.14), depicted as green lines: The double commutator between $\mathcal{E}_{\omega_3}(\mathrm{i}B_2)$ and $G^{\tau,\tau''}_{-j,-j}$ results in an operator, which contains the three purple lines shown in the left panel. The four purple lines in the next panel depict the result of the double commutator between $\mathcal{E}_{\omega_3}(\mathrm{i}B_2)$ and $G^{\tau,\tau''}_{-j+1,-j+1}$, and so on.

and commuting with iH also that

$$G^{\tau,\tau''}_{-j,-j} + G^{\tau,\tau''}_{j,j}, G^{\tau,\tau''}_{-j+1,-j+1} + G^{\tau,\tau''}_{j-1,j-1}, \ldots, G^{\tau,\tau''}_{0,0} \in \mathrm{L}. \tag{4.5.12}$$

To separate the sum over m from that over $-m$ in (4.5.12), we take double commutators with matrices the of Eq. (4.5.9), that is,

$$\left[\left[G^{\tau,\tau''}_{-m,-m} + G^{\tau,\tau''}_{m,m}, G^{\tau,\tau'}_{m,m+1}\right], G^{\tau,\tau'}_{m,m+1}\right] = -G^{\tau,\tau''}_{m,m}, \tag{4.5.13}$$

which is also illustrated in Fig. 4.8. Thus

$$G^{\tau,\tau''}_{-j,-j}, \ldots, G^{\tau,\tau''}_{j,j}, \in \mathrm{L}, \tag{4.5.14}$$

i.e., all basis elements indicated by the green lines in Fig. 4.7(b) are elements of L. Note, that instead of calculating the double commutators as in Eq. (4.5.13), one could also graphically deduce the basis elements: The double commutator between a linear combination of basis elements (indicated by the green lines in Fig. 4.8), and a single basis element (indicated by the blue line) contains only those basis elements of the linear combination, which have a common vertex with the single basis element. We will extensively use this technique in the following steps of the proof.

Step 3: Isolating the basis elements occurring in $\mathcal{E}_{\omega_3}(\mathrm{i}B_2)$

Next, we isolate the basis elements that occur in interaction Hamiltonian $\mathcal{E}_{\omega_3}(\mathrm{i}B_2)$, i.e., the purple lines in Fig. 4.7(c), by means of a graph proof. Taking double commutators of $\mathcal{E}_{\omega_3}(\mathrm{i}B_2)$ with the basis elements obtained in Eq. (4.5.12), we can isolate $2j+1$ groups of interactions within $\mathcal{E}_{\omega_3}(\mathrm{i}B_2)$, where each group is centered around the transition

$$(j, \tau, m) \leftrightarrow (j+1, \tau'', m), \quad m = -j, \ldots, j.$$

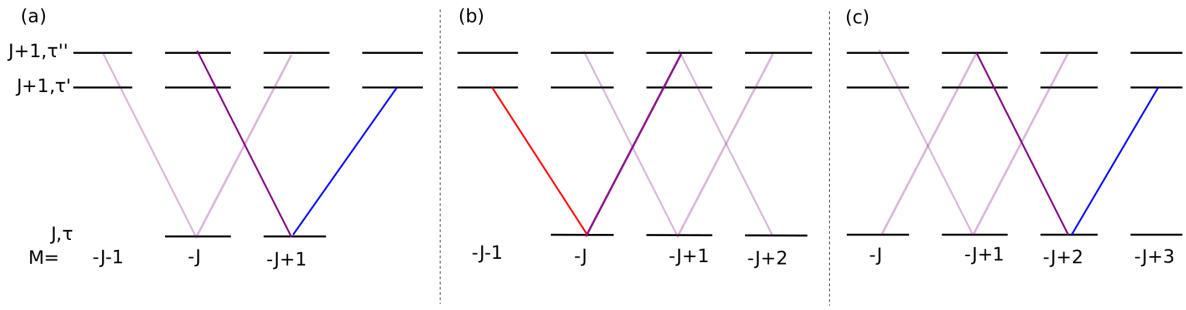


Figure 4.10: A linear combination of the basis elements depicted by the (light and dark) purple lines is an operator $\in$ L. The basis elements depicted by the dark purple lines in (a), (b), and (c) can be isolated by calculating the double commutator with the basis element depicted by the blue (a, c) and red (b) lines.

This is illustrated in Fig. (4.9). We find for all $m \neq \pm j$,

$$\begin{aligned}\left[\left[\mathcal{E}_{\omega_3}(\mathrm{i}B_2), G^{\tau,\tau''}_{m,m}\right], G^{\tau,\tau''}_{m,m}\right] = &-\sqrt{\frac{1}{2}(j+m+1)(j+m)}G^{\tau,\tau''}_{m-1,m} - \sqrt{\frac{1}{2}(j+m+2)(j+m+1)}G^{\tau,\tau''}_{m,m+1} \\ &+ \sqrt{\frac{1}{2}(j-m+1)(j-m)}G^{\tau,\tau''}_{m+1,m} + \sqrt{\frac{1}{2}(j-m+2)(j-m+1)}G^{\tau,\tau''}_{m,m-1},\end{aligned} \tag{4.5.15}$$

with the resulting four matrices indicated by the purple lines in the second panel from the left in Fig. 4.9. If $m = -j$,

$$\left[\left[\mathcal{E}_{\omega_3}(\mathrm{i}B_2), G^{\tau,\tau''}_{-j,-j}\right], G^{\tau,\tau''}_{-j,-j}\right] = \sqrt{(j+1)(2j+1)}G^{\tau,\tau''}_{-j,-j-1} + \sqrt{j(2j+1)}G^{\tau,\tau''}_{-j+1,-j} - G^{\tau,\tau''}_{-j,-j+1}, \tag{4.5.16}$$

where three generalized Pauli matrices are shown as purple lines in the left panel of Fig. 4.9. Finally, if $m = j$,

$$\left[\left[\mathcal{E}_{\omega_3}(\mathrm{i}B_2), G^{\tau,\tau''}_{j,j}\right], G^{\tau,\tau''}_{j,j}\right] = -\sqrt{(j+1)(2j+1)}G^{\tau,\tau''}_{j,j+1} - \sqrt{j(2j+1)}G^{\tau,\tau''}_{j-1,j} + G^{\tau,\tau''}_{j,j-1}, \tag{4.5.17}$$

with the three matrices shown in the right panel of Fig. 4.9.

Next, we show by induction on m that each of the purple lines in Fig. 4.9 can be isolated. As basis for the inductive argument, we first show that the transitions around $(j,\tau,-j) \leftrightarrow (j+1,\tau'',-j)$ and $(j,\tau,-j+1) \leftrightarrow (j+1,\tau'',-j+1)$, indicated by the purple lines in the left and second-left panel of Fig. 4.9, can be isolated. We then carry out the inductive step, that is, we prove that, if we can isolate each of the four basis elements around the transition $(j,\tau,m) \leftrightarrow (j+1,\tau'',m)$, then we can do the same for the basis elements around the transition $(j,\tau,m+1) \leftrightarrow (j,\tau'',m+1)$ for all $m < j-1$.

Step 4: Basis of induction

Since $G^{\tau,\tau'}_{-j+1,-j+2} \in$ L, cf. Eq. (4.5.9), we start by computing the double commutator of (4.5.16) with $G^{\tau,\tau'}_{-j+1,-j+2}$. As indicated in Fig. 4.10(a), this operation yields

$$G^{\tau,\tau''}_{-j+1,-j} \in \mathrm{L}\,. \tag{4.5.18}$$

Moreover, according to Eq. (4.5.10), we can compute the double commutators of (4.5.15) for $M = -j+1$ with $G^{\tau,\tau'}_{-j,-j-1}$. The action of this double commutator is depicted in Fig. 4.10(b) and results in

$$G^{\tau,\tau''}_{-j,-j+1} \in \mathrm{L}\,. \tag{4.5.19}$$

Taking the double commutator of (4.5.15) for $M = -j+1$ with $G^{\tau,\tau'}_{-j+2,-j+3}$ we find that

$$G^{\tau,\tau''}_{-j+2,-j+1} \in \mathrm{L}, \tag{4.5.20}$$

which is illustrated in Fig. 4.10(c). Now, subtracting a suitable linear combination of Eqs. (4.5.18), (4.5.19), and (4.5.20) from (4.5.15) for $m = -j+1$ results in

$$G^{\tau,\tau''}_{-j+1,-j+2} \in \mathrm{L}\,. \tag{4.5.21}$$

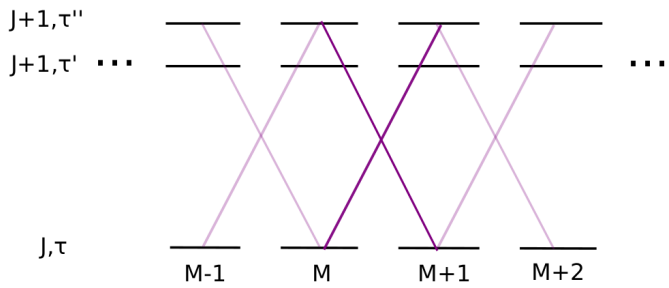


Figure 4.11: The dark purple lines are part of the set of basis elements centered around the $(j, \tau, M) \leftrightarrow (j+1, \tau'', M)$-transition as well as of the set of basis elements centered around the $(j, \tau, M+1) \leftrightarrow (j+1, \tau'', M+1)$-transition.

We have thus shown that the generalized Pauli matrices corresponding to the four purple lines in the second-left panel of Fig. 4.9 can be isolated. Subtracting a suitable linear combination of Eqs. (4.5.18) and (4.5.19) from (4.5.16), we find that

$$G^{\tau,\tau''}_{-j,-j-1} \in \mathrm{L}\,. \tag{4.5.22}$$

Thus, also the three generalized Pauli matrices indicated by the purple lines in the first panel of Fig. 4.9 can be isolated. This concludes the basis of the induction.

Step 5: Inductive step

We now prove the inductive step, that is, if we can isolate each of the basis elements presented by the four lines around the transition $(j, \tau, m) \leftrightarrow (j+1, \tau'', m)$, then we can do the same with the basis elements around the transition $(j, \tau, m+1) \leftrightarrow (j+1, \tau'', m+1)$ for all $m < j-1$. Indeed, inspection of Fig. 4.11 reveals that the transitions $(j, \tau, m) \leftrightarrow (j+1, \tau'', m+1)$ and $(j, \tau, m+1) \leftrightarrow (j+1, \tau'', m)$ are common for both sets of transitions. Thus the inductive hypothesis implies that we are left to show that the sum of basis elements

$$\begin{aligned}&\sqrt{\frac{1}{2}(j+m+3)(j+m+2)}G^{\tau,\tau''}_{m+1,m+2}\\&+\sqrt{\frac{1}{2}(j-m)(j-m-1)}G^{\tau,\tau''}_{m+2,m+1} \in \mathrm{L}\end{aligned}$$

can be separated. This can be done by taking double commutators with $G^{\tau,\tau'}_{m+2,m+3} \in \mathrm{L}$ and $G^{\tau,\tau'}_{m+1,m} \in \mathrm{L}$, as illustrated in Fig. 4.12. Thus, it remains to be shown that the basis elements depicted by purple lines in the right panel in Fig. 4.10 can be isolated. Since it has already been shown that the basis elements corresponding to the transitions $(j, \tau, j-1) \leftrightarrow (j+1, \tau'', j)$ and $(j, \tau, j) \leftrightarrow (j+1, \tau'', j-1)$ can be isolated, the remaining basis element corresponding to the transition $(j, \tau, j) \leftrightarrow (j+1, \tau'', j+1)$ can be isolated by subtracting these two elements. We have thus demonstrated that all generalized Pauli matrices appearing in $\mathcal{E}_{\omega_3}(\mathrm{i}B_2)$, i.e. all basis elements depicted by purple lines in Fig. 4.7(c) are in L. From here one easily concludes the proof of part (i).

Proof of part (ii)

After showing that each single enantiomer is controllable with a set of four fields, we now add

$$\mathcal{E}_{\omega_2}(\mathrm{i}B_l^{\chi}) = \begin{pmatrix} \mathcal{E}_{\omega_2}(\mathrm{i}B_l) & 0 \\ 0 & -\mathcal{E}_{\omega_2}(\mathrm{i}B_l) \end{pmatrix}, \tag{4.5.23}$$

where $l \in \{1, 2, 3\}$, assuming that the sign inversion is in the dipole component $\delta_2^{(+)} = -\delta_2^{(-)}$. We then apply Lemma 3.2.4: here $K = 2$ is the number of enantiomers, which we denote by $(+)$ and $(-)$, the two Hilbert spaces are $\mathbb{C}^{6j+7}$, $m = 5$ is the number of interaction Hamiltonians, and

$$\begin{aligned}
H_0^{(+)} &= H_0^{(-)} = H\,, \qquad H_1^{(+)} = H_1^{(-)} = \mathcal{E}_{\omega_1}(B_1),\\
H_2^{(+)} &= H_2^{(-)} = \mathcal{E}_{\omega_1}(B_2)\,, \quad H_3^{(+)} = H_3^{(-)} = \mathcal{E}_{\omega_3}(B_2)\,,\\
H_4^{(+)} &= H_4^{(-)} = \mathcal{E}_{\omega_3}(B_3)\,, \quad H_5^{(+)} = -H_5^{(-)} = \mathcal{E}_{\omega_2}(B_l)\,.
\end{aligned}$$

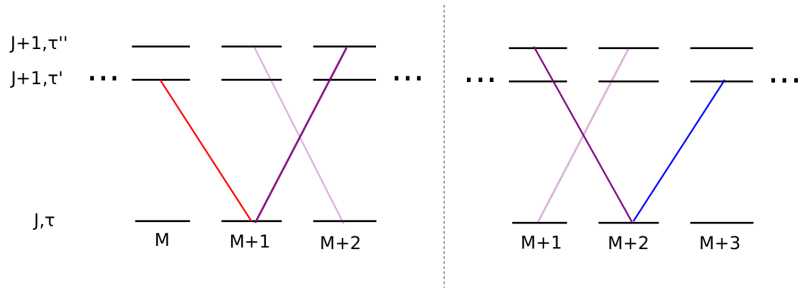


Figure 4.12: A linear superposition of the basis elements depicted by the (light and dark) purple lines is an operator $\in$ L. The basis elements depicted by the dark purple lines in both panels can be isolated by calculating the double commutator with the basis element depicted by the blue and red lines.

We will prove enantiomer-selective controllability by showing that L^{chiral} contains operators of the form $A \oplus 0$, with $A \neq 0$. This means that the control can induce a nontrivial unitary transformation acting on the first enantiomer while inducing the identity on the second one. Lemma 3.2.4 guarantees that this is enough to establish simultaneous evolution operator-controllability. Indeed, if an isomorphism f between $\mathfrak{su}(6j+7)$ and itself were to match the condition of Lemma 3.2.4 then it would necessarily verify $f(A) = 0$, which is impossible because $A \neq 0$ and any isomorphism is injective.

We denote

$$L^{\chi} := \mathrm{Lie}\left\{\mathrm{i}H^{\chi}, \mathcal{E}_{\omega_1}(\mathrm{i}B_1^{\chi}), \mathcal{E}_{\omega_1}(\mathrm{i}B_2^{\chi}), \mathcal{E}_{\omega_3}(\mathrm{i}B_2^{\chi}), \mathcal{E}_{\omega_3}(\mathrm{i}B_3^{\chi}), \mathcal{E}_{\omega_2}(B_l^{\chi})\right\},$$

and we are left to prove that L^{χ} contains operators of the form $A \oplus 0$, with $A \neq 0$. So far we proved that

$$\mathrm{Lie}\{\mathrm{i}H^{\chi}, \mathcal{E}_{\omega_1}(\mathrm{i}B_1^{\chi}), \mathcal{E}_{\omega_1}(\mathrm{i}B_2^{\chi}), \mathcal{E}_{\omega_3}(\mathrm{i}B_2^{\chi}), \mathcal{E}_{\omega_3}(\mathrm{i}B_3^{\chi})\} = \left\{\begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} \mid A \in \mathfrak{su}(6j+7)\right\},$$

and in particular that

$$\begin{pmatrix} \mathcal{E}_{\omega_2}(\mathrm{i}B_l) & 0 \\ 0 & \mathcal{E}_{\omega_2}(\mathrm{i}B_l) \end{pmatrix} \in \mathrm{L}^{\chi}.$$

Thus,

$$\begin{aligned} &\begin{pmatrix} \mathcal{E}_{\omega_2}(\mathrm{i}B_l) & 0 \\ 0 & -\mathcal{E}_{\omega_2}(\mathrm{i}B_l) \end{pmatrix} + \begin{pmatrix} \mathcal{E}_{\omega_2}(\mathrm{i}B_l) & 0 \\ 0 & \mathcal{E}_{\omega_2}(\mathrm{i}B_l) \end{pmatrix} \\ &= \begin{pmatrix} 2\mathcal{E}_{\omega_2}(\mathrm{i}B_l) & 0 \\ 0 & 0 \end{pmatrix} \in \mathrm{L}^{\chi}, \end{aligned}$$

which concludes the proof.

Chapter 5

Non-self-adjointness of the curvature Laplacian on 2D almost-Riemannian manifolds

In this Chapter we study the self-adjointness of a geometric perturbation of the Laplace-Beltrami operator on two-dimensional almost-Riemannian structures (ARSs for brevity) of step 2.

ARSs can be seen as generalizations of the Grushin plane. They are generalized Riemannian structures for which the vectors of a local orthonormal frame can become parallel. Under the 2-step assumption the singular set $\mathcal{Z}$, where the structure is not Riemannian, is a 1D embedded submanifold. While approaching the singular set, all Riemannian quantities diverge. A remarkable property of these structures is that the geodesics can cross the singular set without singularities, but the heat and the solution of the Schrödinger equation (with the Laplace-Beltrami operator Δ) cannot. This is due to the fact that (under a natural compactness hypothesis), the Laplace-Beltrami operator is essentially self-adjoint on a connected component of the manifold without the singular set (as recalled in the Introduction, Theorem 1.6.2, proved in [30]). In the literature such phenomenon is called quantum confinement.

Here, we study the self-adjointness of the curvature Laplacian, namely $-\Delta + cK$, for $c > 0$, where K is the Gaussian curvature, which originates in coordinate-free quantization procedures (as for instance in path-integral or covariant Weyl quantization). The Chapter is devoted to the proof of Theorem 5.1.1, which states that there is no quantum confinement for this type of operators.

It is organized as follows: in Section 5.1 we recall the main original results of the Chapter, already described in the Introduction. In Section 5.2 we recall some key definitions and results for 2-ARS. In Section 5.3 we introduce the basic concepts to study the self-adjointness of symmetric operators and give a proof of an original results on the quantum confinement of curvature Laplacians on α-Grushin surfaces, $\alpha \in \mathbb{R}$ (see Proposition 5.1.2). The proof of Theorem 5.1.1 spans Sections 5.4 and 5.5. A local version around a singular region is studied in Section 5.4, where a description of the closure and adjoint curvature Laplacian operators is given. The main tools needed for our proof are a characterization of the closure of inverse square potential perturbations of the Laplace-Beltrami on 2D-ARSs recently found in [20], and Sturm-Liouville theory applied here in the context of 2D operators. We then extend the results on the whole manifold in Section 5.5.

The results of this chapter are in the paper [21].

5.1 Main results

The main original result of the Chapter reads as follows:

Theorem 5.1.1. *Let M be a compact oriented 2-dimensional manifold equipped with a genuine 2-step 2-ARS. Let Ω be a connected component of $M \setminus Z$, where Z is the singular set. Let g be the Riemannian metric induced by the 2-ARS on Ω, ω be the corresponding Riemannian area, K the corresponding Gaussian curvature and $\Delta = \mathrm{div}_\omega \circ \mathrm{grad}_g$ the Laplace-Beltrami operator. Let $c \geq 0$. The curvature Laplacian $-\Delta + cK$ with domain $C_0^\infty(\Omega)$, is essentially self-adjoint on $L^2(\Omega, \omega)$ if and only if c=0. Moreover, if $c > 0$, the curvature Laplacian has infinite deficiency indices.*

To illustrate that results are in general different if one removes the 2-step assumption, we also study the self-adjoitness of the curvature Laplacian on the α-Grushin cylinder, which for $\alpha \in \mathbb{N}$ in particular is a $(\alpha + 1)$-step

ARS:

Proposition 5.1.2. *Fix $\alpha \in \mathbb{R}$. On $\mathbb{R} \times S^1$ consider the generalized Riemannian structure for which an orthonormal frame is given by*

$$X_1(x, y) = \frac{\partial}{\partial x}, \qquad X_2^{(\alpha)}(x, y) = x^\alpha \frac{\partial}{\partial y}, \qquad \text{here } x \in \mathbb{R}, \ \ y \in S^1.$$

Let $c \geq 0$. On $\mathbb{R}^+ \times S^1$ the structure is Riemannian with Riemannian area $\frac{1}{|x|^\alpha} dx\, dy$. Let $-\Delta_\alpha + cK_\alpha$ be the curvature Laplacian with domain $C_0^\infty(\mathbb{R}^+ \times S^1)$ acting on $L^2(\mathbb{R}^+ \times S^1, \frac{1}{|x|^\alpha} dx\, dy)$. Denote by

$$\alpha_{c,\pm} = \frac{(-2c + 1) \pm 2\sqrt{(c - 2 + \sqrt{3})(c - 2 - \sqrt{3})}}{4c - 1}.$$

- *If $0 \leq c < 1/4$,* $\quad -\Delta_\alpha + cK_\alpha$ *is essentially self-adjoint if and only if $\alpha \geq \alpha_{c,+}$ or $\alpha \leq \alpha_{c,-}$;*
- *if $c = 1/4$,* $\quad -\Delta_\alpha + cK_\alpha$ *is essentially self-adjoint if and only if $\alpha \geq 3$;*
- *if $1/4 < c \leq 2 - \sqrt{3}$,* $\quad -\Delta_\alpha + cK_\alpha$ *is essentially self-adjoint if and only if $\alpha_{c,-} \leq \alpha \leq \alpha_{c,+}$;*
- *if $2 - \sqrt{3} < c < 2 + \sqrt{3}$,* $\quad -\Delta_\alpha + cK_\alpha$ *is not essentially self-adjoint $\forall \alpha \in \mathbb{R}$;*
- *if $c \geq 2 + \sqrt{3}$,* $\quad -\Delta_\alpha + cK_\alpha$ *is essentially self-adjoint if and only if $\alpha_{c,-} \leq \alpha \leq \alpha_{c,+}$;*

The proof of Proposition 5.1.2, which is instructive since it is simple and presents already some crucial ingredients necessary for the general theory, is given in Section 5.3.

5.2 2D almost-Riemannian structures

Definition 5.2.1. Let M be a 2D connected smooth manifold. A 2-dimensional almost-Riemannian Structure (2-ARS) on M is a pair $(\mathbf{U}, f)$ as follows:

1. $\mathbf{U}$ is an Euclidean bundle over M of rank 2. We denote each fiber by U_q, the scalar product on U_q by $(\cdot \mid \cdot)_q$ and the norm of $u \in U_q$ as $|u| = \sqrt{(u \mid u)_q}$.
2. $f : \mathbf{U} \to TM$ is a smooth map that is a morphism of vector bundles i.e., $f(U_q) \subseteq T_qM$ and f is linear on fibers.
3. the *distribution* $\mathcal{D} = \{f(\sigma) \mid \sigma : M \to \mathbf{U} \text{ smooth section}\}$, is a family of vector fields satisfying the Hörmander condition, i.e., defining $\mathcal{D}_1 := \mathcal{D}$, $\mathcal{D}_{i+1} := \mathcal{D}_i + [\mathcal{D}_1, \mathcal{D}_i]$, for $i \geq 1$, there exists $s \in \mathbb{N}$ such that $\mathcal{D}_s(q) = T_qM$.

A particular case of 2-ARSs is given by Riemannian surfaces. In this case $\mathbf{U} = TM$ and f is the identity.
Let us recall few key definitions and facts. We refer to [4] for more details.

- Let $\mathcal{D}_p = \{X(p) \mid X \in \mathcal{D}\} = f(U_p) \subseteq T_pM$. The set of points in M such that $\dim(\mathcal{D}_p) < 2$ is called *singular set* and it is denoted by Z. Since $\mathcal{D}$ satisfies the Hörmander condition, the subspace $\mathcal{D}_p$ is nontrivial for every p and Z coincides with the set of points p where $\mathcal{D}$ is one-dimensional. The 2-ARS is said to be *genuine* if $Z \neq \emptyset$. The 2-ARS is said to be 2-*step* if for every $p \in M$ we have $\mathcal{D}_p + [\mathcal{D}, \mathcal{D}]_p = T_pM$.
- The *(almost-Riemannian) norm* of a vector $v \in \mathcal{D}_p$ is

$$\|v\| := \min\{|u|,\ u \in U_p \ \text{ s.t. } \ v = f(p, u)\}.$$

- An *admissible curve* is a Lipschitz curve $\gamma : [0, T] \to M$ such that there exists a measurable and essentially bounded function $u : [0, T] \ni t \mapsto u(t) \in U_{\gamma(t)}$, called *control function*, such that $\dot\gamma(t) = f(\gamma(t), u(t))$, for a.e. $t \in [0, T]$. Notice there may be more than one control corresponding to the same admissible curve.
- If γ is admissible then $t \to \|\dot\gamma(t)\|$ is measurable. The *(almost-Riemannian) length* of an admissible curve $\gamma : [0, T] \to M$ is

$$\ell(\gamma) := \int_0^T \|\dot\gamma(t)\| dt.$$

- The *(almost-Riemannian) distance* between two points $p_0, p_1 \in M$ is

$$d(p_0, p_1) = \inf\{\ell(\gamma) \,|\, \gamma : [0, T] \to M \text{ admissible}, \ \gamma(0) = p_0, \ \gamma(T) = p_1\}.$$

  Thanks to the bracket-generating condition, the Chow-Rashevskii theorem guarantees that (M, d) is a metric space and that the topology induced by (M, d) is equivalent to the manifold topology.

- Given a local trivialization $\Omega \times \mathbb{R}^2$ of $\mathbf{U}$, an *orthonormal frame* for the 2-ARS on Ω is the pair of vector fields $\{F_1, F_2\} := \{f \circ \sigma_1, f \circ \sigma_2\}$ where $\{\sigma_1, \sigma_2\}$ is an orthonormal frame for $(\cdot \,|\, \cdot)_q$ on $\Omega \times \mathbb{R}^2$ of $\mathbf{U}$. On a local trivialization the map f can be written as $f(p, u) = u_1 F_1(p) + u_2 F_2(p)$. When this can be done globally (i.e., when $\mathbf{U}$ is the trivial bundle) we say that the 2-ARS is *free*.

  Notice that orthonormal frames in the sense above are orthonormal frames in the Riemannian sense out of the singular set.

- Locally, for a 2-ARS, it is always possible to find a system of coordinates and an orthonormal frame that in these coordinates has the form

$$F_1(x, y) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad F_2(x, y) = \begin{pmatrix} 0 \\ \mathfrak{f}(x, y) \end{pmatrix}, \tag{5.2.1}$$

  where $\mathfrak{f} : \Omega \to \mathbb{R}$ is a smooth function. In these coordinates we have that $Z = \{(x, y) \in \Omega \mid \mathfrak{f}(x, y) = 0\}$. Using this orthonormal frame one immediately gets:

  Proposition 5.2.2. *The 2-ARS is 2-step in Ω if and only if for every $(x, y) \in \Omega$ such that $\mathfrak{f}(x, y) = 0$, we have $\partial_x \mathfrak{f}(x, y) \neq 0$.*

  Moreover, the implicit function theorem applied to the function $\mathfrak{f}$ directly implies:

  Proposition 5.2.3. *If the 2-ARS is genuine and 2-step then Z is a closed embedded one dimensional submanifold.*

  In particular if Z is compact, each connected component of Z is diffeomorphic to S^1.

- Out of the singular set Z, the structure is Riemannian and the Riemannian metric, the Riemannian area, the Riemannian curvature, and the Laplace-Beltrami operator are easily expressed in the orthonormal frame given by (5.2.1):

$$g_{(x,y)} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{\mathfrak{f}(x,y)^2} \end{pmatrix}, \tag{5.2.2}$$

$$\omega_{(x,y)} = \frac{1}{|\mathfrak{f}(x, y)|} dx\, dy, \tag{5.2.3}$$

$$K(x, y) = \frac{\mathfrak{f}(x, y)\partial_x^2 \mathfrak{f}(x, y) - 2\,(\partial_x \mathfrak{f}(x, y))^2}{\mathfrak{f}(x, y)^2}, \tag{5.2.4}$$

$$\Delta = \partial_x^2 + \mathfrak{f}^2 \partial_y^2 - \frac{\partial_x \mathfrak{f}}{\mathfrak{f}} \partial_x + \mathfrak{f}(\partial_y \mathfrak{f})\partial_y. \tag{5.2.5}$$

- To prove the main results of this paper, the following normal forms are going to be important.

  Proposition 5.2.4 ([6])**.** *Consider a 2-step 2-ARS. For every $p \in M$ there exist a neighborhood U of p, a system of coordinates in U, and an orthonormal frame $\{X_1, X_2\}$ for the ARS on U, such that $p = (0, 0)$ and $\{X_1, X_2\}$ has one of the following forms:*

  F1. $X_1(x, y) = \dfrac{\partial}{\partial x}, \qquad X_2(x, y) = e^{\phi(x,y)} \dfrac{\partial}{\partial y},$

  F2. $X_1(x, y) = \dfrac{\partial}{\partial x}, \qquad X_2(x, y) = x e^{\phi(x,y)} \dfrac{\partial}{\partial y},$

  where ϕ is a smooth function such that $\phi(0, y) = 0$.

A point $p \in M$ is said to be a *Riemannian point* if $\mathcal{D}_p$ is two-dimensional, and hence a local description around p is given by F1. A point p such that $\mathcal{D}_p$ is one-dimensional, and thus $\mathcal{D}_p + [\mathcal{D}, \mathcal{D}]_p$ is two-dimensional, is called a *Grushin point* and a local description around p is given by F2.

When M is compact orientable, each connected component of Z is diffeomorphic to S^1 and admits a tubular neighborhood diffeomorphic to $\mathbb{R} \times S^1$. In this case the normal form F2 can be extended to the whole neighborhood.

Proposition 5.2.5 ([30])**.** *Consider a* 2*-step* 2*-ARS on a compact orientable manifold. Let W be a connected component of Z. Then there exist a tubular neighborhood U of W diffeomorphic to $\mathbb{R} \times S^1$, a system of coordinates in U, and an orthonormal frame $\{X_1, X_2\}$ of the 2-ARS on U such that $W = \{(0, y),\ y \in S^1\}$ and $\{X_1, X_2\}$ has the form*

$$X_1(x, y) = \frac{\partial}{\partial x}, \qquad X_2(x, y) = x e^{\phi(x,y)} \frac{\partial}{\partial y}. \tag{5.2.6}$$

5.3 Self-adjointness of operators

Let A be a linear operator on a separable Hilbert space $\mathcal{H}$, $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. The linear subspace of $\mathcal{H}$ where the action of A is well-defined is called the domain of A, denoted by $\mathcal{D}(A)$. We shall always assume that $\mathcal{D}(A)$ is dense in $\mathcal{H}$. Following [100], we recall several definitions and properties of linear operators:

- A is said to be *symmetric* if $\langle Au, v \rangle_{\mathcal{H}} = \langle u, Av \rangle_{\mathcal{H}}$ for all $u, v \in \mathcal{D}(A)$.
- A is said to be *closed* if $\mathcal{D}(A)$ with the norm $\| \cdot \|_A := \| \cdot \|_{\mathcal{H}} + \|A \cdot \|_{\mathcal{H}}$ is complete.
- A linear operator B, $\mathcal{D}(B)$ such that $\mathcal{D}(A) \subset \mathcal{D}(B)$ and $Bu = Au$ for all $u \in \mathcal{D}(A)$ is called an *extension* of A. In this case we write $A \subset B$.
- If A is symmetric and densely defined, there exists a minimal closed symmetric extension $\overline{A}$ of A, which is said to be the *closure* of A. We describe this construction: take any sequence $(u_n)_n \subset \mathcal{D}(A)$ which converges to a limit $u \in \mathcal{H}$, and for which the sequence $(Au_n)_n$ converges to a limit $w \in \mathcal{H}$. Then, by symmetry of A, we have that

  $$\langle w, v \rangle_{\mathcal{H}} = \lim_{n\to\infty} \langle Au_n, v \rangle_{\mathcal{H}} = \lim_{n\to\infty} \langle u_n, Av \rangle_{\mathcal{H}} = \langle u, Av \rangle_{\mathcal{H}}, \quad \forall v \in \mathcal{D}(A). \tag{5.3.1}$$

  Since $\mathcal{D}(A)$ is dense in $\mathcal{H}$, w is uniquely determined by u. The closure of A is defined by setting $\overline{A}u = w$, and the domain $\mathcal{D}(\overline{A})$ is the closure of $\mathcal{D}(A)$ with respect to the norm $\| \cdot \|_A$. One can easily see that $\overline{A}$ is closed, symmetric, and any closed extension of A is an extension of $\overline{A}$ as well.
- Given a densely defined linear operator A, the domain $\mathcal{D}(A^*)$ of the adjoint operator A^* is the set of all $v \in \mathcal{H}$ such that there exists $w \in \mathcal{H}$ with $\langle Au, v \rangle_{\mathcal{H}} = \langle u, w \rangle_{\mathcal{H}}$ for all $u \in \mathcal{D}(A)$. The adjoint of A is defined by setting $A^* v = w$.
- A is said to be *self-adjoint* if $A^* = A$, that is, A is symmetric and $\mathcal{D}(A^*) = \mathcal{D}(A)$.
- A is said to be *essentially self-adjoint* if its closure is self-adjoint.
- If B is a closed symmetric extension of A, then $A \subset \overline{A} \subset B \subset A^*$.
- If a densely defined operator B is such that $\mathcal{D}(A) \subset \mathcal{D}(B)$ and there exist $a, b \geq 0$ such that

  $$\|Bu\| \leq a\|Au\| + b\|u\|, \qquad \forall u \in \mathcal{D}(A), \tag{5.3.2}$$

  then B is said to be *small with respect to* A. The infimum of the set of $a \geq 0$ such that (5.3.2) holds is called the A-bound of B. If a can be chose arbitrarily small, B is said to be *infinitesimally* small w.r.t A.

We will need the following classical result in perturbation theory:

Proposition 5.3.1 (Kato-Rellich's Theorem)**.** *Let A, B be two densely defined operators and assume that B is small with respect to A. Then $D(\overline{A}) \subset D(\overline{A + B})$. If moreover $a < 1$ in* (5.3.2)*, then $D(\overline{A}) = D(\overline{A + B})$.*

To study the self-adjointness and more in general describe the extensions of a symmetric operator A, one has the fundamental Von Neumann decomposition ([100, Chapter X])

$$\mathcal{D}(A^*) = \mathcal{D}(\overline{A}) \oplus_A \ker(A^* + \mathrm{i}) \oplus_A \ker(A^* - \mathrm{i}), \tag{5.3.3}$$

where the sum is orthogonal with respect to the scalar product $\langle \cdot, \cdot \rangle_A = \langle \cdot, \cdot \rangle_{\mathcal{H}} + \langle A^* \cdot, A^* \cdot \rangle_{\mathcal{H}}$. As a first direct consequence of (5.3.3), one has the fundamental spectral criterion for self-adjointness:

Proposition 5.3.2. *Let A, $\mathcal{D}(A)$, be a symmetric operator, densely defined on the Hilbert space $\mathcal{H}$. The following are equivalent:*

(a) A is essentially self-adjoint;

(b) $\mathrm{Ran}(A \pm \mathrm{i})$ *is dense in $\mathcal{H}$;*

(c) $\ker(A^* \pm \mathrm{i}) = \{0\}$.

- The dimensions of the vector spaces $\ker(A^* + \mathrm{i})$ and $\ker(A^* - \mathrm{i})$ are called *deficiency indices* of A.

Always using (5.3.3), one can deduce that A admits self-adjoint extensions if and only if its deficiency indices are equal ([100, Corollary to Theorem X.2]).

Another immediate consequence of (5.3.3) is the following fact concerning 1D operators: let A be a 1D Sturm-Liouville operator $-\frac{d^2}{dx^2} + V(x)$, where V is a continuous real function on $\mathbb{R}^+$, acting on $L^2(\mathbb{R}^+, dx)$ with domain $C_0^\infty(\mathbb{R}^+)$ (for a general introduction to 1D Sturm-Liouville operators, see e.g. [102, Chapter 15]). Then, since the eigenvalue equation

$$-u''(x) + V(x)u(x) = \pm \mathrm{i}\, u(x)$$

has always two linearly independent solutions, the quotient $\mathcal{D}(A^*)/\mathcal{D}(\overline{A})$ has at most dimension four. Moreover, let us recall the *limit point-limit circle* Weyl's Theorem (see, e.g, [100, Appendix to Chapter X.1]) which says that the self-adjointness of a 1D Sturm-Liouville operator can be deduced by regarding the solutions to the ODE

$$-u''(x) + V(x)u(x) = 0. \tag{5.3.4}$$

- If all solutions to (5.3.4) are square-integrable near 0 (respectively ∞), then V is said to be in the limit circle case at 0 (resp. ∞). If V is not in the limit circle case at 0 (resp. ∞), it is said to be in the limit point case at 0 (resp. ∞).

Proposition 5.3.3 (Weyl's Theorem)**.** *The operator $-\frac{d^2}{dx^2} + V(x)$ with domain $C_0^\infty(\mathbb{R}^+)$ has deficiency indices*

- $(2, 2)$ *if V is in the limit circle case at both* 0 *and* ∞*;*
- $(1, 1)$ *if V is in the limit circle case at one end point and in the limit point at the other;*
- $(0, 0)$ *if V is in the limit point case at both* 0 *and* ∞.

In particular, $-\frac{d^2}{dx^2} + V(x)$ is essentially self-adjoint on $L^2(\mathbb{R}^+, dx)$ if and only if V is in the limit point case at both 0 *and* ∞.

Some useful criteria to determine whether a potential V is in the limit point or limit circle case (it is also said to be quantum-mechanically complete or incomplete, respectively) at 0 and ∞ are the following:

Proposition 5.3.4. *Let $V \in C^1(\mathbb{R}^+)$ be real and bounded above by a constant E on $[1, \infty)$. Suppose that $\int_1^\infty \frac{1}{\sqrt{E - V(x)}} dx = \infty$ and $V'/|V|^{3/2}$ is bounded near ∞. Then V is in the limit point case at ∞.*

Proposition 5.3.5. *Let $V \in C^0(\mathbb{R}^+)$ be real and positive near* 0*. If $V(x) \geq \frac{3}{4x^2}$ near* 0 *then V is in the limit point case at* 0*. If for some $\epsilon > 0$, $V(x) \leq (\frac{3}{4} - \epsilon)\frac{1}{x^2}$ near* 0*, then V is in the limit circle case at* 0*.*

Proposition 5.3.6. *Let $V \in C^0(\mathbb{R}^+)$ be real, and suppose that it decreases as $x \downarrow 0$. Then V is in the limit circle case at* 0*.*

Weyl's Theorem and these criteria are, respectively, [100, Theorem X.7, Corollary to Theorem X.8, Theorem X.10 and Problem X.7].

Here we give the proof of Proposition 5.1.2, which makes use of the limit point-limit circle argument.

Proof. of Proposition 5.1.2 The Laplace-Beltrami operator (with domain $C_0^\infty(\mathbb{R}^+ \times S^1)$) and the curvature associated with the orthonormal frame $X_1, X_2^{(\alpha)}$ are given by

$$\Delta_\alpha = \frac{\partial^2}{\partial x^2} + x^{2\alpha}\frac{\partial^2}{\partial y^2} - \frac{\alpha}{x}\frac{\partial}{\partial x}, \quad K_\alpha = -\frac{\alpha(\alpha+1)}{x^2}.$$

We perform a unitary transformation

$$U_\alpha : L^2\Big(\mathbb{R}^+ \times S^1, \frac{1}{|x|^\alpha}dx\,dy\Big) \to L^2(\mathbb{R}^+ \times S^1, dx\,dy), \quad \psi \mapsto |x|^{-\alpha/2}\psi,$$

which gives the operator

$$L_{\alpha,c} := U_\alpha(-\Delta_\alpha + cK_\alpha)U_\alpha^{-1} = -\frac{\partial^2}{\partial x^2} - x^{2\alpha}\frac{\partial^2}{\partial y^2} + \frac{(1-4c)\alpha^2 + (2-4c)\alpha}{4x^2}.$$

Via Fourier transform with respect to the variable $y \in S^1$, one considers the direct sum operator

$$\widetilde{L}_{\alpha,c} := \oplus_{k\in\mathbb{Z}}(L_{\alpha,c})_k, \quad (L_{\alpha,c})_k := -\frac{\partial^2}{\partial x^2} + x^{2\alpha}k^2 + \frac{(1-4c)\alpha^2 + (2-4c)\alpha}{4x^2},$$

acting on the Hilbert space $\ell^2(L^2(\mathbb{R}^+))$, with domain $\mathcal{D}(\widetilde{L}_{\alpha,c}) = \{(f_k)_{k\in\mathbb{Z}} \in \ell^2(L^2(\mathbb{R}^+)) \mid f_k \in \mathcal{D}((L_{\alpha,c})_k)\ \forall k \in \mathbb{Z}, f_k = 0$ for almost every $k\}$, where $\mathcal{D}\Big((L_{\alpha,c})_k\Big) = C_0^\infty(\mathbb{R}^+)$ for all k. Moreover, as a general fact concerning direct sum operators, $\widetilde{L}_{\alpha,c}$ is essentially self-adjoint if and only if $(L_{\alpha,c})_k$ is so for all k ([34, Proposition 2.3]). Let us thus study the essential self-adjointness of $(L_{\alpha,c})_0$: it is a Sturm-Liouville operator of the form $-\frac{d^2}{dx^2} + V_{\alpha,c}(x)$, where

$$V_{\alpha,c}(x) = \frac{(1-4c)\alpha^2 + (2-4c)\alpha}{4x^2} =: \frac{k(\alpha,c)}{x^2}. \tag{5.3.5}$$

The potential $V_{\alpha,c}$ is quantum-mechanically complete at infinity, for all $(\alpha, c) \in \mathbb{R} \times [0,\infty)$ (as one can check by applying Proposition 5.3.4). So, applying Propositions 5.3.5 and 5.3.6, we can conclude that $(L_{\alpha,c})_0$ is essentially self-adjoint if and only if $V_{\alpha,c}(x) \geq \frac{3}{4x^2}$ near zero, since $V_{\alpha,c}(x) = k(\alpha,c)/x^2$ and when $k(\alpha,c) < 0$ then $V_{\alpha,c}$ decreases for $x \downarrow 0$. By using the explicit formula (5.3.5) for $V_{\alpha,c}$, we obtain $k(\alpha,c) \geq 3/4$ which yields the values of (α, c) given in the statement. For what we said before, when $(L_{\alpha,c})_0$ is not essentially self-adjoint, neither is so $\widetilde{L}_{\alpha,c}$. Finally, when $(L_{\alpha,c})_0$ is essentially self-adjoint, then

$$x^{2\alpha}k^2 + \frac{(1-4c)\alpha^2 + (2-4c)\alpha}{4x^2} \geq \frac{3}{4x^2},$$

so $(L_{\alpha,c})_k$ is essentially self-adjoint too, for all k, and hence $\widetilde{L}_{\alpha,c}$ is so. □

Remark 5.3.7. As a by-product of the proof of Proposition 5.1.2 we obtain that for the Grushin cylinder ($\alpha = 1$) with $c > 0$ all Fourier components of $-\Delta_1 + cK_1$ are not essentially self-adjoint, due to the inequality $x^2k^2 + (\frac{3}{4} - 2c)\frac{1}{x^2} < \frac{3}{4x^2}$ which holds near zero for all $k \in \mathbb{Z}$. Hence $-\Delta_1 + cK_1$ has infinite deficiency indices, for any $c > 0$. Theorem 5.1.1 extends this result to any two-dimensional almost Riemannian manifold of step 2 (under some natural topological assumptions).

However, from this proof we can also point out that this is not always the case for the α-Grushin cylinder, as for instance in the case of a flat cone ($\alpha = -1$) with $c \geq 0$ (note that this is not an ARS). In that case, the inequality $(k^2 - \frac{1}{4})\frac{1}{x^2} \geq \frac{3}{4x^2}$ implies that the k-th's Fourier components of $-\Delta_{-1} + cK_{-1}$ are essentially self-adjoint for all $k \neq 0$, even if $(-\Delta_{-1} + cK_{-1})_0$ is not. This means that $-\Delta_{-1} + cK_{-1}$ has deficiency indices equal to 1, for all $c \geq 0$.

We conclude this Section by considering a Riemannian manifold (M, g) without boundary, with associated Riemannian volume form ω, and Laplace-Beltrami operator $\Delta = \mathrm{div}_\omega \circ \mathrm{grad}_g$ acting on the Hilbert space $L^2(M,\omega)$, with domain $\mathcal{D}(\Delta) = C_0^\infty(M)$. Green's identity implies

(i) $\int_M \overline{u}\,\Delta v\,d\omega = \int_M \overline{\Delta u}\,v\,d\omega$, for all $u, v \in C_0^\infty(M)$, i.e., Δ is a symmetric operator.

(ii) $\mathcal{D}(\Delta^*) = \{u \in L^2(M,\omega) \mid \Delta u \in L^2(M,\omega)$ in the sense of distributions$\}$.

Letting F be a real-valued continuous function locally $L^2(M,\omega)$ seen as a multiplicative operator with domain $C_0^\infty(M)$, (i) and (ii) still hold true for the operator $\Delta + F$ instead of Δ.

Remark 5.3.8. Being $\Delta + F$ a real operator (that is, it commutes with complex conjugation), its deficiency indices are equal ([100, Theorem X.3]) and thus it always admits self-adjoint extensions.

5.4 Grushin zone

We focus now our attention around a Grushin point. We thus define the Riemannian manifold $\Omega = \{(x, y) \in \mathbb{R} \times S^1 \mid x \neq 0\}$ with metric $g = \mathrm{diag}(1, x^{-2}e^{-2\phi(x,y)})$, where ϕ is a smooth function which is constant for large $|x|$. The smoothness of ϕ is guaranteed by Proposition 5.2.4, and even if it is only defined locally, we extend it constantly in the coordinates (x, y), since what matters is the analysis close to $x = 0$. Note that X_1, X_2 given by Proposition 5.2.4 (F2) is an orthonormal frame for g. We then consider also the two connected components $\Omega_+ = \{(x, y) \in \mathbb{R} \times S^1 \mid x > 0\}$ and $\Omega_- = \{(x, y) \in \mathbb{R} \times S^1 \mid x < 0\}$. We start by proving the following key result:

Theorem 5.4.1. *Consider the Riemannian manifold (Ω_+, g), with associated Riemannian volume form ω, curvature K and Laplace-Beltrami operator Δ. Let $c > 0$. Consider the curvature Laplacian $-\Delta + cK$, with domain $C_0^\infty(\Omega_+)$, acting on $L^2(\Omega_+, \omega)$. Then for every $\epsilon > 0$ there exists a function $h_{\epsilon,c} \in L^2(\Omega_+, \omega) \cap C^\infty(\Omega_+)$ such that*

(i) $h_{\epsilon,c} \in \mathcal{D}((-\Delta + cK)^*)$;

(ii) $h_{\epsilon,c} \notin \mathcal{D}(\overline{-\Delta + cK})$;

(iii) $\mathrm{supp}(h_{\epsilon,c}) \subset (0, \epsilon) \times S^1$.

In particular, $-\Delta + cK$ is not essentially self-adjoint (here $c > 0$). The same conclusions hold if we replace Ω_+ with Ω_- or Ω.

What we can actually prove is the following stronger version of Theorem 5.4.1:

Theorem 5.4.2. *With the same notations of Theorem 5.4.1,* $\dim \mathcal{D}((-\Delta + cK)^*)/\mathcal{D}(\overline{-\Delta + cK}) = \infty$, *i.e., $-\Delta + cK$ has infinite deficiency indices.*

The proofs of Theorems 5.4.1 and 5.4.2 span Sections 5.4.1 and 5.4.3, where we shall describe respectively the closure and the adjoint of $-\Delta + cK$.

5.4.1 Closure operator

We shall work on the manifold Ω_+, being the case Ω_- analogous. Then the statement for Ω follows from the decomposition $L^2(\Omega, \omega) = L^2(\Omega_-, \omega) \oplus^\perp L^2(\Omega_+, \omega)$.

For a metric g of the form $\mathrm{diag}(1, \mathfrak{f}(x, y)^{-2})$, plugging $\mathfrak{f}(x, y) = xe^{\phi(x,y)}$ into (5.2.3), (5.2.4), and (5.2.5) one has the following:

$$\begin{aligned}
\omega_{(x,y)} &= \frac{1}{xe^{\phi(x,y)}} dxdy, \\
K(x, y) &= -\frac{2}{x^2} - \frac{2\partial_x\phi(x, y)}{x} + \partial_x^2\phi(x, y) - (\partial_x\phi(x, y))^2, \\
\Delta &= \partial_x^2 + x^2e^{2\phi(x,y)}\partial_y^2 - \frac{1}{x}\partial_x - \partial_x\phi(x, y)\partial_x + \partial_y\phi(x, y)x^2e^{2\phi(x,y)}\partial_y.
\end{aligned}$$

We perform a unitary transformation

$$U : L^2(\Omega_+, \omega) \to L^2(\Omega_+, dxdy), \quad \psi \mapsto (xe^\phi)^{-1/2}\psi, \tag{5.4.1}$$

and the corresponding transformed Laplacian is given by

$$\begin{aligned}
L &= U\Delta U^{-1} \\
&= \partial_x^2 + x^2e^{2\phi}\partial_y^2 + 2x^2e^{2\phi}(\partial_y\phi)\partial_y - \frac{3}{4x^2} - \frac{\partial_x\phi}{2x} - \frac{1}{4}(\partial_x\phi)^2 + \frac{1}{2}\partial_x^2\phi + \frac{3}{4}x^2(\partial_y\phi)^2e^{2\phi} + \frac{1}{2}x^2(\partial_y^2\phi)e^{2\phi}.
\end{aligned}$$

We shall analyze the self-adjointness of the operator

$$\begin{aligned}
-L + cK &= U(-\Delta + cK)U^{-1} \\
&= -\partial_x^2 - x^2e^{2\phi}\partial_y^2 - 2x^2e^{2\phi}(\partial_y\phi)\partial_y + \left(\frac{3}{4} - 2c\right)\frac{1}{x^2} + \frac{1 - 4c}{2}\frac{\partial_x\phi}{x} + \left(\frac{1}{4} - c\right)(\partial_x\phi)^2 \\
&\quad + \left(c - \frac{1}{2}\right)\partial_x^2\phi - \frac{3}{4}x^2(\partial_y\phi)^2e^{2\phi} - \frac{1}{2}x^2(\partial_y^2\phi)e^{2\phi} \\
&= H_c + \eta_c, \qquad (5.4.2)
\end{aligned}$$

where we have defined the operator

$$H_c = -\partial_x^2 - x^2 e^{2\phi}\partial_y^2 - 2x^2 e^{2\phi}(\partial_y\phi)\partial_y + \left(\frac{3}{4} - 2c\right)\frac{1}{x^2} + \left(\frac{1-4c}{2}\right)\frac{\partial_x\phi}{x}, \tag{5.4.3}$$

and the multiplicative operator

$$\eta_c = \left(\frac{1}{4} - c\right)(\partial_x\phi)^2 + \left(c - \frac{1}{2}\right)\partial_x^2\phi - \frac{3}{4}x^2(\partial_y\phi)^2 e^{2\phi} - \frac{1}{2}x^2(\partial_y^2\phi)e^{2\phi}, \tag{5.4.4}$$

both with domain $C_0^\infty(\Omega_+)$, acting on the Hilbert space $L^2(\Omega_+, dxdy) =: L^2(\Omega_+)$. For later convenience, we also define the operator

$$T_c = -\partial_x^2 - x^2 e^{2\phi}\partial_y^2 - 2x^2 e^{2\phi}(\partial_y\phi)\partial_y + \left(\frac{3}{4} - 2c\right)\frac{1}{x^2}, \quad \mathcal{D}(T_c) = C_0^\infty(\Omega_+), \quad \text{acting on } L^2(\Omega_+),$$

and

$$S_c = -\frac{d^2}{dx^2} + \left(\frac{3}{4} - 2c\right)\frac{1}{x^2}, \quad \mathcal{D}(S_c) = C_0^\infty(\Omega_+), \quad \text{acting on } L^2(\Omega_+). \tag{5.4.5}$$

As a 1D operator, $-\frac{d^2}{dx^2} + \left(\frac{3}{4} - 2c\right)\frac{1}{x^2}$ is usually called inverse square potential Hamiltonian, or Bessel operator, and its closed extensions have been largely studied in the recent literature both for real and complex values of c (see, e.g., [12, 47] and reference therein). In particular, the domain of its closure is known:

Proposition 5.4.3. *([47, Theorem 4.1, Lemma 4.2]) Let c>0 and consider the 1D operator*

$$s_c := -\frac{d^2}{dx^2} + \left(\frac{3}{4} - 2c\right)\frac{1}{x^2}, \quad \mathcal{D}(s_c) = C_0^\infty(\mathbb{R}^+), \tag{5.4.6}$$

acting on $L^2(\mathbb{R}^+, dx)$. Then, $\mathcal{D}(\overline{s_c}) = H_0^2(\mathbb{R}^+, dx)$.

Moreover the following inequality holds

$$\left\|\frac{f}{x^2}\right\|_{L^2(\mathbb{R}^+)} \le \frac{1}{2c}\|s_c f\|_{L^2(\mathbb{R}^+)}, \quad \forall f \in C_0^\infty(\mathbb{R}^+). \tag{5.4.7}$$

In order to describe the space $\mathcal{D}(\overline{-L + cK})$, for all $c > 0$, we apply a general result on inverse-square potential perturbations of the Laplace-Beltrami operator on 2D-ARS. Consider the vector fields

$$Y_1(x, y) = x\frac{\partial}{\partial x}, \quad Y_2(x, y) = x^2\frac{\partial}{\partial y}, \quad (x, y) \in \Omega_+,$$

and define the Sobolev space $H^2_{Y_1,Y_2}\left(\Omega_+, \frac{dxdy}{x^3}\right)$ as the completion of $C_0^\infty(\Omega_+)$ w.r.t. the norm

$$\|f\|_{H^2_{Y_1,Y_2}\left(\Omega_+, \frac{dxdy}{x^3}\right)} = \|f\|_{L^2\left(\Omega_+, \frac{dxdy}{x^3}\right)} + \sum_{i=1,2}\|Y_i f\|_{L^2\left(\Omega_+, \frac{dxdy}{x^3}\right)} + \sum_{i,j=1,2}\|Y_i Y_j f\|_{L^2\left(\Omega_+, \frac{dxdy}{x^3}\right)}.$$

Moreover we write $u \in xH^2_{Y_1,Y_2}\left(\Omega_+, \frac{dxdy}{x^3}\right)$ if $u/x \in H^2_{Y_1,Y_2}\left(\Omega_+, \frac{dxdy}{x^3}\right)$.

Proposition 5.4.4. *([20, Theorem 1.1]) Let Δ be the Laplace-Beltrami operator of (Ω_+, g) with domain $C_0^\infty((0, \epsilon] \times S^1)$, for $\epsilon > 0$. Suppose that $h \in C^\infty(\Omega_+)$ is such that $h(0, \cdot)$ does not have zeroes. Then,*

$$\mathcal{D}\left(\overline{-\Delta + \frac{h}{x^2}}\right) = xH^2_{Y_1,Y_2}\left(\Omega_+, \frac{dxdy}{x^3}\right).$$

We remark that Proposition 5.4.4 is actually proved in a more general setting in [20, Theorem 1.1], and it holds even in the presence of tangency points. We consider here the domain $C_0^\infty((0, \epsilon] \times S^1)$ (that is, the smooth functions that are compactly supported away from 0, whose support may touch ϵ), in order to avoid the non-compactness of Ω_+, which however does not play any role since we are interested only in the behaviour around $x = 0$. A direct consequence of Proposition 5.4.4 is collected in the next corollary, and will be crucial later:

Corollary 5.4.5. *Let c>0 and $f \in \mathcal{D}(\overline{-L + cK})$ with $\operatorname{supp} f \subset (0, \epsilon) \times S^1$. Then, $f(\cdot, y) = o(x^{3/2})$ as $x \to 0^+$, for a.e. $y \in S^1$.*

Proof. First, $f \in \mathcal{D}(\overline{-L+cK})$ if and only if $g := U^{-1}(f) = (xe^{\phi})^{1/2} f \in \mathcal{D}(\overline{-\Delta + cK})$ (cf. (5.4.1)). We set $h = cKx^2 \in C^\infty(\Omega_+)$, and notice that $h(0,\cdot) = -2c$ does not have zeroes for $c > 0$. Thanks to Proposition 5.4.4,

$$g \in \mathcal{D}\left(\overline{-\Delta + \frac{h}{x^2}}\right) \Leftrightarrow g/x \in H^2_{Y_1,Y_2}\left(\Omega_+, \frac{dxdy}{x^3}\right),$$

which implies that in particular, for any $\epsilon > 0$, and for a.e. $y \in S^1$ the norm

$$\int_0^\epsilon \left|\frac{g(x,y)}{x}\right|^2 \frac{dx}{x^3} < \infty,$$

which is true if and only if $g(\cdot, y) = o(x^2)$ as $x \to 0^+$, for a.e. $y \in S^1$. Finally, coming back to f via $f = U(g) = (xe^{\phi})^{-1/2} g$ and noticing that $\phi(0,y) = 0\ \forall y \in S^1$, we conclude the proof. □

5.4.2 An alternative proof of Corollary 5.4.5, for $c \in (0, 3/8]$

We furnish in this section a different proof of Corollary 5.4.5 for small values of c, which uses only the Hardy inequality and the Fourier transform w.r.t. the y-variable.

Lemma 5.4.6. *Let $c \in [0, 3/8]$ and $f \in L^2(\Omega_+)$ with* $\operatorname{supp} f \subset (0,\epsilon) \times S^1$, *for some $\epsilon > 0$. Then, $f \in \mathcal{D}\left(\overline{-L+cK}\right)$ if and only if $f \in \mathcal{D}(\overline{T_c})$.*

Proof. Since $-L + cK = H_c + \eta_c$, and η_c is a bounded operator on $(0,\epsilon) \times S^1$, Proposition 5.3.1 implies that $f \in \mathcal{D}(\overline{-L+cK})$ if and only if $f \in \mathcal{D}(\overline{H_c})$, for all $c > 0$. Furthermore, we want to show that the singular term $\frac{g_{1,c}}{x} := \left(\frac{1-4c}{2}\right)\frac{\partial_x \phi}{x}$ is infinitesimally small w.r.t. T_c, if $c \in [0, 3/8]$. In order to do this we will use two main ingredients. The first one is Hardy inequality:

$$\int_0^\infty \frac{|u(x)|^2}{x^2} dx \le 4 \int_0^\infty |u'(x)|^2 dx, \quad \forall u \in C_0^\infty(\mathbb{R}^+).$$

The second one is perturbation theory, in particular Proposition 5.3.1.

For all functions $u \in C_0^\infty(\mathbb{R}^+ \times S^1)$ we have

$$\begin{aligned}
\left\|\frac{g_{1,c}u}{x}\right\|^2_{L^2(\mathbb{R}^+\times S^1)} &= \int_{\mathbb{R}^+\times S^1} \frac{|g_{1,c}(x,y)|^2}{x^2}|u(x,y)|^2 dxdy \\
\le& 4\|g^2_{1,c}\|_{L^\infty(\mathbb{R}^+\times S^1)} \int_{\mathbb{R}^+\times S^1} |\partial_x u(x,y)|^2 dxdy \qquad \text{(Fubini + Hardy)} \\
\le& 4\|g^2_{1,c}\|_{L^\infty(\mathbb{R}^+\times S^1)} \int_{\mathbb{R}^+\times S^1} |\partial_x u(x,y)|^2 + x^2 e^{2\phi}|\partial_y u(x,y)|^2 + \left(\frac{3}{4} - 2c\right)\frac{|u(x,y)|^2}{x^2}\, dxdy \\
=& 4\|g^2_{1,c}\|_{L^\infty(\mathbb{R}^+\times S^1)} (T_c u, u)_{L^2(\mathbb{R}^+\times S^1)} \qquad \text{(Parts)} \\
\le& 2\|g^2_{1,c}\|_{L^\infty(\mathbb{R}^+\times S^1)} \left(\delta \|T_c u\|^2_{L^2(\mathbb{R}^+\times S^1)} + \frac{1}{\delta}\|u\|^2_{L^2(\mathbb{R}^+\times S^1)}\right), \qquad \text{(Young)}
\end{aligned}$$

where the last inequality holds for every $\delta > 0$, which proves that $\frac{g_{1,c}}{x}$ is infinitesimally small w.r.t. T_c if $c \in [0, 3/8]$. Proposition 5.3.1 then implies that $D(\overline{H_c}) = D(\overline{T_c})$. □

For any function $f \in L^2(\mathbb{R}^+ \times S^1)$, we denote by $f = \sum_{k\in\mathbb{Z}} \widehat{f_k}(x) e^{iky}$ its Fourier series.

Proposition 5.4.7. *Let $c \in (0, 3/8]$, and let $f \in \mathcal{D}(\overline{-L+cK})$ be a function supported in $(0,\epsilon) \times S^1$, for some $\epsilon > 0$. Then, $\widehat{f_k}(x) = o(x^{\frac{3}{2}})$ for $x \downarrow 0$, for every $k \in \mathbb{Z}$.*

Proof. Let $f \in C_0^\infty((0,\epsilon) \times S^1)$. Lemma 5.4.6 shows that $f \in \mathcal{D}(\overline{-L+cK})$ if and only if $f \in \mathcal{D}(\overline{T_c})$. Thus, we are left to study the behavior near $x = 0$ of a function $f \in \mathcal{D}(\overline{T_c})$. For any $k \in \mathbb{Z}$, we have

$$\widehat{(T_c\ f)}_k = s_c \widehat{f_k} - \frac{1}{2}x^2 \sum_{m+m'=k} (-m^2)\widehat{f_m}\widehat{(e^{2\phi})}_{m'} - x^2 \sum_{m+m'=k} (im)\widehat{f_m}\widehat{(\partial_y \phi\, e^{2\phi})}_{m'},$$

where s_c is defined in (5.4.6), and we compute the norm using the triangular inequality

$$\|\widehat{(T_c\ f)}_k\|_{L^2(\mathbb{R}^+)} \geq \left\|s_c \widehat{f_k}\right\|_{L^2(\mathbb{R}^+)}$$
$$-\left\|\frac{1}{2}x^2 \sum_{m+m'=k} (-m^2)\widehat{f_m}\widehat{(e^{2\phi})}_{m'}\right\|_{L^2(\mathbb{R}^+)} - \left\|x^2 \sum_{m+m'=k} (\mathrm{i}m)\widehat{f_m}\widehat{(\partial_y\phi\, e^{2\phi})}_{m'}\right\|_{L^2(\mathbb{R}^+)}$$

We have,

$$\left\| \sum_{m+m'=k} (-m^2)\widehat{f_m}\widehat{(e^{2\phi})}_{m'}\right\|_{L^2(\mathbf{R}_+)} =$$
$$\left\| \sum_{m+m'=k} (-m'^2)\widehat{f_m}\widehat{(e^{2\phi})}_{m'} - k^2 \sum_{m+m'=k} \widehat{f_m}\widehat{(e^{2\phi})}_{m'} + 2k \sum_{m+m'=k} m'\widehat{f_m}\widehat{(e^{2\phi})}_{m'}\right\|_{L^2(\mathbf{R}_+)} \leq$$
$$\|f\|_{L^2(\mathbf{R}_+\times S^1)}\Big(\sup_{x\in\mathbb{R}_+} \|e^{2\phi}\|_{H^2(S^1)} + k^2 \sup_{x\in\mathbb{R}_+} \|e^{2\phi}\|_{L^2(S^1)} + 2|k| \sup_{x\in\mathbb{R}_+} \|e^{2\phi}\|_{H^1(S^1)} \Big) \leq$$
$$C_{\phi,k}\ \|f\|_{L^2(\mathbf{R}_+\times S^1)}$$

thanks to the Cauchy-Schwartz inequality and the Plancherel formula. Similarly,

$$\left\| \sum_{m+m'=k} (\mathrm{i}m)\widehat{f_m}\widehat{(\partial_y\phi\, e^{2\phi})}_{m'}\right\|_{L^2(\mathbf{R}_+)} \leq$$
$$\|f\|_{L^2(\mathbf{R}_+\times S^1)}\Big(\sup_{x\in\mathbb{R}_+} \|e^{2\phi}\partial_y\phi\|_{H^1(S^1)} + |k| \sup_{x\in\mathbb{R}_+} \|e^{2\phi}\partial_y\phi\|_{L^2(S^1)} \Big) \leq C'_{\phi,k}\ \|f\|_{L^2(\mathbf{R}_+\times S^1)}$$

Thus

$$\begin{aligned} \left\|s_c \widehat{f_k}\right\|_{L^2(\mathbb{R}^+)} &\leq \|\widehat{(T_c\ f)}_k\|_{L^2(\mathbb{R}^+)} + \epsilon^2 C''_{\phi,k}\|f\|_{L^2(\mathbb{R}^+\times S^1)} \\ &\leq \|T_c\ f\|_{L^2(\mathbb{R}^+\times S^1)} + \epsilon^2 C''_{\phi,k}\|f\|_{L^2(\mathbb{R}^+\times S^1)} \quad \forall\ f \in C_0^\infty((0,\epsilon)\times S^1). \end{aligned} \tag{5.4.8}$$

By density, (5.4.8) implies that $f \in \mathcal{D}(\overline{T}_c) \Rightarrow \widehat{f_k} \in \mathcal{D}(\overline{s_c})\, \forall k \in \mathbb{Z}$. Then, the conclusion follows by applying Proposition 5.4.3, since every function $u \in H_0^2(\mathbb{R}_+)$ satisfies $u(x) = o(x^{\frac{3}{2}})$ for $x \to 0$. □

Remark 5.4.8. We remark that the values of $c \in (0, 3/8]$ cover all the cases listed in the introduction, that is $c \in (0, 1/3]$, arising from different quantizations procedures.

5.4.3 Adjoint operator

We first consider the 1D Sturm-Liouville model operator given by

$$A = -\frac{d^2}{dx^2} + \frac{g_2}{x^2} + \frac{g_1}{x}, \qquad g_1, g_2 \in \mathbb{R}. \tag{5.4.9}$$

Moreover, we introduce a C^∞ cut-off function $0 \leq P_\epsilon \leq 1$,

$$P_\epsilon(x) = \begin{cases} 1 & \text{if } x \leq \epsilon/2, \\ 0 & \text{if } x \geq \epsilon. \end{cases} \tag{5.4.10}$$

Lemma 5.4.9. *Let $g_1, g_2 \in \mathbb{R}$, $g_2 < 3/4$. Consider the operator A acting on the Hilbert space $L^2(\mathbb{R}^+)$ with domain $C_0^\infty(\mathbb{R}^+)$. Then,*

(a) for any $f \in \mathcal{D}(\overline{A})$, $f(x) = o(x^{\frac{3}{2}})$, as $x \to 0$;

(b) $\mathcal{D}(A^*) = \mathcal{D}(\overline{A}) + \mathrm{span}\{\psi_+ P_\epsilon, \psi_- P_\epsilon\}$, where P_ϵ is the cut-off function defined in (5.4.10)*, and*

$$\psi_\pm(x) = x^{\alpha_\pm} + a_\pm\, x^{\alpha_\pm+1}, \quad \alpha_\pm = \frac{1}{2} \pm \frac{1}{2}\sqrt{4g_2+1}, \quad a_\pm = \frac{g_1}{(\alpha_\pm+1)\alpha_\pm - g_2},$$

if $g_2 \neq -1/4$ and $g_2 \neq 0$,

$$\psi_+(x) = x^{\frac{1}{2}} + g_1 x^{\frac{3}{2}}, \quad \psi_-(x) = x^{\frac{1}{2}}\log(x) + g_1 x^{\frac{3}{2}}\log(x) + 2x^{\frac{1}{2}},$$

if $g_2 = -1/4$, and

$$\psi_+(x) = x, \quad \psi_-(x) = 1 + g_1 x\log(x),$$

if $g_2 = 0$.

Proof. To prove part (a) of the statement, it suffices to consider functions f that are supported arbitrarily near $x = 0$. Then, we can show that $\frac{g_1}{x}$ is infinitesimally small w.r.t. $-\frac{d^2}{dx^2} + \frac{g_2}{x^2}$. Indeed, notice that (5.4.7) w.r.t. this notation reads

$$\left\|\frac{f}{x^2}\right\|_{L^2(\mathbb{R}^+)} \leq \frac{1}{3/4 - g_2}\left\|\left(-\frac{d^2}{dx^2} + \frac{g_2}{x^2}\right) f\right\|_{L^2(\mathbb{R}^+)} \qquad \forall f \in C_0^\infty(\mathbb{R}^+),$$

which at once implies that for any $\epsilon > 0$ we have

$$\left\|\frac{g_1}{x} f\right\|_{L^2(\mathbb{R}^+)} = \left\|\frac{x g_1}{x^2} f\right\|_{L^2(\mathbb{R}^+)} \leq \epsilon \left\|\left(-\frac{d^2}{dx^2} + \frac{g_2}{x^2}\right) f\right\|_{L^2(\mathbb{R}^+)} \qquad \forall f \in C_0^\infty(0, \delta),$$

where $\delta > 0$ is such that $\sup_{x \in (0,\delta)} |g_1 x|(g_2 - 3/4)^{-1} < \epsilon$. Propositions 5.3.1 and 5.4.3 then imply

$$\mathcal{D}\left(\overline{-\frac{d^2}{dx^2} + \frac{g_2}{x^2} + \frac{g_1}{x}}\right) = \mathcal{D}\left(\overline{-\frac{d^2}{dx^2} + \frac{g_2}{x^2}}\right) = H_0^2(\mathbb{R}^+),$$

that concluded the proof of part (a).

To prove the second statement, we look for the solutions of

$$-u''(x) + \frac{g_2}{x^2} u(x) + \frac{g_1}{x} u(x) = 0. \tag{5.4.11}$$

These are two linearly independent functions which can be expressed via confluent hypergeometric functions, but since we are only interested in their behavior near $x = 0$, we can just use the Frobenius method (see, for instance, [105, Chapter 4]) to understand their asymptotics.

The first step is to write down the indicial polynomial, which is defined as

$$P(\alpha) = (x^{-\alpha+2} A x^\alpha)|_{x=0} = \alpha(\alpha - 1) - g_2.$$

The construction depends whether or not the two roots of this polynomial are separated by an integer. The two roots are given by

$$\alpha_\pm = \frac{1}{2} \pm \frac{1}{2}\sqrt{4g_2 + 1}.$$

Under the stated ranges of g_2 it follows that the only two cases where the two roots are separated by an integer are given by $g_2 = 0$ and $g_2 = -1/4$.

Assume that $g_2 \neq 0$ and $g_2 \neq -1/4$. Then the Frobenius method states that there exist two independent solutions, which can be represented as converging series of the form

$$u_\pm(x) = x^{\alpha_\pm} \sum_{i=0}^{\infty} a_i x^i. \tag{5.4.12}$$

We plug the ansatz (5.4.12) into (5.4.11) and obtain the following conditions for the dominating terms

$$\begin{cases} a_0[\alpha(\alpha - 1) - g_2] = 0, \\ a_1(\alpha + 1)\alpha - a_1 g_2 + a_0 g_1 = 0. \end{cases}$$

Setting $a_0 = 1$, we obtain that $\alpha_\pm$ are exactly the roots of the indicial polynomial, that

$$a_{1,\pm} = \frac{g_1}{(\alpha_\pm + 1)\alpha_\pm - g_2} =: a_\pm,$$

and that the solutions are

$$u_\pm(x) = x^{\alpha_\pm} + a_\pm\, x^{\alpha_\pm + 1} + o(x^{\alpha_\pm + 1}).$$

Assume now that $g_2 = -1/4$ or $g_2 = 0$. Then the Frobenius method tells us that $u_+(x)$ is still a solution of (5.4.11) and the second solutions is given by

$$u_-(x) = C u_+(x) \log(x) + x^{\alpha_-} \sum_{i=0} a_i x^i.$$

Plugging this series expression into (5.4.11) allows us to recover $\psi_\pm$ as the dominating terms of $u_\pm$. Moreover notice that, as a direct consequence of the Frobenius method, $A(u_\pm - \psi_\pm)$ is bounded near $x = 0$, and hence $A\psi_\pm \in L^2(0, 1)$.

So, let $\psi_\pm$ as in the statement. Then

$$(i)\ \ \psi_\pm \in L^2(0,1), \quad (ii)\ \ A\psi_\pm \in L^2(0,1), \quad (iii)\ \ \psi_\pm \notin \mathcal{D}(\overline{A}),$$

where (i) and (ii) imply at once that $\psi_\pm P_\epsilon \in \mathcal{D}(A^*)$ and (iii) follows from part (a) and the asymptotics of $\psi_\pm$ near $x = 0$. Since the functions $\psi_+ P_\epsilon$ and $\psi_- P_\epsilon$ are linearly independent and the quotient $\mathcal{D}(A^*)/\mathcal{D}(\overline{A})$ has dimension at most 2 (as it follows from the fact that A is in the limit point case at ∞, by applying Proposition 5.3.4, which in turns implies that $\ker(A^+ \pm \mathrm{i})$ have at most dimension 1, by applying Proposition 5.3.3), the thesis follows. □

Remark 5.4.10. A result similar to Lemma 5.4.9 (that includes also complex values of g_1, g_2) is proved in [48, Proposition 3.1]. Here we have provided a different proof, that uses perturbative arguments and does not require the introduction of Bessel functions.

Now, we can use Lemma 5.4.9 to obtain informations on the adjoint of the 2D operator we are interested in, that is, $-L + cK$ defined in (5.4.2), and complete the proof of Theorem 5.4.1.

Proof. of Theorem 5.4.1 We take the coefficient of $\frac{1}{x}$ evaluated at $x = 0$ (i.e., on the singularity) and treat the second variable y as a parameter. Indeed, setting

$$g_2 = \frac{3}{4} - 2c, \qquad g_1(y) = \frac{1-4c}{2}\partial_x\phi(0,y) \in C^\infty(S^1) \tag{5.4.13}$$

we obtain from Lemma 5.4.9 two functions $\psi_{\pm,c} \in C^\infty(\Omega)$ of both variables x, y. Then, we get the following:

Proposition 5.4.11. *Let $c > 0$, and define $\widetilde{h}_{\pm,\epsilon,c}(x,y) = \psi_{\pm,c}(x,y)P_\epsilon(x) \in L^2(\Omega_+) \cap C^\infty(\Omega_+)$, where $\psi_{\pm,c}$ have the same form as functions $\psi_\pm$ from Lemma 5.4.9 with g_1, g_2 given by* (5.4.13) *and P_ϵ is defined in* (5.4.10)*. Then,*

(i) $\widetilde{h}_{\pm,\epsilon,c} \in \mathcal{D}((-L+cK)^*)$*;*

(ii) $\widetilde{h}_{\pm,\epsilon,c} \notin \mathcal{D}(\overline{-L+cK})$*;*

(iii) $\mathrm{supp}(\widetilde{h}_{\pm,\epsilon,c}) \subset (0,\epsilon) \times S^1$.

Proof. Part (iii) is obvious, as $\mathrm{supp}(P_\epsilon) \subset (0,\epsilon)$. To prove (i), we consider the operator R on the domain $C_0^\infty(\Omega_+)$, whose action is defined by $R := (-L + cK) - A$, (where A is the operator whose action is defined in (5.4.9), but now is considered on the domain $C_0^\infty(\Omega_+)$, and g_1, g_2 are the functions defined in (5.4.13)), and we claim that $R\widetilde{h}_{\pm,\epsilon,c} \in L^2(\Omega_+)$, in the weak sense. Indeed, we have

$$\begin{aligned} R &= -x^2e^{2\phi}\partial_y^2 - 2x^2e^{2\phi}(\partial_y\phi)\partial_y + \frac{1-4c}{2}\Big(\frac{\partial_x\phi(x,y) - \partial_x\phi(0,y)}{x}\Big) + \eta_c \\ &= -x^2e^{2\phi}\partial_y^2 - 2x^2e^{2\phi}(\partial_y\phi)\partial_y + \widetilde{\eta}_c, \end{aligned}$$

(where η_c and $\widetilde{\eta}_c$ are functions that are bounded on $(0,\epsilon) \times S^1$) and the claim follows from the C^∞-regularity of $\widetilde{h}_{\pm,\epsilon,c}$ w.r.t. y. Then, by the very construction of $\widetilde{h}_{\pm,\epsilon,c}$, we have that $A\widetilde{h}_{\pm,\epsilon,c} \in L^2(\Omega_+)$, which in turns implies that $(-L+cK)\widetilde{h}_{\pm,\epsilon,c} = (R+A)\widetilde{h}_{\pm,\epsilon,c} \in L^2(\Omega_+)$ in the weak sense, and proves part (i).

To prove part (ii) we first notice that for all $c > 0$ and all $y \in S^1$, $\widetilde{h}_{\pm,\epsilon,c}(\cdot,y)$ is not $o(x^{3/2})$ (notice that $x^{\alpha_\pm} = x^{1/2\pm\sqrt{1-2c}}$), and we can apply Corollary 5.4.5 to conclude that $\widetilde{h}_{\pm,\epsilon,c} \notin \mathcal{D}(\overline{-L+cK})$. □

To conclude the proof of Theorem 5.4.1, it suffices to consider $h_{\pm,\epsilon,c} := U^{-1}\widetilde{h}_{\pm,\epsilon,c}$, where U is the unitary transformation defined in (5.4.1). □

The proof of Theorem 5.4.2 is now an immediate consequence:

Proof. of Theorem 5.4.2 It follows by considering the infinite-dimensional vector space spanned by the family of functions $\{h_{\pm,\epsilon,c}e^{\mathrm{i}ky}\}_{k\in\mathbb{Z}} \subset \mathcal{D}((-\Delta+cK)^*) \setminus \mathcal{D}(\overline{-\Delta+cK})$. □

5.5 Proof of Theorem 5.1.1

If $c = 0$, $-\Delta$ is known to be essentially self-adjoint on $L^2(M, \omega)$ ([30, Theorem 1.1]). Then, let $c > 0$.

Let $Z = \coprod_{j \in j} W_j$ be the disjoint union in connected components for the singular set, and $M = \cup_{i \in I} \Omega_i$ be an open cover such that, for every W_j, there exist a unique Ω_{i_j} (Grushin zone) with $W_j \subset \Omega_{i_j}$ and $W_j \cap \Omega_i = \emptyset$ if $i \neq i_j$. Moreover, as previously remarked, we can assume that Ω_{i_j} is a tubular neighborhood of W_j, i.e., $\Omega_{i_j} \cong \mathbb{R} \times S^1$.

Let W be a connected component of Z, and Ω the corresponding Grushin zone. Consider the operator $(-\Delta + cK)_\Omega$ defined as the restriction of $-\Delta + cK$ on the domain $C_0^\infty(\Omega \setminus W)$. In the local chart Ω with coordinates $(x, y) \in \mathbb{R} \times S^1$, $W = \{(x, y) \in \mathbb{R} \times S^1 \mid x = 0\}$, and Theorem 5.4.1 gives a function, e.g. $h_{+,\epsilon,c}$, supported arbitrarily close to W, such that $h_{+,\epsilon,c} \in \mathcal{D}((-\Delta + cK)^*_\Omega) \setminus \mathcal{D}(\overline{(-\Delta + cK)}_\Omega)$.

We define the function

$$F_{\epsilon,c} = \begin{cases} h_{+,\epsilon,c} & \text{on } \Omega, \\ 0 & \text{on } M \setminus \Omega. \end{cases}$$

So we have

$$\begin{aligned} \langle F_{\epsilon,c}, (-\Delta + cK)u \rangle_{L^2(M)} &= \langle F_{\epsilon,c}, (-\Delta + cK)u \rangle_{L^2(\Omega)} + \langle F_{\epsilon,c}, (-\Delta + cK)u \rangle_{L^2(M \setminus \Omega)} \\ &= \langle (-\Delta + cK)^*_\Omega h_{+,\epsilon,c}, u \rangle_{L^2(\Omega)}, \quad \forall u \in C_0^\infty(M \setminus Z), \end{aligned}$$

having integrated by parts ($h_{+,\epsilon,c}$ vanishes away from $\partial\Omega$, and u vanishes away from W), which proves that

$$(-\frac{1}{2}\Delta + cK)^* F_{\epsilon,c} = \begin{cases} (-\Delta + cK)^*_\Omega h_{+,\epsilon,c} & \text{on } \Omega, \\ 0 & \text{on } M \setminus \Omega, \end{cases}$$

and $F_{\epsilon,c} \in \mathcal{D}((-\Delta + cK)^*)$. We are left to prove that $F_{\epsilon,c} \notin \mathcal{D}(\overline{-\Delta + cK})$, which implies the non-self-adjointness of $-\Delta + cK$ on $L^2(M)$.

Suppose by contradiction that $F_{\epsilon,c} \in \mathcal{D}(\overline{-\Delta + cK})$. Then, there exist a sequence $(\phi_n)_{n \in \mathbb{N}} \subset C_0^\infty(M \setminus Z)$ and a function $G_{\epsilon,c} \in L^2(M)$ such that

(i) $\phi_n \to F_{\epsilon,c}$, as $n \to \infty$, in $L^2(M)$,

(ii) $(-\Delta + cK)\phi_n \to G_{\epsilon,c}$, as $n \to \infty$, in $L^2(M)$.

Now, $G_{\epsilon,c}$ must satisfy

$$G_{\epsilon,c} = (\overline{-\Delta + cK})F_{\epsilon,c} = (-\Delta + cK)^* F_{\epsilon,c} = \begin{cases} (-\Delta + cK)^*_\Omega h_{+,\epsilon,c} & \text{on } \Omega, \\ 0 & \text{on } M \setminus \Omega, \end{cases}.$$

So, $F_{\epsilon,c}$ and $G_{\epsilon,c}$ are both supported in $U \subsetneq \Omega$. We then consider the cut-off function $\xi \in C_0^\infty(\Omega)$

$$\xi(x) = \begin{cases} 1 & \text{if } x \in U, \\ 0 & \text{if } x \notin \Omega, \end{cases} \tag{5.5.1}$$

with $0 \leq \xi \leq 1$, and define the sequence $(\widetilde{\phi}_n = \xi\phi_n)_{n \in \mathbb{N}} \subset C_0^\infty(\Omega \setminus W)$. We have the following

Lemma 5.5.1. *$\widetilde{\phi}_n \to h_{+,\epsilon,c}$ and $(-\Delta + cK)\widetilde{\phi}_n = (-\Delta + cK)_\Omega \widetilde{\phi}_n \to G_{\epsilon,c}|_\Omega$, as $n \to \infty$, in $L^2(\Omega)$.*

Thus, we conclude by applying Lemma 5.5.1 which says that $h_{+,\epsilon,c} \in \mathcal{D}(\overline{(-\Delta + cK)}_\Omega)$, which is impossible.

Proof. of Lemma 5.5.1 Because of (i) and (ii), we have as $n \to \infty$

$$\begin{aligned} &(i.1)\ \ \|\phi_n - h_{+,\epsilon,c}\|_{L^2(U)} \to 0\,, \quad (i.2)\ \ \|\phi_n\|_{L^2(M \setminus U)} \to 0, \\ &(ii.1)\ \ \|(-\Delta + cK)\phi_n - G_{\epsilon,c}\|_{L^2(U)} \to 0\,, \quad (ii.2)\ \ \|(-\Delta + cK)\phi_n\|_{L^2(M \setminus U)} \to 0, \end{aligned}$$

since $\mathrm{supp}(h_{+,\epsilon,c})$ and $\mathrm{supp}(G_{\epsilon,c})$ are both contained in U. Then we have (as $n \to \infty$)

$$\|\widetilde{\phi}_n - h_{+,\epsilon,c}\|_{L^2(\Omega)} = \|\phi_n - h_{+,\epsilon,c}\|_{L^2(U)} + \|\xi\phi_n\|_{L^2(\Omega \setminus U)} \leq \|\phi_n - h_{+,\epsilon,c}\|_{L^2(U)} + \|\phi_n\|_{L^2(M \setminus U)} \to 0.$$

Moreover, using that $\Delta(\xi\phi_n) = (\Delta\xi)\phi_n + 2\nabla\xi \cdot \nabla\phi_n + \xi(\Delta\phi_n)$, we have

$$\|(-\Delta + cK)\widetilde{\phi}_n - G_{\epsilon,c}|_\Omega\|_{L^2(\Omega)} \leq \\ \|(-\Delta + cK)\phi_n - G_{\epsilon,c}\|_{L^2(U)} + C\|(-\Delta + cK)\phi_n + |\nabla\phi_n| + \phi_n\|_{L^2(\Omega\setminus U)},$$

where C is a constant such that $C > \|\Delta\xi\|_{L^\infty(\Omega)}, \| \, |\nabla\xi| \, \|_{L^\infty(\Omega)}, \|\xi\|_{L^\infty(\Omega)}$. Since K is a bounded function on $\Omega \setminus U$, we have

$$\|K\phi_n\|_{L^2(\Omega\setminus U)} \leq \|K\|_{L^\infty(\Omega\setminus U)} \cdot \|\phi_n\|_{L^2(\Omega\setminus U)} \to 0, \quad \text{as } n \to \infty,$$

and

$$\|\Delta\phi_n\|_{L^2(\Omega\setminus U)} \leq \|(-\Delta + cK)\phi_n\|_{L^2(\Omega\setminus U)} + \|cK\phi_n\|_{L^2(\Omega\setminus U)} \to 0, \quad \text{as } n \to \infty.$$

Finally, by Sobolev embedding, we have

$$\| \, |\nabla\phi_n| \, \|_{L^2(\Omega\setminus U)} \leq \widetilde{C}(\|\Delta\phi_n\|_{L^2(\Omega\setminus U)} + \|\phi_n\|_{L^2(\Omega\setminus U)}) \to 0, \quad \text{as } n \to \infty.$$

□

To prove that the deficiency indices of $-\Delta + cK$ are infinite if $c > 0$, it suffices to consider the infinite-dimensional vector space spanned by the family of functions $\{F^k_{\epsilon,c}\}_{k\in\mathbb{Z}}$ contained in $\mathcal{D}((-\Delta + cK)^*) \setminus \mathcal{D}(\overline{-\Delta + cK})$ defined by

$$F^k_{\epsilon,c} = \begin{cases} e^{\mathrm{i}ky} h_{+,\epsilon,c} & \text{on } \Omega, \\ 0 & \text{on } M \setminus \Omega. \end{cases}$$

Remark 5.5.2. One can construct such family of functions close to any singular region of M, and each singular region has an infinite family of self-adjoint extensions; this gives room to self-adjoint extensions on the whole manifold, characterized by different boundary conditions to be imposed at each singular region.

This concludes the proof of Theorem 5.1.1.

Chapter 6

Self-adjoint extensions of the Laplacian on anti-conic Grushin surfaces

In this chapter we classifY all the uniformly fibered self-adjoint extension of the Laplace-Beltrami operator on the α-Grushin cylinder, for $\alpha \in [0, 1)$, through the Kreĭn-Višik-Birman (KVB for brevity) theory (see Theorem 6.1.1). These extensions correspond to boundary conditions which are uniform w.r.t. the Fourier decomposition. In this region of α, the Laplace-Beltrami is a non-negative operator, with infinite deficency indices. The Friedrichs and bridging extension were already found in [34], and we recover them as particular cases within our general scheme. As a byproduct of our analysis, we are also able to compute the Sobolev-regularity on the singular set of the Grushin cylinder of functions belonging to different self-adjoint extensions (see Corollary 6.1.2), extending thus the results found in [97] (on the regularity of functions belonging to the deficency spaces).

The chapter is organized as follows: in Section 6.1 we state the main original results of the chapter already presented in the Introduction. In Section 6.2 we formulate the problem in terms of the Fourier decomposition, which yields a direct sum with constant fibre structure to the problem. In Section 6.3 we proved the main result on each half-fibre for the Fourier component (see Theorem 6.3.1); in particular, in Proposition 6.3.8 we characterize the operator closure of each Fourier component and in Theorem 6.3.13 we recall the KVB extension scheme. In Section 6.4 we extend the result of the previous section to the whole fibre, in Theorem 6.4.1. In Section 6.5 we describe how to realize general (i.e. possibly not uniformly fibred) self-adjoint extensions using the KVB scheme, giving in particular a characterization of the adjoint Laplace-Beltrami operator (see Lemma 6.5.2) in terms of the Sobolev-regularity of the Fourier coefficients involved in its decomposition. In Section 6.6 we finally prove the main results of the Chapter in Theorem 6.6.1 and Corollary 6.6.3; in particular, in order to go back from the description in Fourier components to the description w.r.t. the (x, y)-variables, we prove that the second derivative w.r.t. the y-variable is controlled by the Laplace-Beltrami operator (that is Lemma 6.6.11) thanks to a uniform estimate on the inverse of the Friedrichs extension, proved in Lemma 6.3.3(ii).

The results of this chapter are in the paper [64].

6.1 Main results

Let $M = (\mathbb{R} \setminus \{0\}) \times S^1$ and $\omega_\alpha = |x|^{-\alpha} \mathrm{d}x\, \mathrm{d}y$, for $\alpha \in [0, 1)$. We consider the linear differential operator

$$H_\alpha = -\frac{\partial^2}{\partial x^2} - x^{2\alpha} \frac{\partial^2}{\partial y^2} + \frac{\alpha}{x} \frac{\partial}{\partial x},$$

acting on the Hilbert space $L^2(M, \omega_\alpha)$, densely defined on the domain $\mathcal{D}(H_\alpha) = C_0^\infty(M)$. As we have recalled in the Introduction, $-H_\alpha$ is the Laplace-Beltrami operator associated with the generalized almost-Riemannian structure

$$X_1(x, y) = \frac{\partial}{\partial x}, \qquad X_2^{(\alpha)}(x, y) = |x|^\alpha \frac{\partial}{\partial y}, \qquad (x, y) \in \mathbb{R} \times S^1.$$

The main original results of the chapter are a classification of the local self-adjoint extensions of the operator H_α and their Sobolev regularity at the boundary.

Theorem 6.1.1. *Let $\alpha \in [0, 1)$. The operator H_α admits the following families of self-adjoint extensions in $L^2(M, \omega_\alpha)$:*

- *Friedrichs extension*: $H_{\alpha,F}$;
- *Family* $\mathrm{I_R}$: $\{H^{[\gamma]}_{\alpha,R} \mid \gamma \in \mathbb{R}\}$;
- *Family* $\mathrm{I_L}$: $\{H^{[\gamma]}_{\alpha,L} \mid \gamma \in \mathbb{R}\}$;
- *Family* II_a *with* $a \in \mathbb{C}$: $\{H^{[\gamma]}_{\alpha,a} \mid \gamma \in \mathbb{R}\}$;
- *Family* III: $\{H^{[\Gamma]}_{\alpha} \mid \Gamma \equiv (\gamma_1, \gamma_2, \gamma_3, \gamma_4) \in \mathbb{R}^4\}$.

Each operator belonging to any such family is a restriction of H^*_α*, and hence its differential action is precisely* H_α*. The domain of each of the above extensions is qualified as the space of the functions* $f \in L^2(M, \omega_\alpha)$ *satisfying the following properties.*

(i) *Integrability and regularity:*

$$\int_M \left|H_\alpha f\right|^2 \omega_\alpha \;<\; +\infty\,. \tag{6.1.1}$$

(ii) *Boundary condition: The limits*

$$f_0^{\pm}(y) \;=\; \lim_{x\to 0^\pm} f^{\pm}(x,y) \tag{6.1.2}$$

$$f_1^{\pm}(y) \;=\; \pm(1+\alpha)^{-1} \lim_{x\to 0^\pm} \left(\frac{1}{|x|^\alpha}\,\frac{\partial f(x,y)}{\partial x}\right) \tag{6.1.3}$$

exist and are finite for almost every $y \in S^1$*, and depending on the considered type of extension, and for almost every* $y \in S^1$*, they satisfy*

$$f_0^{\pm}(y) \;=\; 0 \qquad \text{if } f \in \mathcal{D}(H_{\alpha,F}), \tag{6.1.4}$$

$$\begin{cases} f_0^-(y) = 0 \\ f_1^+(y) = \gamma f_0^+(y) \end{cases} \qquad \text{if } f \in \mathcal{D}(H^{[\gamma]}_{\alpha,R}), \tag{6.1.5}$$

$$\begin{cases} f_1^-(y) = \gamma f_0^-(y) \\ f_0^+(y) = 0 \end{cases} \qquad \text{if } f \in \mathcal{D}(H^{[\gamma]}_{\alpha,L}), \tag{6.1.6}$$

$$\begin{cases} f_0^+(y) = a\, f_0^-(y) \\ f_1^-(y) + \overline{a}\, f_1^+(y) = \gamma f_0^-(y) \end{cases} \qquad \text{if } f \in \mathcal{D}(H^{[\gamma]}_{\alpha,a}), \tag{6.1.7}$$

$$\begin{cases} f_1^-(y) = \gamma_1 f_0^-(y) + (\gamma_2 + \mathrm{i}\gamma_3) f_0^+(y) \\ f_1^+(y) = (\gamma_2 - \mathrm{i}\gamma_3) f_0^-(y) + \gamma_4 f_0^+(y) \end{cases} \qquad \text{if } f \in \mathcal{D}(H^{[\Gamma]}_{\alpha})\,. \tag{6.1.8}$$

We can also deduce the regularity of the wave-function at the singular boundary S^1, depending on the different physics imposed by different self-adjoint extensions.

Corollary 6.1.2. *Let* f *belong to the domain of one of the self-adjoint extensions of* H_α *listed in Theorem 6.1.1. Then,*

$$f_0^{\pm} \in H^{s_{0,\pm}}(S^1, \mathrm{d}y) \qquad \text{and} \qquad f_1^{\pm} \in H^{s_{1,\pm}}(S^1, \mathrm{d}y) \tag{6.1.9}$$

with

- $s_{1,\pm} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$ *for the Friedrichs extension,*
- $s_{1,-} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$, $s_{0,+} = s_{1,+} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type* I_R*,*
- $s_{1,+} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$, $s_{0,-} = s_{1,-} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type* I_L*,*
- $s_{1,\pm} = s_{0,\pm} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$ *for extensions of type* II_a*,*
- $s_{1,\pm} = s_{0,\pm} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type* III.

6.2 Unitary equivalent reformulation of the problem

Let us introduce a unitarily equivalent re-formulation of the problem of the self-adjoint extensions of H_α in $L^2(M,\omega_\alpha)$.

We recall that H_α is reduced with respect to the decomposition

$$L^2(M,\omega_\alpha) = L^2(\mathbb{R}^+\times S^1,\omega_\alpha)\oplus L^2(\mathbb{R}^-\times S^1,\omega_\alpha) =: L^2(M^+,\omega_\alpha)\oplus L^2(M^-,\omega_\alpha). \tag{6.2.1}$$

hence we will manipulate $H_\alpha^+ := H_\alpha|_{C_0^\infty(M^+)}$ and $H_\alpha^- := H_\alpha|_{C_0^\infty(M^-)}$ separately.

We shall map $L^2(M^\pm,\omega_\alpha)$ unitarily onto the space

$$\mathcal{H}^\pm \;:=\; \bigoplus_{k\in\mathbb{Z}} L^2(\mathbb{R}^\pm,\mathrm{d}x) \;\cong\; \ell^2(\mathbb{Z},L^2(\mathbb{R}^\pm,\mathrm{d}x)) \;\cong\; L^2(\mathbb{R}^\pm,\mathrm{d}x)\otimes\ell^2(\mathbb{Z}). \tag{6.2.2}$$

We first apply the unitary transformation

$$\begin{aligned} U_\alpha^\pm : L^2(\mathbb{R}^\pm\times S^1,|x|^{-\alpha}\mathrm{d}x\mathrm{d}y) &\xrightarrow{\cong} L^2(\mathbb{R}^\pm\times S^1,\mathrm{d}x\mathrm{d}y)\\ f \;&\mapsto\; \psi \;:=\; |x|^{-\frac{\alpha}{2}} f \end{aligned} \tag{6.2.3}$$

(thus restoring the standard Euclidean metric by removing the weight), and then the further unitary transformation

$$\mathcal{F}_2^\pm : L^2(\mathbb{R}^\pm\times S^1,\mathrm{d}x\mathrm{d}y) \xrightarrow{\cong} L^2(\mathbb{R}^\pm,\mathrm{d}x)\otimes\ell^2(\mathbb{Z}) \;=:\; \mathcal{H}^\pm, \tag{6.2.4}$$

consisting of a partial Fourier transform in the y-variable only, that is,

$$\begin{aligned} \psi \;&\mapsto\; (\psi_k)_{k\in\mathbb{Z}}\\ e_k(y) \;:=\; \frac{e^{\mathrm{i}ky}}{\sqrt{2\pi}}, \qquad \psi_k(x) \;&:=\; \int_0^{2\pi}\overline{e_k(y)}\,\phi(x,y)\,\mathrm{d}y, \qquad x\in\mathbb{R}^\pm. \end{aligned} \tag{6.2.5}$$

So we may write $\psi(x,y)=\sum_{k\in\mathbb{Z}}\psi_k(x)e_k(y)$ in the L^2-convergent sense. Each $\psi_k\in L^2(\mathbb{R}^\pm,\mathrm{d}x)$ and $\sum_{k\in\mathbb{Z}}\|\psi_k\|_{L^2}^2 < +\infty$.

Thus,

$$\mathcal{H}^\pm \;=\; \mathcal{F}_2^\pm U_\alpha^\pm L^2(M^\pm,\omega_\alpha) \tag{6.2.6}$$

with a natural *constant-fibre orthogonal sum structure* on such space, namely,

$$\mathcal{H}^\pm \;=\; \bigoplus_{k\in\mathbb{Z}} \mathfrak{h}^\pm, \qquad \mathfrak{h}_\pm \;:=\; L^2(\mathbb{R}^\pm,\mathrm{d}x) \tag{6.2.7}$$

with *constant fiber* $\mathfrak{h}_\pm$ and scalar product

$$\big\langle(\psi_k)_{k\in\mathbb{Z}},(\widetilde{\psi}_k)_{k\in\mathbb{Z}}\big\rangle_{\mathcal{H}^\pm} \;=\; \sum_{k\in\mathbb{Z}}\int_{\mathbb{R}^\pm}\overline{\psi_k(x)}\,\widetilde{\psi}_k(x)\,\mathrm{d}x \;\equiv\; \sum_{k\in\mathbb{Z}}\langle\psi_k,\widetilde{\psi}_k\rangle_{\mathfrak{h}^\pm}. \tag{6.2.8}$$

Analogously, and with self-explanatory notation, $\mathcal{F}_2 := \mathcal{F}_2^-\oplus\mathcal{F}_2^+$, $U_\alpha := U_\alpha^-\oplus U_\alpha^+$, whence $\mathcal{F}_2U_\alpha = \mathcal{F}_2^-U_\alpha^-\oplus\mathcal{F}_2^+U_\alpha^+$, and

$$\mathcal{H} \;:=\; \mathcal{F}_2U_\alpha L^2(M,\omega_\alpha) \;\cong\; \ell^2(\mathbb{Z},L^2(\mathbb{R},\mathrm{d}x)) \;\cong\; \mathcal{H}^-\oplus\mathcal{H}^+ \;\cong\; \bigoplus_{k\in\mathbb{Z}}\mathfrak{h} \tag{6.2.9}$$

with *bilateral fibre*

$$\mathfrak{h} \;:=\; L^2(\mathbb{R}^-,\mathrm{d}x)\oplus L^2(\mathbb{R}^+,\mathrm{d}x) \;\cong\; L^2(\mathbb{R},\mathrm{d}x). \tag{6.2.10}$$

By means of (6.2.3) and (6.2.4) we obtain the operators

$$\mathsf{H}_\alpha^\pm \;:=\; U_\alpha^\pm H_\alpha^\pm (U_\alpha^\pm)^{-1} \tag{6.2.11}$$

acting on $L^2(\mathbb{R}^\pm\times S^1,\mathrm{d}x\mathrm{d}y)$ as

$$\begin{aligned} \mathcal{D}(\mathsf{H}_\alpha^\pm) \;&=\; C_0^\infty(\mathbb{R}_x^\pm\times S_y^1)\\ \mathsf{H}_\alpha^\pm\phi \;&=\; \Big(-\frac{\partial^2}{\partial x^2} - |x|^{2\alpha}\frac{\partial^2}{\partial y^2} + \frac{\alpha(2+\alpha)}{4x^2}\Big)\phi, \end{aligned} \tag{6.2.12}$$

as well as the operators

$$\mathscr{H}_\alpha^\pm \;:=\; \mathcal{F}_2^\pm\, U_\alpha^\pm\, H_\alpha^\pm\, (U_\alpha^\pm)^{-1}(\mathcal{F}_2^\pm)^{-1} \;=\; \mathcal{F}_2^\pm\, \mathsf{H}_\alpha^\pm(\mathcal{F}_2^\pm)^{-1} \tag{6.2.13}$$

acting on $\mathcal{H}^\pm$ as

$$\begin{aligned} \mathcal{D}(\mathscr{H}_\alpha^\pm) \;&=\; \Big\{\psi \equiv (\psi_k)_{k\in\mathbb{Z}} \in \bigoplus_{k\in\mathbb{Z}} L^2(\mathbb{R}^\pm, \mathrm{d}x) \,\Big|\, \psi \in \mathcal{F}_2^\pm C_0^\infty(\mathbb{R}_x^\pm \times S_y^1)\Big\} \\ \mathscr{H}_\alpha^\pm\psi \;&=\; \Big(\Big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2|x|^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2}\Big)\psi_k\Big)_{k\in\mathbb{Z}}\,. \end{aligned} \tag{6.2.14}$$

Completely analogous formulas hold for H_α and $\mathscr{H}_\alpha$, defined in the obvious way.

In particular, for each $\psi^\pm \in \mathcal{D}(\mathscr{H}_\alpha^\pm)$ the component functions $\psi_k^\pm(\cdot)$ are compactly supported in x inside $\mathbb{R}^\pm$ for every $k \in \mathbb{Z}$, and moreover

$$\begin{aligned} &\sum_{k\in\mathbb{Z}} \Big\|\Big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2|x|^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2}\Big)\psi_k^\pm\Big\|^2_{L^2(\mathbb{R}^\pm,\mathrm{d}x)} \\ &\qquad = \|\mathscr{H}_\alpha^\pm\psi^\pm\|^2_{\mathcal{H}^\pm} \;=\; \|(\mathcal{F}_2^\pm)^{-1}\mathscr{H}_\alpha^\pm\mathcal{F}_2^\pm\phi^\pm\|^2_{L^2(\mathbb{R}_x^\pm\times S_y^1)} \\ &\qquad = \Big\|\Big(-\frac{\partial^2}{\partial x^2} - |x|^{2\alpha}\frac{\partial^2}{\partial y^2} + \frac{\alpha(2+\alpha)}{4x^2}\Big)\phi^\pm\Big\|^2_{L^2(\mathbb{R}_x^\pm\times S_y^1)} \;<\; +\infty\,, \end{aligned} \tag{6.2.15}$$

where $\phi^\pm = \mathcal{F}_2^\pm\psi \in C_0^\infty(\mathbb{R}_x^\pm \times S_y^1)$.

The above construction establishes a unitarily equivalent version of the operators of interest. Thus, the self-adjointness problem for $H_\alpha^\pm$ in $L^2(M^\pm, \omega_\alpha)$ is equivalent to the self-adjointness problem for $\mathscr{H}_\alpha^\pm$ in $\mathcal{H}^\pm$, and the same holds for H_α with respect to $\mathscr{H}_\alpha$. Furthermore, when non-trivial self-adjoint extensions exist for $H_\alpha^\pm$ (resp., H_α), they can be equivalently (and in practice more conveniently) identified as self-adjoint extensions of $\mathscr{H}_\alpha^\pm$ (resp., $\mathscr{H}_\alpha$).

In fact, such an analysis for $\mathscr{H}_\alpha^\pm$ (resp., $\mathscr{H}_\alpha$) is naturally boiled down to the analysis of such operators *on each fibre* and a subsequent recombination of the information over the whole *constant-fibre orthogonal sum*.

To develop this approach, it is convenient to introduce on each fibre $\mathfrak{h}_\pm$, thus for each $k \in \mathbb{Z}$, the operators

$$A_\alpha^\pm(k) \;:=\; -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2|x|^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2}\,, \qquad \mathcal{D}(A_\alpha(k)) \;:=\; C_0^\infty(\mathbb{R}^+)\,, \tag{6.2.16}$$

and similarly on $\mathfrak{h}$ we define

$$\begin{aligned} \mathcal{D}(A_\alpha(k)) \;&:=\; C_0^\infty(\mathbb{R}^-) \boxplus C_0^\infty(\mathbb{R}^+) \\ A_\alpha(k) \;&:=\; A_\alpha^-(k) \oplus A_\alpha^+(k)\,, \end{aligned} \tag{6.2.17}$$

where the notation '$\boxplus$' simply indicates the direct sum of two (non-complete) subspaces of each summand of the orthogonal sum of two Hilbert spaces.

By construction the map $\mathbb{Z} \ni k \mapsto A_\alpha(k)$ has values in the space of densely defined, symmetric, non-negative operators on $\mathfrak{h}$, *all* with the *same* domain irrespectively of k. In each $A_\alpha(k)$ the integer k plays the role of a fixed parameter. Moreover, all the $A_\alpha(k)$'s are closable and each $\overline{A_\alpha(k)}$ is non-negative and with the same dense domain in $\mathfrak{h}$.

As non-trivial self-adjoint extensions are suitable restrictions of the adjoints, let us characterise the latter operators. The adjoint of H_α is the maximal realisation of the same differential operator, that is,

$$\begin{aligned} \mathcal{D}((\mathsf{H}_\alpha^\pm)^*) \;&=\; \left\{ \begin{array}{c} \phi \in L^2(\mathbb{R}^\pm \times S^1, \mathrm{d}x\mathrm{d}y) \text{ such that} \\ \Big(-\frac{\partial^2}{\partial x^2} - |x|^{2\alpha}\frac{\partial^2}{\partial y^2} + \frac{\alpha(2+\alpha)}{4x^2}\Big)\phi \in L^2(\mathbb{R}^\pm \times S^1, \mathrm{d}x\mathrm{d}y) \end{array} \right\} \\ (\mathsf{H}_\alpha^\pm)\phi \;&=\; \Big(-\frac{\partial^2}{\partial x^2} - |x|^{2\alpha}\frac{\partial^2}{\partial y^2} + \frac{\alpha(2+\alpha)}{4x^2}\Big)\phi\,. \end{aligned} \tag{6.2.18}$$

This, and the unitary equivalence (6.2.13), yields at once

$$\begin{aligned} \mathcal{D}((\mathscr{H}_\alpha^\pm)^*) \;&=\; \left\{ \begin{array}{c} \psi \equiv (\psi_k)_{k\in\mathbb{Z}} \in \bigoplus_{k\in\mathbb{Z}} L^2(\mathbb{R}^\pm, \mathrm{d}x) \;\text{ such that} \\ \displaystyle\sum_{k\in\mathbb{Z}} \Big\|\Big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2|x|^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2}\Big)\psi_k\Big\|^2_{L^2(\mathbb{R}^\pm,\mathrm{d}x)} \;<\; +\infty \end{array} \right\} \\ (\mathscr{H}_\alpha^\pm)^*\psi \;&=\; \Big(\Big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2|x|^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2}\Big)\psi_k\Big)_{k\in\mathbb{Z}}\,. \end{aligned} \tag{6.2.19}$$

Clearly, $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ is a weak second derivative in (6.2.19) and a classical second derivative in (6.2.14). Furthermore, with respect to the decomposition (6.2.9),

$$(\mathscr{H}_\alpha)^* \;=\; (\mathscr{H}_\alpha^-)^* \oplus (\mathscr{H}_\alpha^+)^* \,. \tag{6.2.20}$$

Analogously to (6.2.19), one has

$$\begin{aligned} \mathcal{D}(A_\alpha^\pm(k)^*) \;&=\; \left\{ \begin{array}{c} g^\pm \in L^2(\mathbb{R}^\pm, \mathrm{d}x) \;\text{ such that} \\ \big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2|x|^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2}\big) g^\pm \in L^2(\mathbb{R}^\pm, \mathrm{d}x) \end{array} \right\} \\ A_\alpha^\pm(k)^* g^\pm \;&=\; \Big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2|x|^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2}\Big) g^\pm \,, \end{aligned} \tag{6.2.21}$$

and

$$A_\alpha(k)^* \;=\; A_\alpha^-(k)^* \oplus A_\alpha^+(k)^* \,. \tag{6.2.22}$$

6.3 Extensions of the differential operator on each half-fibre

In this Section and in the next one we classify the self-adjoint extensions of the right-fibre operators $A_\alpha(k)^+$ defined in (6.2.16) for $\alpha \in [0,1)$ and $k \in \mathbb{Z}$, with respect to the fibre Hilbert space $L^2(\mathbb{R}^+, \mathrm{d}x)$.

For simplicity of notation, we shall temporarily drop the superscript '+' and simply write $A_\alpha(k)$ for $A_\alpha(k)^+$, and $\langle \cdot, \cdot \rangle_{L^2}$ and $\| \cdot \|_{L^2}$ for scalar products and norms taken in $L^2(\mathbb{R}^+)$, with analogous notation for the Sobolev norms. Obviously, the whole discussion is completely analogous for $A_\alpha(k)^-$ in $L^2(\mathbb{R}^-)$ instead of $A_\alpha(k)^+$.

As already recalled from [63, Corollary 3.8], for each fixed $\alpha \in [0,1)$ and $k \in \mathbb{Z}$, $A_\alpha(k)$ has deficiency index 1, hence admits a one-(real-)parameter family of self-adjoint extensions. We reconstruct and classify this family by means of the KVB extension theory [62].

When $\alpha = 0$ the operator $A_\alpha(k)$ is the minimally defined, shifted Laplacian $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2$ on $L^2(\mathbb{R}^+)$: the family of its self-adjoint realisations is well-known (see, e.g., [66, 46]) and the extension formulas that we find for $\alpha \in (0,1)$ take indeed the usual form for the extensions of the Laplacian in the limit $\alpha \downarrow 0$.

Let us observe preliminarily that $A_\alpha(k)$ has strictly positive lower bound for every non-zero k. Indeed,

$$\min_{x \in \mathbb{R}^+} \Big(k^2 x^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2} \Big) \;=\; (1+\alpha)\big(\tfrac{2+\alpha}{4}\big)^{\frac{\alpha}{1+\alpha}} |k|^{\frac{2}{1+\alpha}} \;=:\; M_{\alpha,k} \,,$$

whence

$$\langle h, A_\alpha(k) h \rangle_{L^2} \;\geqslant\; M_{\alpha,k} \|h\|_{L^2}^2 \qquad \forall h \in \mathcal{D}(A_\alpha(k)) \,. \tag{6.3.1}$$

Instead, when $k = 0$ one sees that

$$\inf_{h \in \mathcal{D}(A_\alpha(0)) \setminus \{0\}} \frac{\langle h, A_\alpha(0) h \rangle_{L^2}}{\|h\|_{L^2}^2} \;=\; 0 \,. \tag{6.3.2}$$

Therefore, as long as $k \neq 0$, owing to (6.3.1) we can apply the KVB extension theory directly in the setting of a *strictly positive operator*. This programme will be completed in the present Section. The special case $k = 0$ is deferred to the appendix of this chapter, where we highlight the main steps that need be modified – starting from the auxiliary shifted operator $A_\alpha(0) + \mathbb{1}$, which has again strictly positive bottom.

For convenience of notation let us set

$$C_\alpha \;:=\; \frac{\alpha(2+\alpha)}{4} \,. \tag{6.3.3}$$

Then $C_\alpha \in [0, \frac{3}{4})$. Let us also refer to

$$S_{\alpha,k} \;:=\; -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2 x^{2\alpha} + \frac{C_\alpha}{x^2} \,, \tag{6.3.4}$$

as the differential operator (with no domain specification) representing the action of both $A_\alpha(k)$ and $A_\alpha(k)^*$, where the derivative is classical or weak depending on the context.

Clearly, in order to characterise the operator closure $\overline{A_\alpha(k)}$ of $A_\alpha(k)$, its Friedrichs extension $A_{\alpha,F}(k)$, as well as any other self-adjoint extension, it suffices to indicate the corresponding domains, for all such operators are restrictions of the adjoint $A_\alpha(k)^*$ and as such they all act with the action of the differential operator $S_{\alpha,k}$.

Here is the main result of this Section.

Theorem 6.3.1. *Let $\alpha \in [0,1)$ and $k \in \mathbb{Z}\setminus\{0\}$.*

(i) The operator closure of $A_\alpha(k)$ has domain

$$\mathcal{D}(\overline{A_\alpha(k)}) \;=\; H^2_0(\mathbb{R}^+) \cap L^2(\mathbb{R}^+, \langle x\rangle^{4\alpha}\,\mathrm{d}x)\,. \tag{6.3.5}$$

(ii) The adjoint of $A_\alpha(k)$ has domain

$$\begin{aligned} \mathcal{D}(A_\alpha(k)^*) \;&=\; \left\{ \begin{array}{c} g \in L^2(\mathbb{R}^+) \;\; \textit{such that} \\ \big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2x^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2}\big)g \in L^2(\mathbb{R}^+) \end{array} \right\} \\ &=\; \mathcal{D}(\overline{A_\alpha(k)}) \dotplus \mathrm{span}\{\Psi_{\alpha,k}\} \dotplus \mathrm{span}\{\Phi_{\alpha,k}\}\,, \end{aligned} \tag{6.3.6}$$

where $\Phi_{\alpha,k}$ and $\Psi_{\alpha,k}$ are two smooth functions on $\mathbb{R}^+$ explicitly defined, in terms of modified Bessel functions, respectively by formula (6.3.12) *and by formulas* (6.3.21)*,* (6.3.23)*,* (6.3.26)*, and* (6.3.28) *below. Moreover,*

$$\ker A_\alpha(k)^* \;=\; \mathrm{span}\{\Phi_{\alpha,k}\}\,. \tag{6.3.7}$$

(iii) The Friedrichs extension of $A_\alpha(k)$ has operator domain

$$\begin{aligned} \mathcal{D}(A_{\alpha,F}(k)) \;&=\; \big\{g \in \mathcal{D}(A_\alpha(k)^*)\,\big|\, g(x) \overset{x\downarrow 0}{=} g_1x^{1+\frac{\alpha}{2}} + o(x^{\frac{3}{2}}),\; g_1 \in \mathbb{C}\big\} \\ &=\; \mathcal{D}(\overline{A_\alpha(k)}) \dotplus \mathrm{span}\{\Psi_{\alpha,k}\} \end{aligned} \tag{6.3.8}$$

and form domain

$$\mathcal{D}[A_{\alpha,F}(k)] \;=\; H^1_0(\mathbb{R}^+) \cap L^2(\mathbb{R}^+, \langle x\rangle^{2\alpha}\,\mathrm{d}x)\,. \tag{6.3.9}$$

Moreover, $A_{\alpha,F}(k)$ is the only self-adjoint extension of $A_\alpha(k)$ whose operator domain is entirely contained in $\mathcal{D}(x^{-1})$, namely the self-adjointness domain of the operator of multiplication by x^{-1}.

(iv) The self-adjoint extensions of $A_\alpha(k)$ in $L^2(\mathbb{R}^+)$ form the family

$$\{A^{[\gamma]}_\alpha(k)\,|\,\gamma \in \mathbb{R}\cup\{\infty\}\}\,.$$

The extension with $\gamma = \infty$ is the Friedrichs extension, and for generic $\gamma \in \mathbb{R}$ one has

$$\mathcal{D}(A^{[\gamma]}_\alpha(k)) \;=\; \big\{g \in \mathcal{D}(A_\alpha(k)^*)\,\big|\, g(x) \overset{x\downarrow 0}{=} g_0x^{-\frac{\alpha}{2}} + \gamma g_0 x^{1+\frac{\alpha}{2}} + o(x^{\frac{3}{2}}),\; g_0 \in \mathbb{C}\big\}\,. \tag{6.3.10}$$

It is interesting to immediately point out that the asymptotics near $x = 0$ of functions belonging to $\mathcal{D}(A^{[\gamma]}_\alpha(k))$ depend on α, but do not depend on k.

The proof of Theorem 6.3.1 requires an amount of preparatory material that is presented in Sections 6.3.1-6.3.5 and will be finally completed in Section 6.3.6.

Despite the technical hypothesis $k \neq 0$ in Theorem 6.3.1, the same conclusions hold for $k = 0$, by considering the shifted operator $A_\alpha(0) + \mathbb{1}$, which is now strictly positive (the details are given in the Appendix, see Theorem 6.7.11).

6.3.1 Homogeneous differential problem: kernel of $A_\alpha(k)^*$

Let us qualify the kernel of the adjoint $A_\alpha(k)^*$.

To this aim, we make use of the modified Bessel functions K_ν and I_ν [2, Sect. 9.6], that are two explicit, linearly independent, smooth solutions to the modified Bessel equation

$$z^2w'' + zw' - (z^2+\nu^2)w \;=\; 0, \qquad z \in \mathbb{R}^+ \tag{6.3.11}$$

with parameter $\nu \in \mathbb{C}$. In particular, in terms of $K_{\frac{1}{2}}$ and $I_{\frac{1}{2}}$ we define the functions

$$\begin{aligned} \Phi_{\alpha,k}(x) \;&:=\; \sqrt{x}\,K_{\frac{1}{2}}\big(\tfrac{|k|}{1+\alpha}\,x^{1+\alpha}\big) \\ F_{\alpha,k}(x) \;&:=\; \sqrt{x}\,I_{\frac{1}{2}}\big(\tfrac{|k|}{1+\alpha}\,x^{1+\alpha}\big)\,. \end{aligned} \tag{6.3.12}$$

Explicitly, as can be deduced from [2, Eq. (10.2.4), (10.2.13), and (10.2.14)],

$$\begin{aligned} \Phi_{\alpha,k}(x) &:= \sqrt{\tfrac{\pi(1+\alpha)}{2|k|}}\, x^{-\alpha/2}\, e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}} \\ F_{\alpha,k}(x) &:= \sqrt{\tfrac{2(1+\alpha)}{\pi|k|}}\, x^{-\alpha/2}\, \sinh\big(\tfrac{|k|}{1+\alpha}\, x^{1+\alpha}\big)\,. \end{aligned} \tag{6.3.13}$$

From (6.3.13) we obtain the short-distance asymptotics

$$\begin{aligned} \Phi_{\alpha,k}(x) &\overset{x\downarrow 0}{=} \sqrt{\tfrac{\pi(1+\alpha)}{2|k|}}\, x^{-\frac{\alpha}{2}} - \sqrt{\tfrac{\pi\,|k|}{2(1+\alpha)}}\, x^{1+\frac{\alpha}{2}} + \sqrt{\tfrac{\pi\,|k|^3}{8(1+\alpha)^3}}\, x^{2+\frac{3}{2}\alpha} + O(x^{3+\frac{5}{2}\alpha}) \\ F_{\alpha,k}(x) &\overset{x\downarrow 0}{=} \sqrt{\tfrac{2|k|}{(1+\alpha)\pi}}\, x^{1+\frac{\alpha}{2}} + O(x^{3+\frac{5}{2}\alpha}), \end{aligned} \tag{6.3.14}$$

and the large-distance asymptotics

$$\begin{aligned} \Phi_{\alpha,k}(x) &\overset{x\to+\infty}{=} \sqrt{\tfrac{\pi(1+\alpha)}{2|k|}}\, e^{-\frac{|k|x^{1+\alpha}}{1+\alpha}}\, x^{-\frac{\alpha}{2}}(1+O(x^{-(1+\alpha)})) \\ F_{\alpha,k}(x) &\overset{x\to+\infty}{=} \sqrt{\tfrac{1+\alpha}{2\pi|k|}}\, e^{\frac{|k|x^{1+\alpha}}{1+\alpha}}\, x^{-\frac{\alpha}{2}}(1+O(x^{-(1+\alpha)})), \end{aligned} \tag{6.3.15}$$

as well as the norm

$$\|\Phi_{\alpha,k}\|_{L^2}^2 \;=\; \pi\,(1+\alpha)^{\frac{1-\alpha}{1+\alpha}}\,\Gamma\big(\tfrac{1-\alpha}{1+\alpha}\big)\,(2|k|)^{-\frac{2}{1+\alpha}}\,. \tag{6.3.16}$$

Lemma 6.3.2. *Let $\alpha \in (0,1)$ and $k \in \mathbb{Z}\backslash\{0\}$. One has*

$$\ker A_\alpha(k)^* \;=\; \mathrm{span}\{\Phi_{\alpha,k}\}\,. \tag{6.3.17}$$

Proof. Owing to (6.2.21), a generic $h \in \ker A_\alpha(k)^*$ belongs to $L^2(\mathbb{R}^+)$ and satisfies

$$S_{\alpha,k}\, h \;=\; -h'' + k^2 x^{2\alpha} h + C_\alpha\, x^{-2} h \;=\; 0\,. \tag{i}$$

Setting

$$z \;:=\; \frac{|k|}{1+\alpha}\, x^{1+\alpha}, \qquad w(z) \;:=\; \frac{h(x)}{\sqrt{x}}, \qquad \nu \;:=\; \frac{\sqrt{1+4C_\alpha}}{2(1+\alpha)} \;=\; \frac{1}{2}, \tag{ii}$$

the ordinary differential equation (i) takes precisely the form (6.3.11) with the considered ν. The two linearly independent solutions $K_{\frac{1}{2}}$ and $I_{\frac{1}{2}}$ to (6.3.11) yield, through the transformation (ii) above, the two linearly independent solutions (6.3.12) to (i). In fact, only $\Phi_{\alpha,k}$ is square-integrable, whereas $F_{\alpha,k}$ fails to be so at infinity (as is seen from (6.3.16)-(6.3.15)). Formula (6.3.17) is thus proved. □

6.3.2 Non-homogeneous inverse differential problem

Let us now focus on the non-homogeneous problem

$$S_{\alpha,k}\, u \;=\; g \tag{6.3.18}$$

in the unknown u for given g. With respect to the fundamental system $\{F_{\alpha,k}, \Phi_{\alpha,k}\}$ given by (6.3.12), of solutions for the problem $S_{\alpha,k}\, u = 0$, the general solution is given by

$$u \;=\; c_1 F_{\alpha,k} + c_2 \Phi_{\alpha,k} + u_{\mathrm{part}} \tag{6.3.19}$$

for $c_1, c_2 \in \mathbb{C}$ and some particular solution u_{part}, i.e., $S_{\alpha,k}\, u_{\mathrm{part}} = g$.

The Wronskian

$$W(\Phi_{\alpha,k}, F_{\alpha,k})(r) \;:=\; \det\begin{pmatrix} \Phi_{\alpha,k}(r) & F_{\alpha,k}(r) \\ \Phi'_{\alpha,k}(r) & F'_{\alpha,k}(r) \end{pmatrix} \tag{6.3.20}$$

relative to the fundamental system $\{F_{\alpha,k}, \Phi_{\alpha,k}\}$ is clearly constant in r, since it is evaluated on solutions to the homogeneous differential problem, with a value that can be computed by means of the asymptotics (6.3.14) or (6.3.15) and amounts to

$$W(\Phi_{\alpha,k}, F_{\alpha,k}) \;=\; 1+\alpha \;=:\; W\,. \tag{6.3.21}$$

A standard application of the method of variation of constants [111, Section 2.4] shows that we can take u_{part} to be

$$u_{\text{part}}(r) \;=\; \int_0^{+\infty} G_{\alpha,k}(r,\rho) g(\rho)\,\mathrm{d}\rho\,, \tag{6.3.22}$$

where

$$G_{\alpha,k}(r,\rho) \;:=\; \frac{1}{W}\begin{cases}\Phi_{\alpha,k}(r)F_{\alpha,k}(\rho) & \text{if } 0<\rho<r\\ F_{\alpha,k}(r)\Phi_{\alpha,k}(\rho) & \text{if } 0<r<\rho\,.\end{cases} \tag{6.3.23}$$

For $a \in \mathbb{R}$ and $k \in \mathbb{Z}\backslash\{0\}$, let $R^{(a)}_{G_{\alpha,k}}$ be the integral operator acting on functions g on $\mathbb{R}^+$ as

$$\begin{aligned}\big(R^{(a)}_{G_{\alpha,k}} g\big)(x) \;&:=\; \int_0^{+\infty} \mathscr{G}^{(a)}_{\alpha,k}(x,\rho)\, g(\rho)\,\mathrm{d}\rho\\ \mathscr{G}^{(a)}_{\alpha,k}(x,\rho) \;&:=\; x^a\, k^2\, G_{\alpha,k}(x,\rho)\,,\end{aligned} \tag{6.3.24}$$

and let

$$R_{G_{\alpha,k}} \;:=\; |k|^{-2}\, R^{(0)}_{G_{\alpha,k}}\,, \tag{6.3.25}$$

whence

$$(R_{G_{\alpha,k}} g)(x) \;=\; \int_0^{+\infty} G_{\alpha,k}(x,\rho)\, g(\rho)\,\mathrm{d}\rho\,. \tag{6.3.26}$$

The following property holds.

Lemma 6.3.3. *Let $\alpha \in (0,1)$ and $k \in \mathbb{Z}\backslash\{0\}$.*

(i) For each $a \in (-\frac{1-\alpha}{2}, 2\alpha]$, $R^{(a)}_{G_{\alpha,k}}$ can be realised as an everywhere defined, bounded operator on $L^2(\mathbb{R}^+,\mathrm{d}x)$, which is also self-adjoint if $a = 0$.

(ii) When $a = 2\alpha$, the operator $R^{(2\alpha)}_{G_{\alpha,k}}$ is bounded uniformly in k.

Remark 6.3.4. The uniformity in k of the norm of $R^{(2\alpha)}_{G_{\alpha,k}}$ will be useful in Subsect. 6.6.5. In fact, it is to prove the boundedness claim (i) in a form that implies the k-uniformity of claim (ii) that we have to do a somewhat lengthy proof, given in the Appendix 6.7.3.

A relevant consequence of Lemma 6.3.3 is the following large-distance decaying behaviour of a generic function of the form $R_{G_{\alpha,k}} u$.

Corollary 6.3.5. *Let $\alpha \in (0,1)$ and $k \in \mathbb{Z}\backslash\{0\}$. Then*

$$\operatorname{ran} R_{G_{\alpha,k}} \;\subset\; L^2(\mathbb{R}^+, \langle x\rangle^{4\alpha}\mathrm{d}x)\,. \tag{6.3.27}$$

Proof. By Lemma 6.3.3 we know that both $x^{2\alpha}R_{G_{\alpha,k}}$ and $R_{G_{\alpha,k}}$ are bounded in $L^2(\mathbb{R}^+,\mathrm{d}x)$. Therefore, for any $u \in L^2(\mathbb{R}^+,\mathrm{d}x)$ one has that both $R_{G_{\alpha,k}}u$ and $x^{2\alpha}R_{G_{\alpha,k}}u$ must belong to $L^2(\mathbb{R}^+,\mathrm{d}x)$, whence indeed $R_{G_{\alpha,k}}u \in L^2(\mathbb{R}^+,(1+x^{4\alpha})\mathrm{d}x)$. □

Moreover, we recognise that $R_{G_{\alpha,k}}$ inverts a self-adjoint extension of $A_\alpha(k)$.

Lemma 6.3.6. *Let $\alpha \in (0,1)$ and $k \in \mathbb{Z}\backslash\{0\}$. There exists a self-adjoint extension $\mathscr{A}_\alpha(k)$ of $A_\alpha(k)$ in $L^2(\mathbb{R}^+)$ which has everywhere defined and bounded inverse and such that $\mathscr{A}_\alpha(k)^{-1} = R_{G_{\alpha,k}}$.*

Proof. $R_{G_{\alpha,k}}$ is bounded and self-adjoint (Lemma 6.3.3), and by construction satisfies $S_{\alpha,k}\, R_{G_{\alpha,k}}\, g = g\ \forall g \in L^2(\mathbb{R}^+)$. Therefore, $R_{G_{\alpha,k}} g = 0$ for some $g \in L^2(\mathbb{R}^+)$ implies $g = 0$, i.e., $R_{G_{\alpha,k}}$ is injective. Then $R_{G_{\alpha,k}}$ has dense range ($(\operatorname{ran} R_{G_{\alpha,k}})^\perp = \ker R_{G_{\alpha,k}}$). As a consequence (see, e.g., [102, Theorem 1.8(iv)]), $\mathscr{A}_\alpha(k) := R^{-1}_{G_{\alpha,k}}$ is self-adjoint. One thus has $R_{G_{\alpha,k}} = \mathscr{A}_\alpha(k)^{-1}$ and from the identity $A_\alpha(k)^* R_{G_{\alpha,k}} = \mathbb{1}$ on $L^2(\mathbb{R}^+)$ one deduces that for any $h \in \mathcal{D}(\mathscr{A}_\alpha(k))$, say, $h = R_{G_{\alpha,k}} g = \mathscr{A}_\alpha(k)^{-1} g$ for some $g \in L^2(\mathbb{R}^+)$, the identity $A_\alpha(k)^* h = \mathscr{A}_\alpha(k) h$ holds. This means that $A_\alpha(k)^* \supset \mathscr{A}_\alpha(k)$, whence also $\overline{A_\alpha(k)} = A_\alpha(k)^{**} \subset \mathscr{A}_\alpha(k)$, i.e., $\mathscr{A}_\alpha(k)$ is a self-adjoint extension of $A_\alpha(k)$. □

We conclude this Subsection by examining the function

$$\Psi_{\alpha,k} \;:=\; R_{G_{\alpha,k}}\Phi_{\alpha,k}\,. \tag{6.3.28}$$

We prove the following useful asymptotics.

Lemma 6.3.7. *Let $\alpha \in (0,1)$ and $k \in \mathbb{Z}\backslash\{0\}$. Then*

$$\Psi_{\alpha,k}(x) \overset{x\downarrow 0}{=} \sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\,\|\Phi_{\alpha,k}\|_{L^2}^2\,x^{1+\alpha/2} + o(x^{3/2})\,. \tag{6.3.29}$$

Proof. Owing to (6.3.23) and (6.3.26),

$$\Psi_{\alpha,k}(x) \;=\; \frac{1}{W}\Big(\Phi_{\alpha,k}(x)\int_0^x F_{\alpha,k}(\rho)\Phi_{\alpha,k}(\rho)\mathrm{d}\rho + F_{\alpha,k}(x)\int_x^{+\infty}\Phi_{\alpha,k}(\rho)^2\mathrm{d}\rho\Big)\,.$$

By means of (6.3.14) we then find

$$\Phi_{\alpha,k}(x)\int_0^x F_{\alpha,k}(\rho)\Phi_{\alpha,k}(\rho)\mathrm{d}\rho \overset{x\downarrow 0}{=} \sqrt{\tfrac{\pi(1+\alpha)}{8|k|}}x^{-\frac{\alpha}{2}+2} + o(x^3) \overset{x\downarrow 0}{=} o(x^{3/2})$$

(having explicitly used that $\alpha \in (0,1)$), and

$$\begin{aligned} F_{\alpha,k}(x)\int_x^{+\infty}\Phi_{\alpha,k}(\rho)^2\mathrm{d}\rho &\overset{x\downarrow 0}{=} F_{\alpha,k}(x)\Big(\|\Phi_{\alpha,k}\|_{L^2}^2 - \int_0^x \Phi_{\alpha,k}(\rho)^2\mathrm{d}\rho\Big) \\ &\overset{x\downarrow 0}{=} \sqrt{\tfrac{2|k|}{\pi(1+\alpha)}}\,\|\Phi_{\alpha,k}\|_{L^2}^2\,x^{1+\frac{\alpha}{2}} + O(x^{2-\frac{\alpha}{2}})\,. \end{aligned}$$

The latter quantity is leading, and using the expression (6.3.21) for W yields (6.3.29). □

In fact, using (6.3.21), (6.3.23), and (6.3.26) as in the proof above, and using the explicit expression (6.3.13) for $\Phi_{\alpha,k}$ and $F_{\alpha,k}$, one finds

$$\begin{aligned} \Psi_{\alpha,k}(x) \;=\; \sqrt{\tfrac{\pi(1+\alpha)}{2|k|^3}}\Big(& x^{-\frac{\alpha}{2}}\,e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}}\int_0^x \mathrm{d}\rho\,\rho^{-\alpha}\sinh\big(\tfrac{|k|}{1+\alpha}\rho^{1+\alpha}\big)\,e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}} \\ &+ x^{-\frac{\alpha}{2}}\sinh\big(\tfrac{|k|}{1+\alpha}x^{1+\alpha}\big)\int_x^{+\infty}\mathrm{d}\rho\,\rho^{-\alpha}\,e^{-\frac{2|k|}{1+\alpha}\rho^{1+\alpha}}\Big) \end{aligned} \tag{6.3.30}$$

or also, with a change of variable $\rho \mapsto |k|^{\frac{1}{1+\alpha}}\rho$,

$$\begin{aligned} \Psi_{\alpha,k}(x) \;=\; & \sqrt{\tfrac{\pi(1+\alpha)}{2}}|k|^{-\frac{5+\alpha}{2(1+\alpha)}}\times \\ &\times\Big(x^{-\frac{\alpha}{2}}\,e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}}\int_0^{x|k|^{\frac{1}{1+\alpha}}}\mathrm{d}\rho\,\rho^{-\alpha}\sinh\big(\tfrac{\rho^{1+\alpha}}{1+\alpha}\big)\,e^{-\frac{\rho^{1+\alpha}}{1+\alpha}} \\ &\quad + x^{-\frac{\alpha}{2}}\sinh\big(\tfrac{|k|}{1+\alpha}x^{1+\alpha}\big)\int_{x|k|^{\frac{1}{1+\alpha}}}^{+\infty}\mathrm{d}\rho\,\rho^{-\alpha}\,e^{-\frac{2\rho^{1+\alpha}}{1+\alpha}}\Big)\,. \end{aligned} \tag{6.3.31}$$

However, we will not need such an explicit expression for $\Psi_{\alpha,k}$ until Subsect. 6.7.8.

6.3.3 Operator closure $\overline{A_\alpha(k)}$

The next fundamental ingredient for the KVB extension scheme is the qualification of the operator closure $\overline{A_\alpha(k)}$ of $A_\alpha(k)$.

In this Subsection we establish the following result.

Proposition 6.3.8. *Let $\alpha \in (0,1)$ and $k \in \mathbb{Z}\backslash\{0\}$. Then*

$$\mathcal{D}(\overline{A_\alpha(k)}) \;=\; H_0^2(\mathbb{R}^+)\cap L^2(\mathbb{R}^+,\langle x\rangle^{4\alpha}\,\mathrm{d}x)\,. \tag{6.3.32}$$

Here, by definition,

$$\mathcal{D}(\overline{A_\alpha(k)}) \;=\; \overline{C_0^\infty(\mathbb{R}^+)}^{\|\,\|_{A_\alpha(k)}}, \tag{6.3.33}$$

where the norm $\|\cdot\|_{A_\alpha(k)}$ is defined by

$$\begin{aligned} \|\varphi\|^2_{A_\alpha(k)} \;&:=\; \|-\varphi'' + k^2x^{2\alpha}\varphi + C_\alpha x^{-2}\varphi\|^2_{L^2(\mathbb{R}^+)} + \|\varphi\|^2_{L^2(\mathbb{R}^+)} \\ &\qquad \forall\varphi\in\mathcal{D}(A_\alpha(k)) = C_0^\infty(\mathbb{R}^+)\,. \end{aligned} \tag{6.3.34}$$

In order to prove Proposition 6.3.8 we shall need several lemmas, whose proves follow standard ODE arguments and are given in the Appendix.

First, we need a useful representation of $\mathcal{D}(A_\alpha(k)^*)$ based on the differential nature (6.2.21) of the adjoint $A_\alpha(k)^*$.

Lemma 6.3.9. *Let $\alpha\in(0,1)$ and $k\in\mathbb{Z}\backslash\{0\}$.*

(i) For each $g\in\mathcal{D}(A_\alpha(k)^*)$ there exist uniquely determined constants $a_0^{(g)}, a_\infty^{(g)}\in\mathbb{C}$ and functions

$$\begin{aligned} b_0^{(g)}(x) \;&:=\; \frac{1}{W}\int_0^x F_{\alpha,k}(\rho)(A_\alpha(k)^*g)(\rho)\,\mathrm{d}\rho \\ b_\infty^{(g)}(x) \;&:=\; -\frac{1}{W}\int_0^x \Phi_{\alpha,k}(\rho)(A_\alpha(k)^*g)(\rho)\,\mathrm{d}\rho \end{aligned} \tag{6.3.35}$$

on $\mathbb{R}^+$ such that

$$g \;=\; a_0^{(g)}F_{\alpha,k} + a_\infty^{(g)}\Phi_{\alpha,k} + b_\infty^{(g)}F_{\alpha,k} + b_0^{(g)}\Phi_{\alpha,k} \tag{6.3.36}$$

with $\Phi_{\alpha,k}$ and $F_{\alpha,k}$ defined in (6.3.12) *and $W=-(1+\alpha)$ as in* (6.3.21).

(ii) The functions $b_0^{(g)}$ and $b_\infty^{(g)}$ satisfy the properties

$$b_0^{(g)}, b_\infty^{(g)} \in AC(\mathbb{R}^+) \tag{6.3.37}$$

$$b_0^{(g)}(x) \overset{x\downarrow 0}{=} o(1), \quad b_\infty^{(g)}(x) \overset{x\downarrow 0}{=} o(1) \tag{6.3.38}$$

$$b_\infty^{(g)}(x)F_{\alpha,k}(x) + b_0^{(g)}(x)\Phi_{\alpha,k}(x) \overset{x\downarrow 0}{=} o(x^{3/2})\,. \tag{6.3.39}$$

Next, proceeding towards the proof of Proposition 6.3.8, we introduce, for any two functions in $\mathcal{D}(A_\alpha(k)^*)$, the Wronskian

$$\mathbb{R}^+\ni x\mapsto W_x(g,h) \;:=\; \det\begin{pmatrix} g(x) & h(x) \\ g'(x) & h'(x)\end{pmatrix}, \qquad g,h\in\mathcal{D}(A_\alpha(k)^*) \tag{6.3.40}$$

and the boundary form

$$\omega(g,h) \;:=\; \langle A_\alpha(k)^*g, h\rangle_{L^2} - \langle g, A_\alpha(k)^*h\rangle_{L^2}, \qquad g,h\in\mathcal{D}(A_\alpha(k)^*). \tag{6.3.41}$$

The boundary form is anti-symmetric, i.e.,

$$\omega(h,g) = -\overline{\omega(g,h)}, \tag{6.3.42}$$

and it is related to the Wronskian by

$$\omega(g,h) \;=\; -\lim_{x\downarrow 0} W_x(\overline{g},h)\,. \tag{6.3.43}$$

Indeed,

$$\begin{aligned} \omega(g,h) \;&=\; \int_0^{+\infty}(\overline{A_\alpha(k)^*g})(\rho)\,h(\rho)\,\mathrm{d}\rho - \int_0^{+\infty}\overline{g(\rho)}\,(A_\alpha(k)^*h)(\rho)\mathrm{d}\rho \\ &=\; \lim_{x\downarrow 0}\Big(\int_x^{+\infty}(\overline{-g''(\rho)}\,h(\rho)\,\mathrm{d}\rho + \int_x^{+\infty}\overline{g(\rho)}\,h''(\rho)\,\mathrm{d}\rho\Big) \\ &=\; \lim_{x\downarrow 0}\Big(\overline{g'(x)}h(x) - \overline{g(x)}h'(x)\Big) \;=\; -\lim_{x\downarrow 0} W_x(\overline{g},h)\,. \end{aligned}$$

It is also convenient to refer to the two-dimensional space of solutions to the differential problem $S_{\alpha,k}\, u = 0$ as the space

$$\mathcal{L} \;:=\; \{u : \mathbb{R}^+ \to \mathbb{C} \,|\, S_{\alpha,k}\, u = 0\} \;=\; \mathrm{span}\,\{\Phi_{\alpha,k}, F_{\alpha,k}\}\,, \tag{6.3.44}$$

where the second identity follows from what argued in the proof of Lemma 6.3.2. As well known, $x \mapsto W_x(u,v)$ is constant whenever $u, v \in \mathcal{L}$, and this constant is zero if and only if u and v are linearly dependent. Clearly, any $u \in \mathcal{L}$ is square-integrable around $x = 0$, as follows from the asymptotics (6.3.14).

Lemma 6.3.10. *Let $\alpha \in (0,1)$ and $k \in \mathbb{Z}\backslash\{0\}$. For given $u \in \mathcal{L}$,*

$$\begin{aligned} L_u : \mathcal{D}(A_\alpha(k)^*) &\to \mathbb{C} \\ g \mapsto L_u(g) \;&:=\; \lim_{x\downarrow 0} W_x(\overline{u}, g) \end{aligned} \tag{6.3.45}$$

defines a linear functional on $\mathcal{D}(A_\alpha^*(k))$ which vanishes on $\mathcal{D}(\overline{A_\alpha(k)})$.

With this preparatory material at hand, we can characterise the space $\mathcal{D}(\overline{A_\alpha(k)})$ as follows.

Lemma 6.3.11. *Let $\alpha \in (0,1)$, $k \in \mathbb{Z}\backslash\{0\}$, and $\varphi \in \mathcal{D}(A_\alpha(k)^*)$. The following conditions are equivalent:*

(i) $\varphi \in \mathcal{D}(\overline{A_\alpha(k)})$,

(ii) $\omega(\varphi, g) = 0$ *for all* $g \in \mathcal{D}(A_\alpha(k)^*)$,

(iii) $L_u(\varphi) = 0$ *for all* $u \in \mathcal{L}$,

(iv) in the decomposition (6.3.36) *of φ one has* $a_0^{(\varphi)} = a_\infty^{(\varphi)} = 0$.

We can now characterise the short-distance behaviour of the functions in $\mathcal{D}(\overline{A_\alpha(k)})$ and of their derivative.

Lemma 6.3.12. *Let $\alpha \in (0,1)$ and $k \in \mathbb{Z}\setminus\{0\}$. If $\varphi \in \mathcal{D}(\overline{A_\alpha(k)})$, then $\varphi(x) = o(x^{3/2})$ and $\varphi'(x) = o(x^{1/2})$ as $x \downarrow 0$.*

Proof. Owing to Lemma 6.3.11,

$$\varphi \;=\; b_\infty^{(\varphi)} F_{\alpha,k} + b_0^{(\varphi)} \Phi_{\alpha,k}\,.$$

Thus, $\varphi = o(x^{\frac{3}{2}})$ follows from (6.3.39) of Lemma 6.3.9. Moreover,

$$\varphi' \;=\; \big(b_\infty^{(\varphi)} F_{\alpha,k} + b_0^{(\varphi)} \Phi_{\alpha,k}\big)' \;=\; b_\infty^{(\varphi)} F'_{\alpha,k} + b_0^{(\varphi)} \Phi'_{\alpha,k}\,,$$

thanks to the cancellation $(b_\infty^{(\varphi)})' F_{\alpha,k} + (b_0^{(\varphi)})' \Phi_{\alpha,k} = 0$ that follows from (6.3.35). From the short-distance asymptotics (6.3.14) one has

$$\begin{aligned} F_{\alpha,k}(x) \;&=\; O(x^{1+\frac{\alpha}{2}}), \qquad F'_{\alpha,k}(x) = O(x^{\frac{\alpha}{2}}), \\ \Phi_{\alpha,k}(x) \;&=\; O(x^{-\frac{\alpha}{2}}), \qquad \Phi_{\alpha,k}(x)' \;=\; O(x^{-(1+\frac{\alpha}{2})}), \end{aligned}$$

whence

$$\begin{aligned} |b_\infty^{(\varphi)}(x) F'_{\alpha,k}(x)| \;&\lesssim\; x^{\frac{\alpha}{2}}\, \|A_\alpha(k)^*\varphi\|_{L^2((0,x))} \Big(\int_0^x |\rho^{-\frac{\alpha}{2}}|^2 \mathrm{d}\rho\Big)^{\frac{1}{2}} \\ &\lesssim\; x^{\frac{1}{2}}\, \|\overline{A_\alpha(k)}\varphi\|_{L^2((0,x))} \;=\; o(x^{\frac{1}{2}}), \end{aligned}$$

and also

$$\begin{aligned} |b_0^{(\varphi)}(x) \Phi'_{\alpha,k}(x)| \;&\lesssim\; \frac{1}{x^{1+\frac{\alpha}{2}}}\, \|A_\alpha(k)^*\varphi\|_{L^2((0,x))} \Big(\int_0^x |\rho^{1+\frac{\alpha}{2}}|^2 \mathrm{d}\rho\Big)^{\frac{1}{2}} \\ &\lesssim\; x^{\frac{1}{2}}\, \|\overline{A_\alpha(k)}\varphi\|_{L^2((0,x))} \;=\; o(x^{\frac{1}{2}})\,. \end{aligned}$$

The proof is thus completed. □

We are finally in the condition to prove Proposition 6.3.8.

Proof of Proposition 6.3.8. Let us first prove the inclusion

$$(*) \qquad H^2_0(\mathbb{R}^+) \cap L^2(\mathbb{R}^+, \langle x\rangle^{4\alpha}\,\mathrm{d}x) \;\subset\; \mathcal{D}(\overline{A_\alpha(k)})\,.$$

If φ belongs to the space on the l.h.s. of (*), then $\varphi'' \in L^2(\mathbb{R})$, $x^{2\alpha}\varphi \in L^2(\mathbb{R})$, and $\varphi(x) = o(x^{3/2})$ as $x \downarrow 0$, whence also $x^{-2}\varphi \in L^2(\mathbb{R})$. As a consequence, $-\varphi'' + k^2x^{2\alpha}\varphi + C_\alpha x^{-2}\varphi \in L^2(\mathbb{R})$, i.e., owing to (6.2.21), $\varphi \in \mathcal{D}(A_\alpha(k)^*)$. Representing now φ according to (6.3.36) as

$$\varphi \;=\; a_0^{(\varphi)}F_{\alpha,k} + a_\infty^{(\varphi)}\Phi_{\alpha,k} + b_\infty^{(\varphi)}F_{\alpha,k} + b_0^{(\varphi)}\Phi_{\alpha,k}\,,$$

we deduce that $a_0^{(\varphi)} = a_\infty^{(\varphi)} = 0$, for otherwise the behaviour (6.3.14) of $\Phi_{\alpha,k}$ and $F_{\alpha,k}$ as $x \downarrow 0$ would be incompatible with $\varphi(x) = o(x^{3/2})$. Instead, the component $b_\infty^{(\varphi)}F_{\alpha,k} + b_0^{(\varphi)}\Phi_{\alpha,k}$ displays the $o(x^{3/2})$-behaviour, as we see from (6.3.39). Lemma 6.3.11 then implies $\varphi \in \mathcal{D}(\overline{A_\alpha(k)})$, which proves (*).

Next, let us prove the opposite inclusion

$$(**) \qquad H^2_0(\mathbb{R}^+) \cap L^2(\mathbb{R}^+, \langle x\rangle^{4\alpha}\,\mathrm{d}x) \;\supset\; \mathcal{D}(\overline{A_\alpha(k)})\,.$$

Owing to Lemma 6.3.6 there exists a self-adjoint extension $\mathscr{A}_\alpha(k)$ of $\overline{A_\alpha(k)}$ with $\mathcal{D}(\mathscr{A}_\alpha(k)) = \mathrm{ran}R_{G_{\alpha,k}}$, and owing to Corollary 6.3.5 $\mathrm{ran}R_{G_{\alpha,k}} \subset L^2(\mathbb{R}^+, \langle x\rangle^{4\alpha}\,\mathrm{d}x)$. Therefore, $\mathcal{D}(\overline{A_\alpha(k)}) \subset L^2(\mathbb{R}^+, \langle x\rangle^{4\alpha}\,\mathrm{d}x)$. It remains to prove that $\mathcal{D}(\overline{A_\alpha(k)}) \subset H^2_0(\mathbb{R}^+)$. For $\varphi \in \mathcal{D}(\overline{A_\alpha(k)}) \subset \mathcal{D}(A_\alpha(k)^*)$ formula (6.2.21) prescribes that $g := -\varphi'' + k^2x^{2\alpha}\varphi + C_\alpha x^{-2}\varphi \in L^2(\mathbb{R})$. As proved right above, $x^{2\alpha}\varphi \in L^2(\mathbb{R})$, whereas the property $x^{-2}\varphi \in L^2(\mathbb{R}^+)$ follows from Lemma 6.3.12. Then by linearity $\varphi'' \in L^2(\mathbb{R}^+)$, which also implies $\varphi \in H^2(\mathbb{R}^+)$ by standard arguments [69, Remark 4.21]. Lemma 6.3.12 ensures that $\varphi(0) = \varphi'(0) = 0$, and we conclude that $\varphi \in H^2_0(\mathbb{R}^+)$. This completes the proof of (**). □

6.3.4 Kreĭn-Višik-Birman extension scheme for symmetric positive operators

Following, e.g., [10], and [62], we recall the main theorem of the KVB self-adjoint extension theory.

Let $\mathcal{H}$ be a Hilbert space and H a linear operator that we assume to be symmetric, densely defined, and *positive* (i.e., there exists $c > 0$ such that $(v, Hv) \geq c\|v\|^2$, $\forall v \in \mathcal{H}$). Assume moreover that there exists a self-adjoint extension of H, denoted by $\mathscr{H}$, with everywhere defined bounded inverse. Notice that such an extension always exists when H is positive, since in this case one can take as $\mathscr{H}$ the Friedrich extension [100, Theorem X.32], which is also positive and thus has an everywhere defined bounded inverse.

Theorem 6.3.13 (Kreĭn-Višik-Birman extension Theorem)**.** .

- *The domain of the adjoint H^* can be decomposed as*

$$\mathcal{D}(H^*) \;=\; \mathcal{D}(\overline{H}) \dotplus \mathscr{H}^{-1}\ker H^* \dotplus \ker H^*, \tag{6.3.46}$$

and

$$\mathcal{D}(\mathscr{H}) \;=\; \mathcal{D}(\overline{H}) \dotplus \ker H^*.$$

- *There is a one-to-one correspondence $S \leftrightarrow \mathscr{H}^S$ between the self-adjoint extensions $\mathscr{H}^S$ of H and the self-adjoint operators S defined on Hilbert subspaces of* $\ker H^*$. *If S is any such operator with domain $\mathcal{D}(S) \subset \ker H^*$, the corresponding extension $\mathscr{H}^S$ is given by*

$$\mathcal{D}(\mathscr{H}^S) \;=\; \left\{ \begin{array}{c} \psi = \widetilde{\varphi} + \mathscr{H}^{-1}(Sv + w) + v \\ \textit{such that} \\ \widetilde{\varphi} \in \mathcal{D}(\overline{H}), \quad v \in \mathcal{D}(S), \\ w \in \ker(H^*) \cap \mathcal{D}(S)^\perp \end{array} \right\} \tag{6.3.47}$$

$$\mathscr{H}^S\psi \;=\; \overline{H}\widetilde{\varphi} + Sv + w\,.$$

6.3.5 Distinguished extension and induced classification

We apply here the general Theorem 6.3.13 to the operator $A_\alpha(k)$, exploiting the self-adjoint reference extension $\mathscr{A}_\alpha(k)$ (defined in Lemma 6.3.6), that has everywhere defined bounded inverse. Since (see Lemmas 6.3.2, 6.3.6, and (6.3.28))

$$\ker A_\alpha(k)^* = \mathrm{span}\{\Phi_{\alpha,k}\}\,, \qquad \text{and} \qquad \mathscr{A}_\alpha(k)^{-1}\Phi_{\alpha,k} = \Psi_{\alpha,k}\,,$$

Theorem 6.3.13 gives at once that all self-adjoint extensions of $A_\alpha(k)$ constitute a one-real-parameter-family $\{A_\alpha^{[\beta]}(k)\,|\,\beta\in\mathbb{R}\}$, given by

$$\begin{aligned}\mathcal{D}(A_\alpha^{[\beta]}(k)) &= \big\{\, g=\varphi+c(\beta\,\Psi_{\alpha,k}+\Phi_{\alpha,k})\,\big|\,\varphi\in\mathcal{D}(\overline{A_\alpha(k)}),\ c\in\mathbb{C}\big\}\\ A_\alpha^{[\beta]}(k)g &= A_\alpha(k)^*g \;=\; \overline{A_\alpha(k)}\,\varphi+c\,\beta\,\Phi_{\alpha,k}\end{aligned}\tag{6.3.48}$$

and we have the decomposition

$$\begin{aligned}\mathcal{D}(A_\alpha(k)^*) &= \mathcal{D}(\overline{A_\alpha(k)})\dotplus\operatorname{span}\{\Psi_{\alpha,k}\}\dotplus\operatorname{span}\{\Phi_{\alpha,k}\}\\ \mathcal{D}(\mathscr{A}_\alpha(k)) &= \mathcal{D}(\overline{A_\alpha(k)})\dotplus\operatorname{span}\{\Psi_{\alpha,k}\}\,.\end{aligned}\tag{6.3.49}$$

By comparing (6.3.49) with the short-range asymptotics for $\Phi_{\alpha,k}$ (formula (6.3.14) above), for $\Psi_{\alpha,k}$ (Lemma 6.3.7), and for the elements of $\mathcal{D}(\overline{A_\alpha(k)})$ (Lemma 6.3.12), one deduces that for a function

$$g \;=\; \varphi+c_1\Psi_{\alpha,k}+c_0\Phi_{\alpha,k} \;\in\; \mathcal{D}(A_\alpha(k)^*)\tag{6.3.50}$$

(with $\varphi\in\mathcal{D}(\overline{A_\alpha(k)})$ and $c_0,c_1\in\mathbb{C}$) the limits

$$\begin{aligned}g_0 &:= \lim_{x\downarrow 0}\,x^{\frac{\alpha}{2}}g(x) \;=\; c_0\sqrt{\tfrac{\pi(1+\alpha)}{2|k|}}\\ g_1 &:= \lim_{x\downarrow 0}\,x^{-(1+\frac{\alpha}{2})}(g(x)-g_0x^{-\frac{\alpha}{2}}) \;=\; c_1\sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\,\|\Phi_{\alpha,k}\|_{L^2}^2-c_0\sqrt{\tfrac{\pi|k|}{2(1+\alpha)}}\end{aligned}\tag{6.3.51}$$

exist and are finite, and one has the asymptotics

$$g(x)\;\overset{x\downarrow 0}{=}\;g_0x^{-\frac{\alpha}{2}}+g_1x^{1+\frac{\alpha}{2}}+o(x^{3/2})\,.\tag{6.3.52}$$

In turn, by comparing (6.3.50) with (6.3.48) we see that for given β the domain of the extension $A_\alpha^{[\beta]}(k)$ consists of all those g's in $\mathcal{D}(A_\alpha(k)^*)$ that, decomposed as in (6.3.50), satisfy the condition

$$c_1 \;=\; \beta\,c_0\,.\tag{6.3.53}$$

Moreover, replacing c_0 and c_1 of the expression (6.3.50) with g_0 and g_1 according to (6.3.51), the self-adjointness condition (6.3.53) takes the form

$$g_1 \;=\; \gamma\,g_0\,,\qquad \gamma\;:=\;\tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|_{L^2}^2}{\pi(1+\alpha)}\,\beta-1\Big)\,.\tag{6.3.54}$$

We can therefore equivalently parametrise each extension with the new real parameter γ and write $A_\alpha^{[\gamma]}(k)$ in place of $A_\alpha^{[\beta]}(k)$, with β and γ linked by (6.3.54).

We have thus proved the following.

Proposition 6.3.14. *Let $\alpha\in(0,1)$ and $k\in\mathbb{Z}\setminus\{0\}$. The self-adjoint extensions of $A_\alpha(k)$ in $L^2(\mathbb{R}^+)$ form the family $\{A_\alpha^{[\gamma]}(k)\,|\,\gamma\in\mathbb{R}\cup\{\infty\}\}$. The extension with $\gamma=\infty$ is the reference extension $\mathscr{A}_\alpha(k)=R_{G_{\alpha,k}}^{-1}$, where $R_{G_{\alpha,k}}$ is the operator defined by* (6.3.26)*. For generic $\gamma\in\mathbb{R}$ one has*

$$\begin{aligned}A_\alpha^{[\gamma]}(k) &= A_\alpha(k)^*\Big|_{\mathcal{D}(A_\alpha^{[\gamma]}(k))}\\ \mathcal{D}(A_\alpha^{[\gamma]}(k)) &= \{g\in\mathcal{D}(A_\alpha(k)^*)\,|\,g_1=\gamma g_0\}\,,\end{aligned}\tag{6.3.55}$$

where, for each g, the constants g_0 and g_1 are defined by the limits (6.3.51)*.*

The above classification allows us to finally identify the Friedrich extension $A_{\alpha,F}(k)$:

Proposition 6.3.15. *Let $\alpha\in(0,1)$ and $k\in\mathbb{Z}\setminus\{0\}$. Then $\mathscr{A}_\alpha(k)=A_{\alpha,F}(k)$, and hence $R_{G_{\alpha,k}}=A_{\alpha,F}(k)^{-1}$ and $\Psi_{\alpha,k}=(A_{\alpha,F}(k))^{-1}\Phi_{\alpha,k}$.*

For the proof of Proposition 6.3.15 it is convenient to recall the following.

Lemma 6.3.16. *Let $\alpha\in(0,1)$ and $k\in\mathbb{Z}\setminus\{0\}$. The quadratic form of the Friedrichs extension of $A_\alpha(k)$ is given by*

$$\begin{aligned}\mathcal{D}[A_{\alpha,F}(k)] &= \big\{g\in L^2(\mathbb{R}^+)\,\big|\,\|g'\|_{L^2}^2+\|x^\alpha g\|_{L^2}^2+\|x^{-1}g\|_{L^2}^2<+\infty\big\}\\ A_{\alpha,F}(k)[g,h] &= \int_0^{+\infty}\Big(\overline{g'(x)}h'(x)+k^2x^{2\alpha}\,\overline{g(x)}h(x)+C_\alpha\,\frac{\overline{g(x)}h(x)}{x^2}\Big)\mathrm{d}x\,.\end{aligned}\tag{6.3.56}$$

Proof. It is a standard construction (see, e.g., [62, Theorem 15]), that follows from the fact that $\mathcal{D}[A_{\alpha,F}(k)]$ is the closure of $\mathcal{D}(A_\alpha(k)) = C_0^\infty(\mathbb{R}^+)$ in the norm

$$\begin{aligned}\|g\|_F^2 &:= \langle g, A_\alpha(k)g\rangle_{L^2} + \langle g, g\rangle_{L^2} \\ &= \|g'\|_{L^2}^2 + k^2\|x^\alpha g\|_{L^2}^2 + C_\alpha\|x^{-1}g\|_{L^2}^2 + \|g\|_{L^2}^2 \,.\end{aligned}$$

Then (6.3.56) follows at once from the above formula, since $k^2 > 0$ and $C_\alpha > 0$. □

Proof of Proposition 6.3.15. Let $g \in \mathcal{D}(A_\alpha^{[\gamma]}(k))$ for some $\gamma \in \mathbb{R}$. The short-distance expansion (6.3.52), combined with the self-adjointness condition (6.3.55), yields

$$x^{-1}g(x) \overset{x\downarrow 0}{=} g_0\, x^{-(1+\frac{\alpha}{2})} + \gamma\, g_0\, x^{\frac{\alpha}{2}} + o(x^{\frac{1}{2}})\,.$$

Therefore, in general (namely whenever $g_0 \neq 0$) $x^{-1}g$ is *not* square-integrable at zero. When this is the case, formula (6.3.56) prevents g from belonging to $\mathcal{D}[A_{\alpha,F}(k)]$. This shows that *no* extension $A_\alpha^{[\gamma]}(k)$, $\gamma \in \mathbb{R}$, has operator domain entirely contained in $\mathcal{D}[A_{\alpha,F}(k)]$. The latter statement does not cover $\mathscr{A}_\alpha(k)$ ($\gamma = \infty$). Now, $A_{\alpha,F}(k)$ can be none of the $A_\alpha^{[\gamma]}(k)$'s, $\gamma \in \mathbb{R}$, because the Friedrichs extension has indeed operator domain inside $\mathcal{D}[A_{\alpha,F}(k)]$ – in fact, it is the unique extension with such property. Necessarily the conclusion is that $A_{\alpha,F}(k)$ and $\mathscr{A}_\alpha(k)$ are the same. □

A straightforward consequence of Proposition 6.3.15 (and of its proof) is the following.

Corollary 6.3.17. *Let $\alpha \in (0,1)$ and $k \in \mathbb{Z}\setminus\{0\}$. The Friedrichs extension $A_{\alpha,F}(k)$ of $A_\alpha(k)$ is the only self-adjoint extension whose operator domain is contained in $\mathcal{D}(x^{-1})$.*

6.3.6 Proof of the classification theorem on fibre

Let us collect the results of the preceding discussion and prove Theorem 6.3.1.

Remark 6.3.18. The case $\alpha = 0$ and hence $A_\alpha(k)$ is (a positive shift of) the minimally defined Laplacian, is well known in the literature (see, e.g., [66]) and in this case Theorem 6.3.1 recover this information. In particular, the operator closure has domain $H_0^2(\mathbb{R}^+)$, the adjoint has domain $H^2(\mathbb{R}^+)$, the Friedrichs extension is the Dirichlet Laplacian and has form domain $H_0^1(\mathbb{R}^+)$.

Thus, Theorem 6.3.1 need only be proved when $\alpha \in (0,1)$, the regime in which the analysis of Subsections 6.3.1-6.3.5 was developed.

Part (i) of Theorem 6.3.1 is precisely Proposition 6.3.8. Part (ii) follows from (6.2.21) and (6.3.49) concerning the operator domain, and from Lemma 6.3.2 concerning the kernel.

Part (iv), the actual classification of extensions, is the rephrasing of Proposition 6.3.14, using the fact that the reference extension is $\mathscr{A}_\alpha(k) = A_{\alpha,F}(k)$ (Proposition 6.3.15), and plugging the self-adjointness condition $g_1 = \gamma g_0$ into the general asymptotics (6.3.52).

In part (iii), formula (6.3.8) for the operator domain follows from (6.3.49) (with $\mathscr{A}_\alpha(k) = A_{\alpha,F}(k)$) and from the short-range asymptotics for $\Psi_{\alpha,k}$ (Lemma 6.3.7), and for the elements of $\mathcal{D}(\overline{A_\alpha(k)})$ (Lemma 6.3.12) – which is the same as taking formally $\gamma = \infty$ in the general asymptotics. The distinctive property of $A_{\alpha,F}(k)$ with respect to the space $\mathcal{D}(x^{-1})$ is given by Corollary 6.3.17.

Thus, it remains to prove (6.3.9) for the form domain of $A_{\alpha,F}(k)$. The inclusion $\mathcal{D}[A_{\alpha,F}(k)] \subset H_0^1(\mathbb{R}^+) \cap L^2(\mathbb{R}^+, \langle x\rangle^{2\alpha}\,\mathrm{d}x)$ follows directly from Lemma 6.3.16, as (6.3.56) prescribes that if $g \in \mathcal{D}[A_{\alpha,F}(k)]$, then $g', x^\alpha g, x^{-1}g \in L^2(\mathbb{R}^+)$, and the latter condition implies necessarily $g(0) = 0$. Conversely, if $g \in H_0^1(\mathbb{R}^+)$ *and* $g \in L^2(\mathbb{R}^+, \langle x\rangle^{2\alpha}\,\mathrm{d}x)$, then $g(x) \overset{x\downarrow 0}{=} o(x^{\frac{1}{2}})$ and all three norms $\|g'\|_{L^2}$, $\|x^\alpha g\|_{L^2}$, and $\|x^{-1}g\|_{L^2}$ are finite. Owing to (6.3.56), $g \in \mathcal{D}[A_{\alpha,F}(k)]$.

The proof of Theorem 6.3.1 is completed.

6.4 Bilateral-fibre extensions

In this Section we study the two-sided version of the problem considered in Sections 6.3, namely the problem of the self-adjoint extensions in $L^2(\mathbb{R})$ of the bilateral differential operator

$$\begin{aligned}\mathcal{D}(A_\alpha(k)) &= C_0^\infty(\mathbb{R}^-) \boxplus C_0^\infty(\mathbb{R}^+) \\ A_\alpha(k) &= A_\alpha^-(k) \oplus A_\alpha^+(k)\,,\end{aligned} \tag{6.4.1}$$

already defined in (6.2.17). The Hilbert space $L^2(\mathbb{R})$ is now canonically decomposed into the orthogonal sum

$$L^2(\mathbb{R}, \mathrm{d}x) \;\cong\; L^2(\mathbb{R}^-, \mathrm{d}x) \oplus L^2(\mathbb{R}^+, \mathrm{d}x)\,. \tag{6.4.2}$$

Each $g \in L^2(\mathbb{R})$ reads therefore

$$g \;=\; g^- \oplus g^+ \;\equiv\; \begin{pmatrix} g^- \\ g^+ \end{pmatrix}, \qquad g^\pm(x) \;:=\; g(x) \quad \text{for } x \in \mathbb{R}^\pm, \tag{6.4.3}$$

and

$$A_\alpha(k)g \;=\; S_{\alpha,k}g^- \oplus S_{\alpha,k}g^+, \qquad S_{\alpha,k} \;:=\; -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2|x|^{2\alpha} + \frac{C_\alpha}{x^2}\,. \tag{6.4.4}$$

As $A^\pm_\alpha(k)$ has deficiency index 1 in $L^2(\mathbb{R}^\pm)$, $A_\alpha(k)$ has deficiency index 2 in $L^2(\mathbb{R})$, thus it comes with a richer variety of extensions.

Among them, one has extensions of form

$$B^-_\alpha(k) \oplus B^+_\alpha(k) \tag{6.4.5}$$

where $B^\pm_\alpha(k)$ is a self-adjoint extension of $A^\pm_\alpha(k)$ in $L^2(\mathbb{R}^\pm)$, namely a member of the family determined in the previous Section (Theorem 6.3.1). Extensions of type (6.4.5) are *reduced* with respect to the decomposition (6.4.2) (in the usual sense of, e.g., [102, Sect. 1.4]): they provide *decoupled* self-adjoint realisations of the differential operator $S_{\alpha,k}$, with no constraint between the behaviour as $x \to 0^+$ and $x \to 0^-$. An important extension of this type is the Friedrich extension $A_{\alpha,F}(k)$: indeed, a standard check shows that

$$A_{\alpha,F}(k) \;=\; A^-_{\alpha,F}(k) \oplus A^+_{\alpha,F}(k), \tag{6.4.6}$$

where $A^\pm_{\alpha,F}$ is the Friedrichs extension of $A^\pm_\alpha(k)$ in $L^2(\mathbb{R}^\pm)$, described in Theorem 6.3.1(iii).

Generic extensions, instead, are not reduced as in (6.4.5), and are characterised by *coupled* bilateral boundary conditions. We classify them using again the KVB scheme described in Sec. 6.3.4.

Following the same steps of Sections 6.3 and 6.7.5, we are now interested in self-adjoint *restrictions* of the adjoint $A_\alpha(k)^* = A^-_\alpha(k)^* \oplus A^+_\alpha(k)^*$.

In order to export the one-sided analysis of Sections 6.3 to the present two-sided context, let us introduce a unique expression for the functions of relevance, $\Phi_{\alpha,k}$ and $\Psi_{\alpha,k}$, valid for the left and the right side. Thus, we set

$$\widetilde{\Phi}_{\alpha,k}(x) \;:=\; \Phi_{\alpha,k}(|x|), \qquad \widetilde{\Psi}_{\alpha,k}(x) \;:=\; \Psi_{\alpha,k}(|x|), \tag{6.4.7}$$

understanding $\widetilde{\Phi}_{\alpha,k}$ and $\widetilde{\Psi}_{\alpha,k}$ both as functions on $\mathbb{R}^-$ and on $\mathbb{R}^+$, depending on the context. Let us recall that such functions are defined in (6.3.13) and (6.3.28) when $k \neq 0$, and in (6.7.21) and (6.7.29) when $k = 0$.

Let us discuss the case $k \neq 0$ first. We deduce at once, respectively from Proposition 6.3.8, Lemma 6.3.2, formula (6.3.28), and Proposition 6.3.15, that

$$\mathcal{D}(\overline{A_\alpha(k)}) \;=\; \big(H^2_0(\mathbb{R}^-) \boxplus H^2_0(\mathbb{R}^+)\big) \cap L^2(\mathbb{R}, \langle x\rangle^{4\alpha}\,\mathrm{d}x) \tag{6.4.8}$$

$$\ker A_\alpha(k)^* \;=\; \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} \tag{6.4.9}$$

$$A_{\alpha,F}(k)^{-1} \ker A_\alpha(k)^* \;=\; \mathrm{span}\{\widetilde{\Psi}_{\alpha,k}\} \oplus \mathrm{span}\{\widetilde{\Psi}_{\alpha,k}\}, \tag{6.4.10}$$

whence also [62, Theorem 1]

$$\begin{aligned} \mathcal{D}(A_\alpha(k)^*) \;=\; & \big(H^2_0(\mathbb{R}^-) \boxplus H^2_0(\mathbb{R}^+)\big) \cap L^2(\mathbb{R}, \langle x\rangle^{4\alpha}\,\mathrm{d}x) \\ & \dotplus \mathrm{span}\{\widetilde{\Psi}_{\alpha,k}\} \oplus \mathrm{span}\{\widetilde{\Psi}_{\alpha,k}\} \\ & \dotplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\}, \end{aligned} \tag{6.4.11}$$

namely, the analogue of (6.3.49).

In the notation of (6.4.3), a generic $g \in \mathcal{D}(A_\alpha(k)^*)$ has therefore the short-range asymptotics

$$g(x) \;\equiv\; \begin{pmatrix} g^-(x) \\ g^+(x) \end{pmatrix} \overset{x\to 0}{=} \begin{pmatrix} g^-_0 \\ g^+_0 \end{pmatrix} |x|^{-\frac{\alpha}{2}} + \begin{pmatrix} g^-_1 \\ g^+_1 \end{pmatrix} |x|^{1+\frac{\alpha}{2}} + o(|x|^{\frac{3}{2}}) \tag{6.4.12}$$

for suitable $g^\pm_0, g^\pm_1 \in \mathbb{C}$ given by the limits

$$\begin{aligned} g^\pm_0 \;&=\; \lim_{x\to 0^\pm} |x|^{\frac{\alpha}{2}} g^\pm(x) \\ g^\pm_1 \;&=\; \lim_{x\to 0^\pm} |x|^{-(1+\frac{\alpha}{2})}\big(g^\pm(x) - g^\pm_0|x|^{-\frac{\alpha}{2}}\big)\,. \end{aligned} \tag{6.4.13}$$

Formula (6.4.12) follows from (6.4.11) and the usual short-range asymptotics for $\Phi_{\alpha,k}$, $\Psi_{\alpha,k}$, and $\mathcal{D}(\overline{A_\alpha(k)})$.

Now, the KVB extension Theorem 6.3.13 establishes a one-to-one correspondence between self-adjoint extensions of $A_\alpha(k)$ and self-adjoint operators T in Hilbert subspaces of $\ker A_\alpha(k)^*$: denoting by $A_\alpha^{(T)}(k)$ each such extension, and by $\mathcal{K} \subset \ker A_\alpha(k)^*$ the Hilbert subspace where T acts in, $A_\alpha^{(T)}(k)$ is the restriction of $A_\alpha(k)^*$ to the domain

$$\mathcal{D}\big(A_\alpha^{(T)}(k)\big) \;=\; \left\{ \begin{array}{c} g = \varphi + A_{\alpha,F}(k)^{-1}(Tv+w) + v \\ \text{with} \\ \varphi \in \big(H_0^2(\mathbb{R}^-) \boxplus H_0^2(\mathbb{R}^+)\big) \cap L^2(\mathbb{R}, \langle x\rangle^{4\alpha}\,\mathrm{d}x), \\ v \in \mathcal{K}, \quad w \in \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\}, \quad w \perp v \end{array} \right\}. \tag{6.4.14}$$

Clearly $\dim \mathcal{K}$ can be equal to 0, 1, or 2. The former case corresponds to taking formally '$T = \infty$' on $\mathcal{D}(T) = \{0\}$, and reproduces the Friedrichs extension. The other two cases produce the rest of the family of extensions.

All the preceding discussion has an immediate counterpart when $k = 0$, based on the results of Sect. 6.7.5. The above formulas are valid for $k = 0$ too, except for (6.4.8), that need be replaced with the generic identity

$$\mathcal{D}(\overline{A_\alpha(0)}) \;=\; \mathcal{D}\big(\overline{A_\alpha^-(0)}\big) \oplus \mathcal{D}\big(\overline{A_\alpha^+(0)}\big) \tag{6.4.15}$$

as we did not make the characterisation of $\mathcal{D}\big(\overline{A_\alpha^\pm(0)}\big)$ as explicit as when $k \neq 0$ (nor we need that, for only the asymptotics as $x \to 0$ are relevant for our purposes), and except for (6.4.11), that consequently reads now

$$\begin{aligned} \mathcal{D}(A_\alpha(0)^*) \;=\; & \mathcal{D}\big(\overline{A_\alpha^-(0)}\big) \boxplus \mathcal{D}\big(\overline{A_\alpha^+(0)}\big) \\ & \dotplus \mathrm{span}\{\widetilde{\Psi}_{\alpha,0}\} \oplus \mathrm{span}\{\widetilde{\Psi}_{\alpha,0}\} \\ & \dotplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,0}\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,0}\}\,. \end{aligned} \tag{6.4.16}$$

Thus when $k = 0$ formula (6.4.14) takes the form

$$\mathcal{D}\big(A_\alpha^{(T)}(0)\big) \;=\; \left\{ \begin{array}{c} g = \varphi + (A_{\alpha,F}(0) + \mathbb{1})^{-1}(Tv+w) + v \\ \text{with} \\ \varphi \in \mathcal{D}\big(\overline{A_\alpha^-(0)}\big) \boxplus \mathcal{D}\big(\overline{A_\alpha^+(0)}\big), \\ v \in \mathcal{K}, \quad w \in \mathrm{span}\{\widetilde{\Phi}_{\alpha,0}\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,0}\}, \quad w \perp v \end{array} \right\}, \tag{6.4.17}$$

where now $\mathcal{K}$ is a Hilbert subspace of $\ker(A_\alpha(0)^* + \mathbb{1})$ and T is a self-adjoint operator in $\mathcal{K}$.

We can now formulate the main result of this Section.

Theorem 6.4.1. *Let $\alpha \in [0,1)$ and $k \in \mathbb{Z}$. Each self-adjoint extension $B_\alpha(k)$ of $A_\alpha(k)$ acts as*

$$B_\alpha(k)g \;=\; S_{\alpha,k}\, g^- \oplus S_{\alpha,k}\, g^+ \tag{6.4.18}$$

on a generic g of its domain, written in the notation of (6.4.3) *and* (6.4.12)-(6.4.13). *The family of self-adjoint extensions of $A_\alpha(k)$ is formed by the following sub-families.*

- *Friedrichs extension.*

  It is the operator (6.4.6). *Its domain consists of those functions in $\mathcal{D}(A_\alpha(k)^*)$ whose asymptotics* (6.4.12) *has $g_0^\pm = 0$.*

- *Family* $\mathrm{I_R}$.

  It is the family $\{A_{\alpha,R}^{[\gamma]}(k) \,|\, \gamma \in \mathbb{R}\}$ defined, with respect to the asymptotics (6.4.12), *by*

  $$\mathcal{D}(A_{\alpha,R}^{[\gamma]}(k)) \;=\; \{g \in \mathcal{D}(A_\alpha(k)^*) \,|\, g_0^- = 0,\; g_1^+ = \gamma g_0^+\}\,.$$

- *Family* $\mathrm{I_L}$.

  It is the family $\{A_{\alpha,L}^{[\gamma]}(k) \,|\, \gamma \in \mathbb{R}\}$ defined, with respect to the asymptotics (6.4.12), *by*

  $$\mathcal{D}(A_{\alpha,L}^{[\gamma]}(k)) \;=\; \{g \in \mathcal{D}(A_\alpha(k)^*) \,|\, g_0^+ = 0,\; g_1^- = \gamma g_0^-\}\,.$$

- *Family* II_a *with $a \in \mathbb{C}$.*

  It is the family $\{A_{\alpha,a}^{[\gamma]}(k) \,|\, \gamma \in \mathbb{R}\}$ defined, with respect to the asymptotics (6.4.12), *by*

  $$\mathcal{D}(A_{\alpha,a}^{[\gamma]}(k)) \;=\; \left\{ g \in \mathcal{D}(A_\alpha(k)^*) \,\middle|\, \begin{array}{c} g_0^+ = a\, g_0^- \\ g_1^- + \overline{a}\, g_1^+ = \gamma\, g_0^- \end{array} \right\}.$$

family of extensions	space $\mathcal{K}$	boundary conditions	parameters	notes
Friedrichs	$\{0\} \oplus \{0\}$	$g_0^{\pm} = 0$		bilateral confining
I_{R}	$\{0\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\}$	$g_0^- = 0$ $g_1^+ = \gamma g_0^+$	$\gamma \in \mathbb{R}$	left confining
I_{L}	$\mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} \oplus \{0\}$	$g_1^- = \gamma g_0^-$ $g_0^+ = 0$	$\gamma \in \mathbb{R}$	right confining
II_a $a \in \mathbb{C}$	$\mathrm{span}\{\widetilde{\Phi}_{\alpha,k} \oplus a\widetilde{\Phi}_{\alpha,k}\}$	$g_0^+ = a\, g_0^-$ $g_1^- + \overline{a}\, g_1^+ = \gamma\, g_0^-$	$\gamma \in \mathbb{R}$	bridging for $a = 1$ and $\gamma = 0$
III	$\mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\}$	$g_1^- = \gamma_1 g_0^- + \zeta g_0^+$ $g_1^+ = \overline{\zeta} g_0^- + \gamma_4 g_0^+$ $\zeta := \gamma_2 + \mathrm{i}\gamma_3$	$\gamma_j \in \mathbb{R}$ $j = 1, 2, 3, 4$	

Table 6.1: Summary of all possible boundary conditions of self-adjointness for the bilateral-fibre extensions of $A_\alpha(k)$

- *Family* III.

  It is the family $\{A_\alpha^{[\Gamma]}(k) \,|\, \Gamma \equiv (\gamma_1, \gamma_2, \gamma_3, \gamma_4) \in \mathbb{R}^4\}$ *defined, with respect to the asymptotics* (6.4.12)*, by*

$$\mathcal{D}(A_\alpha^{[\Gamma]}(k)) \;=\; \left\{ g \in \mathcal{D}(A_\alpha(k)^*) \;\middle|\; \begin{array}{c} g_1^- = \gamma_1 g_0^- + \zeta g_0^+ \\ g_1^+ = \overline{\zeta} g_0^- + \gamma_4 g_0^+ \\ \zeta := \gamma_2 + \mathrm{i}\gamma_3 \end{array} \right\}.$$

The families I_{R}, I_{L}, II_a *for all* $a \in \mathbb{C} \setminus \{0\}$*, and* III *are mutually disjoint and, together with the Friedrichs extension, exhaust the family of self-adjoint extensions of* $A_\alpha(k)$*.*

The proof of Theorem 6.4.1 is straightforward, and it is given here in all details for completeness, and also to provide an explicative example of the KVB extension theory for a reader that may be familiar with Von Neumann extension theory or may not be familiar in general with the extension theories (in this example, of operators of deficiency index 2).

Proof of Theorem 6.4.1. Let us consider first $k \neq 0$ and let us exploit the classification formula (6.4.14) in all possible cases.

The choice $\mathcal{K} = \{0\} \oplus \{0\}$ yields to the extension with domain

$$\mathcal{D}(\overline{A_\alpha(k)}) \dotplus A_{\alpha,F}(k)^{-1} \ker A_\alpha(k)^* \;=\; \mathcal{D}(A_{\alpha,F}(k)),$$

namely the Friedrichs extension. Formula (6.3.8) of Theorem 6.3.1, applied on both sides $\mathbb{R}^+$ and $\mathbb{R}^-$, then implies $g_0^+ = 0 = g_0^-$.

The choice $\mathcal{K} = \{0\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\}$ yields to the extensions in the domain of which a function $g = \varphi + A_{\alpha,F}(k)^{-1}(Tv + w) + v$ is decoupled into a component g^- in the domain of $A_{\alpha,F}^-(k)$ (the Friedrichs extension of $A_\alpha^-(k)$) and a component g^+ in the domain of a self-adjoint extension of $A_\alpha^+(k)$ in $L^2(\mathbb{R}^+)$. This identifies a family $\{A_{\alpha,R}^{[\gamma]}(k) \,|\, \gamma \in \mathbb{R}\}$ of extensions with

$$A_{\alpha,R}^{[\gamma]}(k) \;=\; A_{\alpha,F}^-(k) \oplus A_\alpha^{+,[\gamma]}(k),$$

where $A_\alpha^{+,[\gamma]}(k)$ denotes here the generic extension of $A_\alpha^+(k)$, according to the classification of Theorem 6.3.1(iv), for which therefore $g_1^+ = \gamma g_0^+$. The symmetric choice $\mathcal{K} = \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} \oplus \{0\}$ is treated in a completely analogous way.

The next one-dimensional choice is $\mathcal{K} = \mathrm{span}\{\widetilde{\Phi}_{\alpha,k} \oplus a\widetilde{\Phi}_{\alpha,k}\}$ for some $0 \neq a \in \mathbb{C}$. Formula (6.4.14) is now to be specialised with

$$v \in \mathcal{K}, \qquad w \in \mathcal{K}^\perp \cap \big(\mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\}\big) = \mathrm{span}\{\widetilde{\Phi}_{\alpha,k} \oplus (-\overline{a}^{-1})\widetilde{\Phi}_{\alpha,k}\}\,.$$

The generic self-adjoint operator T on $\mathcal{K}$ is now the multiplication by some $\tau \in \mathbb{R}$. Then (6.4.14) reads

$$\begin{aligned} g &= \varphi + A_{\alpha,F}(k)^{-1}\left(\tau c_0 \begin{pmatrix} \widetilde{\Phi}_{\alpha,k} \\ a\widetilde{\Phi}_{\alpha,k} \end{pmatrix} + \widetilde{c}_0 \begin{pmatrix} \widetilde{\Phi}_{\alpha,k} \\ -\overline{a}^{-1}\widetilde{\Phi}_{\alpha,k} \end{pmatrix}\right) + c_0 \begin{pmatrix} \widetilde{\Phi}_{\alpha,k} \\ a\widetilde{\Phi}_{\alpha,k} \end{pmatrix} \\ &= \varphi + \begin{pmatrix} (\tau c_0 + \widetilde{c}_0)\widetilde{\Psi}_{\alpha,k} \\ (\tau c_0 a - \widetilde{c}_0\,\overline{a}^{-1})\widetilde{\Psi}_{\alpha,k} \end{pmatrix} + c_0 \begin{pmatrix} \widetilde{\Phi}_{\alpha,k} \\ a\widetilde{\Phi}_{\alpha,k} \end{pmatrix} \end{aligned}$$

for generic coefficients $c_0, \widetilde{c}_0 \in \mathbb{C}$. From the expression above we find that the limits (6.4.13), computed with the short-range asymptotics (6.3.14) and (6.3.29) (and Lemma 6.3.12), amount to

$$\begin{aligned} g_0^- &= c_0\sqrt{\tfrac{\pi(1+\alpha)}{2|k|}} \\ g_0^+ &= c_0\, a\sqrt{\tfrac{\pi(1+\alpha)}{2|k|}} \\ g_1^- &= (\tau c_0 + \widetilde{c}_0)\sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\|\Phi_{\alpha,k}\|_{L^2}^2 - c_0\sqrt{\tfrac{\pi|k|}{2(1+\alpha)}} \\ g_1^+ &= (\tau c_0 a - \widetilde{c}_0\,\overline{a}^{-1})\sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\|\Phi_{\alpha,k}\|_{L^2}^2 - c_0 a\sqrt{\tfrac{\pi|k|}{2(1+\alpha)}}\,. \end{aligned}$$

Let us stress that here the constant $\|\Phi_{\alpha,k}\|_{L^2}$ is the L^2-norm of $\Phi_{\alpha,k}$ on the sole positive half-line. The first two equations above yield $g_0^+ = a g_0^-$. The last two yield

$$\begin{aligned} g_1^- + \overline{a}\, g_1^+ &= c_0(1+|a|^2)\Big(\tau\sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\|\Phi_{\alpha,k}\|_{L^2}^2 - \sqrt{\tfrac{\pi|k|}{2(1+\alpha)}}\Big) \\ &= g_0^-(1+|a|^2)\tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|_{L^2}^2}{\pi(1+\alpha)}\,\tau - 1\Big), \end{aligned}$$

having replaced $c_0 = g_0^-\sqrt{\frac{2|k|}{\pi(1+\alpha)}}$. We can also write

$$g_1^- + \overline{a}\, g_1^+ = \gamma\, g_0^-$$

after re-parametrising the extension parameter as

$$\gamma := (1+|a|^2)\tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|_{L^2}^2}{\pi(1+\alpha)}\,\tau - 1\Big) \in \mathbb{R}\,. \tag{6.4.19}$$

This completes the identification of the extensions $A_{\alpha,a}^{[\gamma]}(k)$.

The remaining choice is $\mathcal{K} = \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} = \ker A_\alpha(k)^*$. In this case formula (6.4.14) only has v-vectors and no w-vectors, and the self-adjoint T is represented by a generic 2×2 Hermitian matrix

$$T = \begin{pmatrix} \tau_1 & \tau_2 + \mathrm{i}\tau_3 \\ \tau_2 - \mathrm{i}\tau_3 & \tau_4 \end{pmatrix}, \qquad \tau_1, \tau_2, \tau_3, \tau_4 \in \mathbb{R}\,.$$

Then (6.4.14) reads

$$\begin{aligned} g &= \varphi + A_{\alpha,F}(k)^{-1} T \begin{pmatrix} c_0^-\widetilde{\Phi}_{\alpha,k} \\ c_0^+\widetilde{\Phi}_{\alpha,k} \end{pmatrix} + \begin{pmatrix} c_0^-\widetilde{\Phi}_{\alpha,k} \\ c_0^+\widetilde{\Phi}_{\alpha,k} \end{pmatrix} \\ &= \varphi + \begin{pmatrix} (\tau_1 c_0^- + (\tau_2 + \mathrm{i}\tau_3)c_0^+)\widetilde{\Psi}_{\alpha,k} \\ ((\tau_2 - \mathrm{i}\tau_3)c_0^- + \tau_4 c_0^+)\widetilde{\Psi}_{\alpha,k} \end{pmatrix} + \begin{pmatrix} c_0^-\widetilde{\Phi}_{\alpha,k} \\ c_0^+\widetilde{\Phi}_{\alpha,k} \end{pmatrix} \end{aligned}$$

for generic coefficients $c_0^\pm \in \mathbb{C}$. From the expression above we find that the limits (6.4.13), computed with the short-range asymptotics (6.3.14) and (6.3.29) (and Lemma 6.3.12), amount to

$$\begin{aligned} g_0^\pm &= c_0^\pm\sqrt{\tfrac{\pi(1+\alpha)}{2|k|}} \\ g_1^- &= c_0^-\Big(\tau_1\sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\|\Phi_{\alpha,k}\|_{L^2}^2 - \sqrt{\tfrac{\pi|k|}{2(1+\alpha)}}\Big) + c_0^+(\tau_2 + \mathrm{i}\tau_3)\sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\|\Phi_{\alpha,k}\|_{L^2}^2 \\ g_1^+ &= c_0^-(\tau_2 - \mathrm{i}\tau_3)\sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\|\Phi_{\alpha,k}\|_{L^2}^2 + c_0^+\Big(\tau_4\sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\|\Phi_{\alpha,k}\|_{L^2}^2 + \sqrt{\tfrac{\pi|k|}{2(1+\alpha)}}\Big). \end{aligned}$$

Replacing $c_0^{\pm} = g_0^{\pm}\sqrt{\frac{2|k|}{\pi(1+\alpha)}}$ in the last two equations above and re-defining the extension parameters as

$$\begin{aligned} \gamma_1 &:= \tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|_{L^2}^2}{\pi(1+\alpha)}\,\tau_1 - 1\Big) \\ \gamma_2 + \mathrm{i}\gamma_3 &:= (\tau_2 + \mathrm{i}\tau_3)\tfrac{2|k|}{\pi(1+\alpha)^2}\|\Phi_{\alpha,k}\|_{L^2}^2 \\ \gamma_4 &:= \tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|_{L^2}^2}{\pi(1+\alpha)}\,\tau_4 - 1\Big) \end{aligned} \tag{6.4.20}$$

yields the boundary condition that qualifies the extension $A_\alpha^{[\Gamma]}(k)$ with $\Gamma = (\gamma_1, \gamma_2, \gamma_3, \gamma_4)$.

Last, let us repeat the above reasonings when $k = 0$, based now on the classification formula (6.4.17). The only modifications needed are the replacement of $A_{\alpha,F}(k)^{-1}$ with $(A_{\alpha,F}(0) + \mathbb{1})^{-1}$, and the use, instead of the short-range asymptotics given by (6.3.14), (6.3.29), and Lemma 6.3.12 valid for $k \neq 0$, of the short-range asymptotics given by (6.7.22), (6.7.30), and Lemma 6.7.8 valid for $k = 0$.

The net result concerning the extensions of type II_a, namely the extensions $A_{\alpha,a}^{[\gamma]}(0)$, is that (6.4.19) is replaced by

$$\gamma \;:=\; \tfrac{(1+|a|^2)\Gamma(\frac{1-\alpha}{2})}{2^\alpha(1+\alpha)\Gamma(\frac{1+\alpha}{2})}\Big(\tfrac{(1+\alpha)\|\Phi_{\alpha,0}\|_{L^2}^2}{\Gamma(\frac{3+\alpha}{2})\Gamma(\frac{1-\alpha}{2})}\,\tau - 1\Big) \;\in\; \mathbb{R}\,. \tag{6.4.21}$$

Analogously, concerning the extensions of type III, namely the extensions $A_\alpha^{[\Gamma]}(0)$, (6.4.20) is now replaced by

$$\begin{aligned} \gamma_1 &:= \tfrac{\Gamma(\frac{1-\alpha}{2})}{2^\alpha(1+\alpha)\Gamma(\frac{1+\alpha}{2})}\Big(\tfrac{(1+\alpha)\|\Phi_{\alpha,0}\|_{L^2}^2}{\Gamma(\frac{3+\alpha}{2})\Gamma(\frac{1-\alpha}{2})}\,\tau_1 - 1\Big) \\ \gamma_2 + \mathrm{i}\gamma_3 &:= (\tau_2 + \mathrm{i}\tau_3)\tfrac{\|\Phi_{\alpha,0}\|_{L^2}^2}{2^\alpha\Gamma(\frac{3+\alpha}{2})\Gamma(\frac{1+\alpha}{2})} \\ \gamma_4 &:= \tfrac{\Gamma(\frac{1-\alpha}{2})}{2^\alpha(1+\alpha)\Gamma(\frac{1+\alpha}{2})}\Big(\tfrac{(1+\alpha)\|\Phi_{\alpha,0}\|_{L^2}^2}{\Gamma(\frac{3+\alpha}{2})\Gamma(\frac{1-\alpha}{2})}\,\tau_4 - 1\Big)\,. \end{aligned} \tag{6.4.22}$$

The proof is now completed. □

Whereas Theorem 6.4.1 expresses the various conditions of self-adjointness in terms of the representation (6.4.3) and (6.4.12)-(6.4.13) of a generic $g \in \mathcal{D}(A_\alpha(k)^*)$, that is, in terms of the short-range behaviour of g, for the forthcoming analysis it will be convenient to re-formulate the above classification in two further equivalent forms.

The first one refers to the representation (6.4.3), (6.4.11), and (6.4.16) of $g \in \mathcal{D}(A_\alpha(k)^*)$, that is,

$$g \;=\; \begin{pmatrix}\widetilde{\varphi}^-\\ \widetilde{\varphi}^+\end{pmatrix} + \begin{pmatrix}c_1^-\widetilde{\Psi}_{\alpha,k}\\ c_1^+\widetilde{\Psi}_{\alpha,k}\end{pmatrix} + \begin{pmatrix}c_0^-\widetilde{\Phi}_{\alpha,k}\\ c_0^+\widetilde{\Phi}_{\alpha,k}\end{pmatrix} \tag{6.4.23}$$

with $\widetilde{\varphi}^{\pm} \in \mathcal{D}(\overline{A_\alpha^{\pm}(k)})$ and $c_0^{\pm}, c_1^{\pm} \in \mathbb{C}$. Then the proof of Theorem 6.4.1 demonstrates also the following.

Theorem 6.4.2. *Let $\alpha \in [0,1)$ and $k \in \mathbb{Z}$. The family of self-adjoint extensions of $A_\alpha(k)$ is formed by the following sub-families.*

- *<u>Friedrichs extension</u>. It is the operator* (6.4.6). *Its domain consists of those functions in $\mathcal{D}(A_\alpha(k)^*)$ whose representation* (6.4.23) *has $c_0^{\pm} = 0$.*

- *<u>Family $\mathrm{I_R}$</u>. It is the family $\{A_{\alpha,R}^{[\gamma]}(k) \,|\, \gamma \in \mathbb{R}\}$ defined, with respect to the representation* (6.4.23)*, by*

$$\mathcal{D}(A_{\alpha,R}^{[\gamma]}(k)) \;=\; \{g \in \mathcal{D}(A_\alpha(k)^*) \,|\, c_0^- = 0,\; c_1^+ = \beta c_0^+\}\,,$$

  where β and γ are related by (6.3.54) *for $k \neq 0$ and* (6.7.34) *for $k = 0$.*

- *<u>Family $\mathrm{I_L}$</u>. It is the family $\{A_{\alpha,L}^{[\gamma]}(k) \,|\, \gamma \in \mathbb{R}\}$ defined, with respect to the representation* (6.4.23)*, by*

$$\mathcal{D}(A_{\alpha,L}^{[\gamma]}(k)) \;=\; \{g \in \mathcal{D}(A_\alpha(k)^*) \,|\, c_0^+ = 0,\; c_1^- = \beta c_0^-\}\,,$$

  where β and γ are related by (6.3.54) *for $k \neq 0$ and* (6.7.34) *for $k = 0$.*

- *Family* II_a *with* $a \in \mathbb{C}$. *It is the family* $\{A^{[\gamma]}_{\alpha,a}(k) \,|\, \gamma \in \mathbb{R}\}$ *defined by*

$$\mathcal{D}(A^{[\gamma]}_{\alpha,a}(k)) \;=\; \left\{ \begin{array}{c} g \in \mathcal{D}(A_\alpha(k)^*) \text{ with (6.4.23) of the form} \\ g = \begin{pmatrix} \widetilde{\varphi}^- \\ \widetilde{\varphi}^+ \end{pmatrix} + \begin{pmatrix} (\tau c_0 + \widetilde{c}_0)\widetilde{\Psi}_{\alpha,k} \\ (\tau c_0 a - \widetilde{c}_0\, \overline{a}^{-1})\widetilde{\Psi}_{\alpha,k} \end{pmatrix} + c_0 \begin{pmatrix} \widetilde{\Phi}_{\alpha,k} \\ a\widetilde{\Phi}_{\alpha,k} \end{pmatrix} \end{array} \right\},$$

where τ *and* γ *are related by* (6.4.19) *if* $k \neq 0$, *and by* (6.4.21) *if* $k = 0$.

- *Family* III. *It is the family* $\{A^{[\Gamma]}_{\alpha}(k) \,|\, \Gamma \equiv (\gamma_1, \gamma_2, \gamma_3, \gamma_4) \in \mathbb{R}^4\}$ *defined by*

$$\mathcal{D}(A^{[\Gamma]}_{\alpha}(k)) \;=\; \left\{ \begin{array}{c} g \in \mathcal{D}(A_\alpha(k)^*) \text{ satisfying (6.4.23) with} \\ \begin{pmatrix} c_1^- \\ c_1^+ \end{pmatrix} = \begin{pmatrix} \tau_1 & \tau_2 + \mathrm{i}\tau_3 \\ \tau_2 - \mathrm{i}\tau_3 & \tau_4 \end{pmatrix} \begin{pmatrix} c_0^- \\ c_0^+ \end{pmatrix} \end{array} \right\},$$

where $(\tau_1, \tau_2, \tau_3, \tau_4)$ *and* $(\gamma_1, \gamma_2, \gamma_3, \gamma_4)$ *are related by* (6.4.20) *if* $k \neq 0$ *and* (6.4.22) *if* $k = 0$.

The second alternative to the formulation of the conditions of self-adjointness provided by Theorem 6.4.1, is in fact a very close alternative to the formulation of Theorem 6.4.1 itself, with the same short-range parameters $g_0^\pm$ and $g_1^\pm$ and the same classification parameters γ or Γ, except that it is referred to the following representation of g, which is valid identically for any $x \in \mathbb{R} \setminus \{0\}$, and not just as $|x| \to 0$.

To this aim, and also for later convenience, we shall refer to P as a cut-off function in $C_0^\infty(\mathbb{R})$ such that

$$P(x) \;=\; \begin{cases} 1 & \text{if } |x| < 1\,, \\ 0 & \text{if } |x| > 2\,. \end{cases} \tag{6.4.24}$$

In fact, in the following Theorem it is enough that P be smooth, compactly supported, and with $P(0) = 1$, but we keep the general assumption (6.4.24) for later use.

Theorem 6.4.3. *Let* $\alpha \in [0, 1)$ *and let* $k \in \mathbb{Z}$. *Then for any* $g \in \mathcal{D}(A_\alpha(k)^*)$ *there exist a unique* $\varphi \in \mathcal{D}(\overline{A_\alpha(k)})$ *and uniquely determined coefficients* $g_0^\pm, g_1^\pm \in \mathbb{C}$ *such that*

$$g(x) \;=\; \varphi(x) + g_0\, |x|^{-\frac{\alpha}{2}}\, P(x) + g_1\, |x|^{1+\frac{\alpha}{2}}\, P(x) \qquad \forall x \in \mathbb{R} \setminus \{0\} \tag{6.4.25}$$

in the usual notation

$$\varphi(x) \equiv \begin{pmatrix} \varphi^-(x) \\ \varphi^+(x) \end{pmatrix}, \quad g_0 \equiv \begin{pmatrix} g_0^- \\ g_0^+ \end{pmatrix}, \quad g_1 \equiv \begin{pmatrix} g_1^- \\ g_1^+ \end{pmatrix}.$$

Here $g_0^\pm$ *and* $g_1^\pm$ *are precisely the same as in the asymptotics* (6.4.12)-(6.4.13). *Therefore, the same classification of Theorem 6.4.1 in terms of* $g_0^\pm$ *and* $g_1^\pm$ *applies.*

Proof. Let $k \neq 0$ and let us decompose $g \in \mathcal{D}(A_\alpha(k)^*)$ as $g^\pm = \widetilde{\varphi}^\pm + c_1^\pm \widetilde{\Psi}_{\alpha,k} + c_0^\pm \widetilde{\Phi}_{\alpha,k}$ with respect to the decomposition (6.4.23). For short, let us discuss only the component g^+, dropping the '+' superscript: the discussion for g^- is completely analogous. Thus, $g = \widetilde{\varphi} + c_1 \widetilde{\Psi}_{\alpha,k} + c_0 \widetilde{\Phi}_{\alpha,k}$ for all $x > 0$ and uniquely determined $\widetilde{\varphi} \in \mathcal{D}(\overline{A_\alpha(k)})$ and $c_0, c_1 \in \mathbb{C}$. Let us introduce the functions

$$\begin{aligned} L_{0,k}(x) \;&:=\; \left(\sqrt{\tfrac{\pi(1+\alpha)}{2|k|}} - \sqrt{\tfrac{\pi|k|}{2(1+\alpha)}}\, |x|^{1+\alpha} \right) P(x) \\ L_{1,k}(x) \;&:=\; \sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\, \|\Phi_{\alpha,k}\|^2_{L^2}\, P(x) \end{aligned}$$

and re-write

$$\begin{aligned} g \;&=\; \widetilde{\varphi} + c_1(\widetilde{\Psi}_{\alpha,k} - |x|^{1+\frac{\alpha}{2}} L_{1,k}) + c_0(\widetilde{\Phi}_{\alpha,k} - |x|^{-\frac{\alpha}{2}} L_{0,k}) + c_1\, |x|^{1+\frac{\alpha}{2}} L_{1,k} + c_0\, |x|^{-\frac{\alpha}{2}} L_{0,k} \\ &=\; \varphi + \left(c_1 \sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\, \|\Phi_{\alpha,k}\|^2_{L^2} - c_0 \sqrt{\tfrac{\pi|k|}{2(1+\alpha)}} \right) |x|^{1+\frac{\alpha}{2}} P + c_0 \sqrt{\tfrac{\pi(1+\alpha)}{2|k|}}\, |x|^{-\frac{\alpha}{2}} P\,, \end{aligned}$$

having set

$$\varphi \;:=\; \widetilde{\varphi} + c_1(\widetilde{\Psi}_{\alpha,k} - |x|^{1+\frac{\alpha}{2}} L_{1,k}) + c_0(\widetilde{\Phi}_{\alpha,k} - |x|^{-\frac{\alpha}{2}} L_{0,k})\,.$$

Because of the relation (6.3.51) between c_0, c_1 and g_0, g_1, we also have

$$g \;=\; \varphi + g_0\, |x|^{-\frac{\alpha}{2}} P + g_1\, |x|^{1+\frac{\alpha}{2}} P\,.$$

Next, let us argue that $\varphi \in \mathcal{D}(\overline{A_\alpha(k)})$. First, we observe that both $|x|^{-\frac{\alpha}{2}} L_{0,k}$ and $|x|^{1+\frac{\alpha}{2}} L_{1,k}$ belong to $\mathcal{D}(A_\alpha(k)^*)$. The latter statement, owing to (6.2.21) and (6.3.4), is proved by checking the square-integrability of $S_{\alpha,k}(|x|^{-\frac{\alpha}{2}} L_{0,k})$ and of $S_{\alpha,k}(|x|^{1+\frac{\alpha}{2}} L_{1,k})$. Since P localises $L_{0,k}$ and $L_{1,k}$ around $x = 0$, square-integrability must only be checked *locally*. It is then routine to see that

$$\begin{aligned} &-(|x|^{-\frac{\alpha}{2}} L_{0,k})'' + k^2|x|^{2\alpha}(|x|^{-\frac{\alpha}{2}} L_{0,k}) + C_\alpha x^{-2}(|x|^{-\frac{\alpha}{2}} L_{0,k}), \\ &-(|x|^{1+\frac{\alpha}{2}} L_{1,k})'' + k^2|x|^{2\alpha}(|x|^{1+\frac{\alpha}{2}} L_{1,k}) + C_\alpha x^{-2}(|x|^{1+\frac{\alpha}{2}} L_{1,k}), \end{aligned}$$

are both square-integrable around $x = 0$. As a consequence, both $(\widetilde{\Psi}_{\alpha,k} - |x|^{1+\frac{\alpha}{2}} L_{1,k})$ and $(\widetilde{\Phi}_{\alpha,k} - |x|^{-\frac{\alpha}{2}} L_{0,k})$ are elements of $\mathcal{D}(A_\alpha(k)^*)$. Therefore, owing to the representation (6.3.49)-(6.3.51), in order to check that such two functions also belong to $\mathcal{D}(\overline{A_\alpha(k)})$ it suffices to verify the limits

$$\begin{aligned} \lim_{x\to 0} |x|^{\frac{\alpha}{2}}(\widetilde{\Psi}_{\alpha,k} - |x|^{1+\frac{\alpha}{2}} L_{1,k}) &= \lim_{x\to 0} |x|^{\frac{\alpha}{2}}(\widetilde{\Phi}_{\alpha,k} - |x|^{-\frac{\alpha}{2}} L_{0,k}) = 0 \\ \lim_{x\to 0} |x|^{-(1+\frac{\alpha}{2})}(\widetilde{\Psi}_{\alpha,k} - |x|^{1+\frac{\alpha}{2}} L_{1,k}) &= \lim_{x\to 0} |x|^{-(1+\frac{\alpha}{2})}(\widetilde{\Phi}_{\alpha,k} - |x|^{-\frac{\alpha}{2}} L_{0,k}) = 0\,. \end{aligned}$$

The check is obvious, and holds thanks to the short-distance asymptotics that were chosen for $L_{0,k}$ and $L_{1,k}$ precisely so as to suitably match with the short-distance asymptotics (6.3.14) of $\widetilde{\Phi}_{\alpha,k}$ and (6.3.29) of $\widetilde{\Psi}_{\alpha,k}$. This finally shows that $\varphi \in \mathcal{D}(\overline{A_\alpha(k)})$ and establishes (6.4.25). Of course, if conversely a function g of the form (6.4.25) is given with $\varphi \in \mathcal{D}(\overline{A_\alpha(k)})$, unfolding the above arguments one sees that $g \in \mathcal{D}(A_\alpha(k)^*)$.

If instead $k = 0$, the same argument can be repeated decomposing now $g \in \mathcal{D}(A_\alpha(0)^*)$ as $g^\pm = \widetilde{\varphi}^\pm + c_1^\pm \widetilde{\Psi}_{\alpha,0} + c_0^\pm \widetilde{\Phi}_{\alpha,0}$ according to the decomposition (6.4.16), and using now the short-range asymptotics (6.7.22), (6.7.30), and Lemma 6.7.8 valid for $k = 0$. We omit the straightforward details. □

6.5 General extensions of $\mathscr{H}_\alpha$

Let us now come in this Section to the study of the self-adjoint extensions, in the Hilbert space (6.2.9), namely

$$\mathcal{H} \cong \bigoplus_{k\in\mathbb{Z}} \mathfrak{h}_k \cong \ell^2(\mathbb{Z}, \mathfrak{h}), \qquad \mathfrak{h}_k \cong \mathfrak{h} \cong L^2(\mathbb{R}^-) \oplus L^2(\mathbb{R}^+), \tag{6.5.1}$$

of the operator $\mathscr{H}_\alpha$ introduced in (6.2.14) for $\alpha \in (0, 1)$. Such extensions are restrictions of $\mathscr{H}_\alpha^*$, and it is standard that $\mathscr{H}_\alpha^* = \bigoplus_{k\in\mathbb{Z}} A_\alpha(k)^*$ (see also Lemma 6.7.2)

Clearly, $\mathscr{H}_\alpha$ is semi-bounded from below, since $\mathscr{H}_\alpha \subset \bigoplus_{k\in\mathbb{Z}} A_\alpha(k)$ and owing to the uniform semi-boundedness of each $A_\alpha(k)$ (see (6.3.1)). One can then naturally associate to $\mathscr{H}_\alpha$ its Friedrichs extension $\mathscr{H}_{\alpha,F} = \bigoplus_{k\in\mathbb{Z}} A_{\alpha,F}(k)$ (see the Appendix, Sec. 6.7.6 for more details).

There is an obvious peculiarity of the mode $k = 0$ that needs be dealt with separately. Indeed, we know from (6.3.1) that

$$A_{\alpha,F}(k) \geqslant (1+\alpha)\big(\tfrac{2+\alpha}{4}\big)^{\frac{\alpha}{1+\alpha}} \mathbb{1}_k\,, \qquad k \in \mathbb{Z}\setminus\{0\}\,, \tag{6.5.2}$$

whereas the bottom of $A_\alpha(0)$, and hence also of $A_{\alpha,F}(0)$ is precisely zero. Thus, all Friedrichs extensions on fibre have everywhere-defined bounded inverse but the one corresponding to $k = 0$.

It is then convenient to consider a positive shift of $\mathscr{H}_\alpha$ in the zero mode only. Clearly, with $\mathbb{1}_0$ acting as the identity in the 0-th fibre and as the zero operator in all other fibres, the operators $\mathscr{H}_\alpha$ and $\mathscr{H}_\alpha + \mathbb{1}_0$ have precisely the same domain, and so do the respective adjoints and the respective Friedrichs extensions.

Lemma 6.5.1. *Let $\alpha \in [0, 1)$. Let $(\psi_k)_{k\in\mathbb{Z}} \in \mathcal{H} \cong \ell^2(\mathbb{Z}, \mathfrak{h})$. Then:*

(i) $(\psi_k)_{k\in\mathbb{Z}} \in \ker(\mathscr{H}_\alpha + \mathbb{1}_0)^*$ *if and only if*

$$\psi_k = c_{0,k}^- \widetilde{\Phi}_{\alpha,k} \oplus c_{0,k}^+ \widetilde{\Phi}_{\alpha,k} \qquad \forall k \in \mathbb{Z} \tag{6.5.3}$$

for coefficients $c_{0,k}^\pm \in \mathbb{C}$ such that

$$\sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{2}{1+\alpha}} |c_{0,k}^\pm|^2 < +\infty\,. \tag{6.5.4}$$

Furthermore, there is a Hilbert space isomorphism

$$\ker(\mathscr{H}_\alpha + \mathbb{1}_0)^* \cong \ell^2(\mathbb{Z}, \mathbb{C}^2, \mu_k) \tag{6.5.5}$$

with

$$\mu_k := \begin{cases} |k|^{-\frac{2}{1+\alpha}}, & k \neq 0, \\ 1, & k = 0, \end{cases} \tag{6.5.6}$$

(ii) $(\psi_k)_{k\in\mathbb{Z}} \in (\mathscr{H}_\alpha^F + \mathbb{1}_0)^{-1} \ker(\mathscr{H}_\alpha + \mathbb{1}_0)^*$ *if and only if*

$$\psi_k = c_{1,k}^- \widetilde{\Psi}_{\alpha,k} \oplus c_{1,k}^+ \widetilde{\Psi}_{\alpha,k} \qquad \forall k \in \mathbb{Z} \tag{6.5.7}$$

for coefficients $c_{1,k}^\pm \in \mathbb{C}$ *such that*

$$\sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{2}{1+\alpha}} |c_{1,k}^\pm|^2 < +\infty . \tag{6.5.8}$$

Proof. Part (i) follows from the identity $\ker(\mathscr{H}_\alpha + \mathbb{1}_0)^* = \bigoplus_{k\in\mathbb{Z}} \ker(A(k)^* + \delta_{k,0}\mathbb{1}_0)$ (Lemma 6.7.3, eq. (6.7.13)), from $\ker(A(k)^* + \delta_{k,0}\mathbb{1}_0) = \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\} \oplus \mathrm{span}\{\widetilde{\Phi}_{\alpha,k}\}$ (Lemmas 6.3.2 and 6.7.5, and formula (6.4.9)), and from $\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)} \sim |k|^{-\frac{2}{1+\alpha}}$ for $k \neq 0$ (formula (6.3.16)).

Part (ii) follows from the identity

$$\begin{aligned} (\mathscr{H}_\alpha^F + \mathbb{1}_0)^{-1} \ker(\mathscr{H}_\alpha + \mathbb{1}_0)^* &= \bigoplus_{k\in\mathbb{Z}\setminus\{0\}} (A_{\alpha,F}(k))^{-1} \ker A_\alpha(k)^* \\ &\qquad \oplus (A_{\alpha,F}(0) + \mathbb{1}_0)^{-1} \ker(A_\alpha(0)^* + \mathbb{1}_0), \end{aligned}$$

which is a consequence of Lemma 6.7.3 (eq. (6.7.13)) and Lemma 6.7.12, from the identity

$$(A_{\alpha,F}(k) + \delta_{k,0}\mathbb{1}_0)^{-1} \ker(A_\alpha(k)^* + \delta_{k,0}\mathbb{1}_0) = \mathrm{span}\{\widetilde{\Psi}_{\alpha,k}\} \oplus \mathrm{span}\{\widetilde{\Psi}_{\alpha,k}\},$$

which is a consequence of Lemmas 6.3.2 and 6.7.5, and of Propositions 6.3.15 and 6.7.9, from the consequent identity

$$\sum_{k\in\mathbb{Z}\setminus\{0\}} \left\| A_\alpha(k)^* \begin{pmatrix} c_{1,k}^- \widetilde{\Psi}_{\alpha,k} \\ c_{1,k}^+ \widetilde{\Psi}_{\alpha,k} \end{pmatrix} \right\|_{\mathfrak{h}}^2 = \sum_{k\in\mathbb{Z}\setminus\{0\}} \left\| \begin{pmatrix} c_{1,k}^- \widetilde{\Phi}_{\alpha,k} \\ c_{1,k}^+ \widetilde{\Phi}_{\alpha,k} \end{pmatrix} \right\|_{\mathfrak{h}}^2$$

and again from the norm asymptotic $\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)} \sim |k|^{-\frac{2}{1+\alpha}}$.

□

This allows us to characterise the domain of $\mathscr{H}_\alpha^*$ in terms of the representation given by Theorem 6.3.13

$$\begin{aligned} \mathcal{D}(\mathscr{H}_\alpha^*) &= \mathcal{D}((\mathscr{H}_\alpha + \mathbb{1}_0)^*) \\ &= \mathcal{D}(\overline{\mathscr{H}_\alpha + \mathbb{1}_0}) \dotplus (\mathscr{H}_{\alpha,F} + \mathbb{1}_0)^{-1} \ker(\mathscr{H}_\alpha + \mathbb{1}_0)^* \dotplus \ker(\mathscr{H}_\alpha + \mathbb{1}_0)^* \\ &= \mathcal{D}(\overline{\mathscr{H}_\alpha}) \dotplus (\mathscr{H}_{\alpha,F} + \mathbb{1}_0)^{-1} \ker(\mathscr{H}_\alpha^* + \mathbb{1}_0) \dotplus \ker(\mathscr{H}_\alpha^* + \mathbb{1}_0). \end{aligned} \tag{6.5.9}$$

Lemma 6.5.2. *Let* $\alpha \in [0,1)$. *Let* $(g_k)_{k\in\mathbb{Z}} \in \mathcal{H} \cong \ell^2(\mathbb{Z},\mathfrak{h})$. *Then* $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}_\alpha^*)$ *if and only if*

$$g_k = \begin{pmatrix} \widetilde{\varphi}_k^- \\ \widetilde{\varphi}_k^+ \end{pmatrix} + \begin{pmatrix} c_{1,k}^- \widetilde{\Psi}_{\alpha,k} \\ c_{1,k}^+ \widetilde{\Psi}_{\alpha,k} \end{pmatrix} + \begin{pmatrix} c_{0,k}^- \widetilde{\Phi}_{\alpha,k} \\ c_{0,k}^+ \widetilde{\Phi}_{\alpha,k} \end{pmatrix} \qquad \forall k \in \mathbb{Z} \tag{6.5.10}$$

with

$$(\widetilde{\varphi}_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\overline{\mathscr{H}_\alpha}), \qquad \widetilde{\varphi}_k \equiv \begin{pmatrix} \widetilde{\varphi}_k^- \\ \widetilde{\varphi}_k^+ \end{pmatrix} \tag{6.5.11}$$

and

$$\sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{2}{1+\alpha}} |c_{0,k}^\pm|^2 < +\infty \tag{6.5.12}$$

$$\sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{2}{1+\alpha}} |c_{1,k}^\pm|^2 < +\infty . \tag{6.5.13}$$

Proof. From the representation (6.5.9) one deduces at once that in order for $(g_k)_{k\in\mathbb{Z}}$ to belong to $\mathcal{D}(\mathscr{H}_\alpha^*)$ it is necessary and sufficient that

$$(g_k)_{k\in\mathbb{Z}} \;=\; (\widetilde{\varphi}_k)_{k\in\mathbb{Z}} + (\psi_k)_{k\in\mathbb{Z}} + (\xi_k)_{k\in\mathbb{Z}}$$

for some $(\widetilde{\varphi}_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\overline{\mathscr{H}_\alpha})$, $(\psi_k)_{k\in\mathbb{Z}} \in (\mathscr{H}_\alpha^F + \mathbb{1}_0)^{-1}\ker(\mathscr{H}_\alpha^* + \mathbb{1}_0)$, and $(\xi_k)_{k\in\mathbb{Z}} \in \ker(\mathscr{H}_\alpha^* + \mathbb{1}_0)$. The conclusion then follows from Lemma 6.5.1. □

We now present the general family of self-adjoint extensions of $\mathscr{H}_\alpha$ in $\mathcal{H}$, as it follows directly from Theorem 6.3.13. The object of the next Section, is the study of the uniformly fibred extensions of $\mathscr{H}_\alpha$ (see also Prop. 6.7.4). In fact, for the latter a clean and explicit description can be further obtained when going back to the original variables (x, y) of the Grushin cylinder.

Theorem 6.5.3. *Let $\alpha \in [0, 1)$. There is a one-to-one correspondence $S \leftrightarrow \mathscr{H}_\alpha^S$ between the self-adjoint extensions $\mathscr{H}_\alpha^S$ of $\mathscr{H}_\alpha$ and the self-adjoint operators S defined on Hilbert subspaces of* $\ker(\mathscr{H}_\alpha^* + \mathbb{1}_0) \cong \ell^2(\mathbb{Z}, \mathbb{C}^2, \mu_k)$. *If S is any such operator, the corresponding extension $\mathscr{H}_\alpha^S$ is given by*

$$\mathcal{D}(\mathscr{H}_\alpha^S) \;=\; \left\{ \begin{array}{c} \psi = \widetilde{\varphi} + (\mathscr{H}_{\alpha,F} + \mathbb{1}_0)^{-1}(Sv + w) + v \\ \textit{such that} \\ \widetilde{\varphi} \in \mathcal{D}(\overline{\mathscr{H}_\alpha}), \quad v \in \mathcal{D}(S), \\ w \in \ker(\mathscr{H}_\alpha^* + \mathbb{1}_0) \cap \mathcal{D}(S)^\perp \end{array} \right\} \tag{6.5.14}$$

$$(\mathscr{H}_\alpha^S + \mathbb{1}_0)\psi \;=\; (\overline{\mathscr{H}_\alpha} + \mathbb{1}_0)\widetilde{\varphi} + Sv + w\,.$$

Proof. A direct application of the KVB self-adjoint extension theory (see Theorem 6.3.13). The second formula in (6.5.14) follows from the first as $(\mathscr{H}_\alpha^S + \mathbb{1}_0) = (\mathscr{H}_\alpha^* + \mathbb{1}_0) \restriction \mathcal{D}(\mathscr{H}_\alpha^S)$. □

Theorem 6.5.3 encompasses a huge variety of extensions, for $\mathscr{H}_\alpha$ has infinite deficiency index (that is, $\ker(\mathscr{H}_\alpha^* + \mathbb{1}_0)$ is infinite-dimensional). The self-adjointness condition for each $\mathscr{H}_\alpha^S$ is in fact a *restriction condition* on the domain $\mathscr{H}_\alpha^*$: in terms of the representation (6.5.9), such a restriction selects, among the generic elements

$$\psi \;=\; \widetilde{\varphi} + (\mathscr{H}_{\alpha,F} + \mathbb{1}_0)^{-1}\eta + \xi$$

of $\mathcal{D}(\mathscr{H}_\alpha^*)$, only those for which the vectors $\xi, \eta \in \ker(\mathscr{H}_\alpha^* + \mathbb{1}_0)$ (customarily referred to as the '*charges*' of ψ, see e.g. [86] and references therein) satisfy

$$\begin{aligned} \xi \;&=\; v \;\in\; \mathcal{D}(S), \\ \eta \;&=\; Sv + w, \quad w \in \ker(\mathscr{H}_\alpha^* + \mathbb{1}_0) \cap \mathcal{D}(S)^\perp\,. \end{aligned}$$

In this respect, the above condition produces in general a non-fibre-preserving mixing of the charge η with respect to the charge ξ: such a mixing is encoded in the auxiliary operator S.

The class of relevant extensions that we are going to study more in detail is such that the above mixing is absent instead, and the restriction condition of self-adjointness operates *independently in each fibre*. This is the case when

$$S \;=\; \bigoplus_{k\in\mathbb{Z}} S(k) \qquad \text{on} \qquad \ker(\mathscr{H}_\alpha^* + \mathbb{1}_0) \;=\; \bigoplus_{k} \ker(A_\alpha(k)^* + \delta_{k,0}\mathbb{1}_0) \tag{6.5.15}$$

for operators $S(k)$'s each of which is self-adjoint on a (zero-, one-, two-dimensional) subspace $\mathcal{K}$ of the two-dimensional space $\ker(A_\alpha(k)^* + \delta_{k,0}\mathbb{1}_0)$. Extensions (6.5.14) where S is of the form (6.5.15) shall be referred as *fibred extensions*.

Since each fibre of $\ker(\mathscr{H}_\alpha^* + \mathbb{1}_0)$ is isomorphic to $\mathbb{C}^2$, we can identify each self-adjoint component $S(k)$ with an hermitian 2×2-matrix. Then, we shall more precisely study the extensions produced by operators S that act in the same way on each fibre, that are those S such that $S(k) = S(0)$, for all $k \in \mathbb{Z}$: those shall be referred as *uniformly fibred extensions*.

6.6 Uniformly fibred extensions of $\mathscr{H}_\alpha$

From now on we focus on the relevant sub-class of self-adjoint extensions of $\mathscr{H}_\alpha$: those that we refer to as *uniformly fibred extensions*. For such extensions we shall obtain a more explicit and convenient characterisation, namely Theorem 6.6.1 below, as compared to the general classification of Theorem 6.5.3.

6.6.1 Generalities and classification theorem

We are now concerned with extensions that are *fibred*, in the sense discussed in the end of Sect. 6.5, hence given by the direct sum of a self-adjoint extension of $A_\alpha(k)$ on each fibre, and therefore with conditions of self-adjointness that do not couple different fibres, which *in addition* display uniformity.

Let us recall that a generic fibred extension acts on each fibre as a generic self-adjoint realisation of $A_\alpha(k)$ that belongs to one of the families of the classification of Theorem 6.4.1, and is therefore parametrised (apart when it is $A_{\alpha,F}(k)$) by one real parameter or four real parameters. Such extension types and extension parameters may differ fibre by fibre, say, parameter $\gamma^{(k_1)}$ for an extension of type $\mathrm{I_R}$ or $\mathrm{I_L}$ or II_{a_k} on the k_1-th fibre, and parameters $\gamma_1^{(k_2)}, \dots, \gamma_4^{(k_2)}$ for an extension of type III on the k_2-th fibre.

Uniformly fibred extensions are those for which, fibre by fibre, the type of extension of $A_\alpha(k)$ is the same, and all have the same extension parameter(s) γ (and a), or $\gamma_1, \dots, \gamma_4$.

By definition, uniformly fibred extensions can be therefore grouped into sub-families in complete analogy to those of Theorem 6.4.1:

- Friedrichs extension: the operator $\mathscr{H}_{\alpha,F} = \bigoplus_{k\in\mathbb{Z}} A_{\alpha,F}(k)$ (see Lemma 6.7.12);
- Family $\mathrm{I_R}$: operators of the form

$$\mathscr{H}^{[\gamma]}_{\alpha,R} := \bigoplus_{k\in\mathbb{Z}} A^{[\gamma]}_{\alpha,R}(k) \tag{6.6.1}$$

  for some $\gamma \in \mathbb{R}$;
- Family $\mathrm{I_L}$: operators of the form

$$\mathscr{H}^{[\gamma]}_{\alpha,L} := \bigoplus_{k\in\mathbb{Z}} A^{[\gamma]}_{\alpha,L}(k) \tag{6.6.2}$$

  for some $\gamma \in \mathbb{R}$;
- Family II_a for given $a \in \mathbb{C}$: operators of the form

$$\mathscr{H}^{[\gamma]}_{\alpha,a} := \bigoplus_{k\in\mathbb{Z}} A^{[\gamma]}_{\alpha,a}(k) \tag{6.6.3}$$

  for some $\gamma \in \mathbb{R}$;
- Family III: operators of the form

$$\mathscr{H}^{[\Gamma]}_{\alpha} := \bigoplus_{k\in\mathbb{Z}} A^{[\Gamma]}_{\alpha}(k) \tag{6.6.4}$$

  for some $\Gamma \equiv (\gamma_1, \gamma_2, \gamma_3, \gamma_4) \in \mathbb{R}^4$.

Physically, uniformly fibred extensions have surely a special status in that the boundary condition experienced as $x \to 0$ by the quantum particle governed by any such Hamiltonian has both the same form and the same 'magnitude' (hence the same γ-parameter, or γ_j-parameters) irrespective of the transversal momentum, namely the quantum number k.

In addition, from the mathematical point of view uniformly fibred extensions allow for a completely explicit description not only in mixed position-momentum variables (x, k), namely extensions of $\mathscr{H}_\alpha$, but also in the original physical coordinates (x, y), namely extensions of the symmetric operator $\mathsf{H}_\alpha = \mathcal{F}_2^{-1}\mathscr{H}_\alpha\mathcal{F}_2$ acting on $L^2(\mathbb{R}\times S^1, \mathrm{d}x\mathrm{d}y)$, explicitly described in (6.2.12).

This is the content of the main result of the present Section.

Theorem 6.6.1. *Let $\alpha \in [0, 1)$. The densely defined, symmetric operator*

$$\begin{aligned} \mathsf{H}_\alpha &= \mathcal{F}_2^{-1}\mathscr{H}_\alpha\mathcal{F}_2 = -\frac{\partial^2}{\partial x^2} - |x|^{2\alpha}\frac{\partial^2}{\partial y^2} + \frac{\alpha(2+\alpha)}{4x^2} \\ \mathcal{D}(\mathsf{H}^\pm_\alpha) &= C_0^\infty(\mathbb{R}^\pm_x \times S^1_y) \end{aligned}$$

admits the following families of self-adjoint extensions in $L^2(\mathbb{R}\times S^1, \mathrm{d}x\mathrm{d}y)$:

- *<u>Friedrichs extension</u>:* $\mathsf{H}_{\alpha,F}$, *where* $\mathsf{H}_{\alpha,F} = \mathcal{F}_2^{-1}\mathscr{H}_{\alpha,F}\mathcal{F}_2$;
- *<u>Family</u>* $\mathrm{I_R}$*:* $\{\mathsf{H}^{[\gamma]}_{\alpha,R} \mid \gamma \in \mathbb{R}\}$, *where* $\mathsf{H}^{[\gamma]}_{\alpha,R} = \mathcal{F}_2^{-1}\mathscr{H}^{[\gamma]}_{\alpha,R}\mathcal{F}_2$;
- *<u>Family</u>* $\mathrm{I_L}$*:* $\{\mathsf{H}^{[\gamma]}_{\alpha,L} \mid \gamma \in \mathbb{R}\}$, *where* $\mathsf{H}^{[\gamma]}_{\alpha,L} = \mathcal{F}_2^{-1}\mathscr{H}^{[\gamma]}_{\alpha,L}\mathcal{F}_2$;
- *<u>Family</u>* II_a *with* $a \in \mathbb{C}$*:* $\{\mathsf{H}^{[\gamma]}_{\alpha,a} \mid \gamma \in \mathbb{R}\}$, *where* $\mathsf{H}^{[\gamma]}_{\alpha,a} = \mathcal{F}_2^{-1}\mathscr{H}^{[\gamma]}_{\alpha,a}\mathcal{F}_2$;
- *<u>Family</u>* III*:* $\{\mathsf{H}^{[\Gamma]}_{\alpha} \mid \Gamma \equiv (\gamma_1,\gamma_2,\gamma_3,\gamma_4) \in \mathbb{R}^4\}$, *where* $\mathsf{H}^{[\Gamma]}_{\alpha} = \mathcal{F}_2^{-1}\mathscr{H}^{[\Gamma]}_{\alpha}\mathcal{F}_2$.

Each element from any such family is characterised by being the restriction *of the adjoint operator*

$$\begin{aligned} \mathcal{D}(\mathsf{H}^*_\alpha) &= \left\{ \begin{array}{c} \phi \in L^2(\mathbb{R}\times S^1, \mathrm{d}x\mathrm{d}y) \text{ such that} \\ \left(-\frac{\partial^2}{\partial x^2} - |x|^{2\alpha}\frac{\partial^2}{\partial y^2} + \frac{\alpha(2+\alpha)}{4x^2}\right)\phi^\pm \in L^2(\mathbb{R}^\pm\times S^1, \mathrm{d}x\mathrm{d}y) \end{array} \right\} \\ (\mathsf{H}^\pm_\alpha)^*\phi^\pm &= -\frac{\partial^2\phi^\pm}{\partial x^2} - |x|^{2\alpha}\frac{\partial^2\phi^\pm}{\partial y^2} + \frac{\alpha(2+\alpha)}{4x^2}\phi^\pm \end{aligned} \tag{6.6.5}$$

to the functions

$$\phi = \begin{pmatrix}\phi^-\\ \phi^+\end{pmatrix}, \qquad \phi^\pm \in L^2(\mathbb{R}^\pm\times S^1, \mathrm{d}x\mathrm{d}y)$$

for which the limits

$$\phi_0^\pm(y) = \lim_{x\to 0^\pm} |x|^{\frac{\alpha}{2}}\,\phi^\pm(x,y) \tag{6.6.6}$$

$$\begin{aligned} \phi_1^\pm(y) &= \lim_{x\to 0^\pm} |x|^{-(1+\frac{\alpha}{2})}\big(\phi^\pm(x,y) - \phi_0^\pm(y)|x|^{-\frac{\alpha}{2}}\big) \\ &= \pm(1+\alpha)^{-1}\lim_{x\to 0^\pm}|x|^{-\alpha}\partial_x\big(|x|^{\frac{\alpha}{2}}\phi^\pm(x,y)\big) \end{aligned} \tag{6.6.7}$$

exist and are finite for almost every $y \in S^1$*, and satisfy the following boundary conditions, depending on the considered type of extension, for almost every* $y \in \mathbb{R}$*:*

$$\phi_0^\pm(y) = 0 \qquad \text{if } \phi \in \mathcal{D}(\mathsf{H}_{\alpha,F}), \tag{6.6.8}$$

$$\begin{cases} \phi_0^-(y) = 0 \\ \phi_1^+(y) = \gamma\phi_0^+(y) \end{cases} \qquad \text{if } \phi \in \mathcal{D}(\mathsf{H}^{[\gamma]}_{\alpha,R}), \tag{6.6.9}$$

$$\begin{cases} \phi_1^-(y) = \gamma\phi_0^-(y) \\ \phi_0^+(y) = 0 \end{cases} \qquad \text{if } \phi \in \mathcal{D}(\mathsf{H}^{[\gamma]}_{\alpha,L}), \tag{6.6.10}$$

$$\begin{cases} \phi_0^+(y) = a\,\phi_0^-(y) \\ \phi_1^-(y) + \overline{a}\,\phi_1^+(y) = \gamma\phi_0^-(y) \end{cases} \qquad \text{if } \phi \in \mathcal{D}(\mathsf{H}^{[\gamma]}_{\alpha,a}), \tag{6.6.11}$$

$$\begin{cases} \phi_1^-(y) = \gamma_1\phi_0^-(y) + (\gamma_2 + \mathrm{i}\gamma_3)\phi_0^+(y) \\ \phi_1^+(y) = (\gamma_2 - \mathrm{i}\gamma_3)\phi_0^-(y) + \gamma_4\phi_0^+(y) \end{cases} \qquad \text{if } \phi \in \mathcal{D}(\mathsf{H}^{[\Gamma]}_{\alpha}). \tag{6.6.12}$$

Moreover,

$$\phi_0^\pm \in H^{s_{0,\pm}}(S^1, \mathrm{d}y) \qquad \text{and} \qquad \phi_1^\pm \in H^{s_{1,\pm}}(S^1, \mathrm{d}y) \tag{6.6.13}$$

with

- $s_{1,\pm} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$ *for the Friedrichs extension,*
- $s_{1,-} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$, $s_{0,+} = s_{1,+} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type* I_R*,*
- $s_{1,+} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$, $s_{0,-} = s_{1,-} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type* I_L*,*
- $s_{1,\pm} = s_{0,\pm} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$ *for extensions of type* II_a*,*
- $s_{1,\pm} = s_{0,\pm} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type* III.

6.6.2 General strategy

The proof of Theorem 6.6.1 is going to require quite a detailed analysis, as we shall now explain. All the preparation is developed in Subsect. 6.6.2 through 6.7.8, and the proof will be discussed in Subsect. 6.6.6.

The trivial part is of course the reconstruction of each uniformly fibred extension of $\mathscr{H}_\alpha$ through a direct sum of self-adjoint extensions of the $A_\alpha(k)$'s. Instead, the difficult part is to extract the appropriate information so as to export the boundary conditions of self-adjointness from the mixed position-momentum variables (x, k) to the physical coordinates (x, y). The inverse Fourier transform $\mathcal{F}_2^{-1}$ is indeed a non-local operation, and in order to 'add up' the boundary conditions initially available k by k, one needs suitable *uniformity* controls in k.

Let $\mathscr{H}_\alpha^{\mathrm{u.f.}}$ be a uniformly fibred extension of $\mathscr{H}_\alpha$. A generic element $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}_\alpha^{\mathrm{u.f.}})$ can be represented as in (6.5.10) with the 'summability' conditions (6.5.11)-(6.5.12) that guarantee $(g_k)_{k\in\mathbb{Z}}$ to belong to $\mathcal{D}(\mathscr{H}_\alpha^*)$ (Lemma 6.5.2), plus additional constraints among the coefficients $c_{0,k}^\pm$ and $c_{1,k}^\pm$ that guarantee that $\mathcal{D}(\mathscr{H}_\alpha^{\mathrm{u.f.}})$ is indeed a domain of self-adjointness.

However, the above-mentioned representation (6.5.10) for the elements of $\mathcal{D}(\mathscr{H}_\alpha^{\mathrm{u.f.}})$ seems problematic when one needs to describe $\mathcal{F}_2^{-1}\mathcal{D}(\mathscr{H}_\alpha^{\mathrm{u.f.}})$.

We shall follow a second route inspired to the alternative representation (6.4.25) (Theorem 6.4.3).

Now the generic element $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}_\alpha^{\mathrm{u.f.}})$ is represented for each k as

$$g_k \;=\; \begin{pmatrix}\varphi_k^-\\ \varphi_k^+\end{pmatrix} + \begin{pmatrix}g_{0,k}^-\\ g_{0,k}^+\end{pmatrix}|x|^{-\frac{\alpha}{2}}\,P + \begin{pmatrix}g_{1,k}^-\\ g_{1,k}^+\end{pmatrix}|x|^{1+\frac{\alpha}{2}}\,P \tag{6.6.14}$$

where each $\varphi_k \in \mathcal{D}(\overline{A_\alpha(k)})$ and P is the short-scale cut-off (6.4.24).

The evident advantage of (6.6.14) is that computing

$$\phi \;:=\; \mathcal{F}_2^{-1}(g_k)_{k\in\mathbb{Z}} \tag{6.6.15}$$

and using the linearity of $\mathcal{F}_2^{-1}$ yields *formally*

$$\phi(x,y) \;=\; \varphi(x,y) + g_1(y)|x|^{1+\frac{\alpha}{2}}P(x) + g_0(y)|x|^{-\frac{\alpha}{2}}P(x) \tag{6.6.16}$$

with

$$\varphi \;:=\; \mathcal{F}_2^{-1}(\varphi_k)_{k\in\mathbb{Z}} \tag{6.6.17}$$

$$g_0 \;:=\; \mathcal{F}_2^{-1}(g_{0,k})_{k\in\mathbb{Z}} \tag{6.6.18}$$

$$g_1 \;:=\; \mathcal{F}_2^{-1}(g_{1,k})_{k\in\mathbb{Z}}\,. \tag{6.6.19}$$

In (6.6.16) the function φ is expected to retain the regularity in x and the fast vanishing properties, as $x \to 0$, of each φ_k, and hence φ is expected to be a subleading term when taking $\lim_{x\to 0}\phi(x,y)$ and $\lim_{x\to 0}\partial_x\phi(x,y)$; on the other hand, the regularity and short-distance behaviour in x of the other two summands in the r.h.s. of (6.6.16) are immediately read out. Moreover, since $\mathscr{H}_\alpha^{\mathrm{u.f.}}$ is a *uniformly fibred* extension, the boundary condition of self-adjointness in (6.6.14) (namely a condition among those listed in the third column of Table 6.1) takes the same form, with the same extension parameter, irrespective of k, and therefore is immediately exported, in the same form and with the same extension parameter, between $g_0(y)$ and $g_1(y)$ for almost every $y \in S^1$.

Clearly, so far (6.6.16) is only formal: one must guarantee that (6.6.17)-(6.6.19) are actually well-posed and define square-integrable functions in the corresponding variables, with the desired properties.

As we shall comment further on (Subsect. 6.7.7), such a strategy will lead to the following singular circumstance: whereas Lemma 6.5.2 guarantees that applying $\mathcal{F}_2^{-1}$ on $(g_k)_{k\in\mathbb{Z}}$ represented as in (6.5.10) yields three distinct functions, each of which belongs to $\mathcal{F}_2^{-1}\mathcal{D}(\mathscr{H}_\alpha^*) = \mathcal{D}(\mathsf{H}_\alpha^*)$, the three summands in the r.h.s. of (6.6.16) will be proved to belong to $L^2(\mathbb{R}\times S^1, \mathrm{d}x\mathrm{d}y)$, *none* of which being however in $\mathcal{D}(\mathsf{H}_\alpha^*)$ in general – only their sum is, due to cancellations of singularities. This explains why the analysis is going to be onerous.

6.6.3 Integrability and Sobolev regularity of g_0 and g_1

Following the programme outlined in the previous Subsection, let us show that (6.6.18) and (6.6.19) indeed defines functions in $L^2(S^1, \mathrm{d}y)$ with suitable regularity.

Proposition 6.6.2. *Let $\alpha \in [0,1)$ and let $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}_\alpha^{\mathrm{u.f.}})$, where $\mathscr{H}_\alpha^{\mathrm{u.f.}}$ is one of the operators* (6.7.39) *or* (6.6.1)-(6.6.4)*, for given parameters $\gamma \in \mathbb{R}$, $a \in \mathbb{C}$, $\Gamma \in \mathbb{R}^4$, depending on the type. With respect to the representation* (6.6.14) *of each g_k, one has the following.*

(i) If $\mathscr{H}_\alpha^{\text{u.f.}}$ is the Friedrichs extension, then

$$\sum_{k\in\mathbb{Z}} |k|^{\frac{1-\alpha}{1+\alpha}} |g_{1,k}^{\pm}|^2 \;<\; +\infty, \qquad g_{0,k}^{\pm} \;=\; 0\,. \tag{6.6.20}$$

(ii) If $\mathscr{H}_\alpha^{\text{u.f.}}$ is of type I_R, then

$$\begin{aligned} &\sum_{k\in\mathbb{Z}} |k|^{\frac{1-\alpha}{1+\alpha}} |g_{1,k}^{-}|^2 \;<\; +\infty, \qquad g_{0,k}^{-} \;=\; 0, \\ &\sum_{k\in\mathbb{Z}} |k|^{\frac{3+\alpha}{1+\alpha}} |g_{1,k}^{+}|^2 \;<\; +\infty, \qquad \sum_{k\in\mathbb{Z}} |k|^{\frac{3+\alpha}{1+\alpha}} |g_{0,k}^{+}|^2 \;<\; +\infty\,. \end{aligned} \tag{6.6.21}$$

(iii) If $\mathscr{H}_\alpha^{\text{u.f.}}$ is of type I_L, then

$$\begin{aligned} &\sum_{k\in\mathbb{Z}} |k|^{\frac{1-\alpha}{1+\alpha}} |g_{1,k}^{+}|^2 \;<\; +\infty, \qquad g_{0,k}^{+} \;=\; 0, \\ &\sum_{k\in\mathbb{Z}} |k|^{\frac{3+\alpha}{1+\alpha}} |g_{1,k}^{-}|^2 \;<\; +\infty, \qquad \sum_{k\in\mathbb{Z}} |k|^{\frac{3+\alpha}{1+\alpha}} |g_{0,k}^{-}|^2 \;<\; +\infty\,. \end{aligned} \tag{6.6.22}$$

(iv) If $\mathscr{H}_\alpha^{\text{u.f.}}$ is of type II_a, then

$$\begin{aligned} &\sum_{k\in\mathbb{Z}} |k|^{\frac{1-\alpha}{1+\alpha}} |g_{1,k}^{\pm}|^2 \;<\; +\infty, \qquad \sum_{k\in\mathbb{Z}} |k|^{\frac{3+\alpha}{1+\alpha}} |g_{0,k}^{\pm}|^2 \;<\; +\infty, \\ &\sum_{k\in\mathbb{Z}} |k|^{\frac{3+\alpha}{1+\alpha}} |g_{1,k}^{-} + \overline{a} g_{1,k}^{+}|^2 \;<\; +\infty\,. \end{aligned} \tag{6.6.23}$$

(v) If $\mathscr{H}_\alpha^{\text{u.f.}}$ is of type III, then

$$\sum_{k\in\mathbb{Z}} |k|^{\frac{3+\alpha}{1+\alpha}} |g_{0,k}^{\pm}|^2 \;<\; +\infty, \qquad \sum_{k\in\mathbb{Z}} |k|^{\frac{3+\alpha}{1+\alpha}} |g_{1,k}^{\pm}|^2 \;<\; +\infty\,. \tag{6.6.24}$$

Corollary 6.6.3. *Under the assumptions of Proposition 6.6.2, $(g_{0,k}^{\pm})_{k\in\mathbb{Z}}$ and $(g_{1,k}^{\pm})_{k\in\mathbb{Z}}$ belong $\ell^2(\mathbb{Z})$. Hence,* (6.6.18) *and* (6.6.19) *define functions $y \mapsto g_0^{\pm}(y)$ and $y \mapsto g_1^{\pm}(y)$ that belong to $L^2(S^1, \mathrm{d}y)$. In particular, the summability properties* (6.6.20)-(6.6.24) *imply that $g_0^{\pm} \in H^{s_{0,\pm}}(S^1, \mathrm{d}y)$ and $g_1^{\pm} \in H^{s_{1,\pm}}(S^1, \mathrm{d}y)$, where the order of such Sobolev spaces is, respectively,*

(i) $s_{1,\pm} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$ *for the Friedrichs extension,*

(ii) $s_{1,-} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$, $s_{0,+} = s_{1,+} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type I_R,*

(iii) $s_{1,+} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$, $s_{0,-} = s_{1,-} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type I_L,*

(iv) $s_{1,\pm} = s_{0,\pm} = \frac{1}{2}\frac{1-\alpha}{1+\alpha}$ *for extensions of type II_a,*

(v) $s_{1,\pm} = s_{0,\pm} = \frac{1}{2}\frac{3+\alpha}{1+\alpha}$ *for extensions of type* III.

Proof of Proposition 6.6.2. For each case, the proof is organised in two levels. First, we consider each family of extensions as characterised by Theorem 6.4.2 in terms of certain self-adjointness constraints between the coefficients $c_0^{\pm}$ and $c_1^{\pm}$ of the representation (6.5.9)-(6.5.10) of the elements of $\mathscr{D}(\mathscr{H}_\alpha^*)$, and we show that owing to such constraints the a priori summability (6.5.12)-(6.5.13) of the $c_0^{\pm}$'s and $c_1^{\pm}$'s is actually enhanced (see also Remark 6.6.5 below). Then, we export the resulting summability of the $c_0^{\pm}$'s and $c_1^{\pm}$'s on to the $g_0^{\pm}$'s and $g_1^{\pm}$'s by means of the relations

$$g_{0,k}^{\pm} \;=\; c_{0,k}^{\pm}\sqrt{\tfrac{\pi(1+\alpha)}{2|k|}} \tag{6.6.25}$$

$$g_{1,k}^{\pm} \;=\; c_{1,k}^{\pm}\sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\,\|\Phi_{\alpha,k}\|_{L^2(\mathbb{R}^+)}^2 - c_{0,k}^{\pm}\sqrt{\tfrac{\pi|k|}{2(1+\alpha)}} \tag{6.6.26}$$

valid for $k \neq 0$ (see (6.3.51) above).

Let us also recall from (6.3.16) that

$$\|\Phi_{\alpha,k}\|_{L^2(\mathbb{R}^+)}^2 \;\sim\; |k|^{-\frac{2}{1+\alpha}}\,,$$

namely for some multiplicative constant depending only on α.

(i) Theorem 6.4.2 states that for this case $c^{\pm}_{0,k} = 0$. This, together with (6.5.12) and (6.6.26), yields

$$+\infty \;>\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{2}{1+\alpha}} |c^{\pm}_{1,k}|^2 \;\sim\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{1-\alpha}{1+\alpha}} |g^{\pm}_{1,k}|^2 \,.$$

(ii) Theorem 6.4.2 states that for this case $c^{+}_{0,k} = 0$ and $c^{+}_{1,k} = \beta_k c^{+}_{0,k}$ with β_k given for $k \neq 0$ by

$$\gamma \;=\; \tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|^2_{L^2}}{\pi(1+\alpha)}\,\beta_k - 1\Big)$$

(see (6.3.54) above), that is, $\beta_k \sim |k|^{\frac{2}{1+\alpha}}$ at the leading order in k. (Here the operator of multiplication by β_k is what we denoted in abstract by $S(k)$ in the discussion following Theorem (6.5.3) – see (6.5.15) above.) This, together with (6.5.13) and (6.6.25) yields

$$+\infty \;>\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{2}{1+\alpha}} |c^{+}_{1,k}|^2 \;=\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{2}{1+\alpha}} |\beta_k c^{+}_{0,k}|^2 \;\sim\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{3+\alpha}{1+\alpha}} |g^{+}_{0,k}|^2 \,.$$

From this one also obtains

$$\sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{3+\alpha}{1+\alpha}} |g^{+}_{1,k}|^2 \;<\; +\infty\,,$$

owing to the self-adjointness condition in the form $g^{+}_{1,k} = \gamma g^{+}_{0,k}$ (Theorem 6.4.1). As for the summability of the $c^{-}_{1,k}$, one proceeds precisely as in case (i).

(iii) The reasoning for this case is completely analogous as for case (ii), upon exchanging the '+' coefficients with the '−' coefficients.

(iv) Theorem 6.4.2 states for this case

$$\begin{aligned} c^{-}_{0,k} \;&=\; c_{0,k}\,, & c^{-}_{1,k} \;&=\; \tau_k c_{0,k} + \widetilde{c}_{0,k}\,, \\ c^{+}_{0,k} \;&=\; a c_{0,k}\,, & c^{+}_{1,k} \;&=\; \tau_k a c_{0,k} - \overline{a}^{-1}\widetilde{c}_{0,k}\,, \end{aligned}$$

with τ_k given for $k \neq 0$ by

$$\gamma \;:=\; (1+|a|^2)\tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|^2_{L^2}}{\pi(1+\alpha)}\,\tau_k - 1\Big),$$

(see (6.4.19) above), that is $\tau_k \sim |k|^{\frac{2}{1+\alpha}}$ at the leading order in k. This, together with the a priori bounds (6.5.13), and with (6.6.25), yields

$$\begin{aligned} +\infty \;&>\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{2}{1+\alpha}} |c^{-}_{1,k} + \overline{a} c^{+}_{1,k}|^2 \;=\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{2}{1+\alpha}} |(1+|a|^2)\tau_k c_{0,k}|^2 \\ &\sim\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{3+\alpha}{1+\alpha}} |g^{-}_{0,k}|^2 \,. \end{aligned}$$

From this, and self-adjointness conditions $g^{+}_{0,k} = a g^{-}_{0,k}$ and $g^{-}_{1,k} + \overline{a} g^{+}_{1,k} = \gamma g^{-}_{0,k}$ (Theorem 6.4.1), one obtains the last two conditions in (6.6.23). As for establishing the first condition in (6.6.23), one has

$$\begin{aligned} &\sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{1-\alpha}{1+\alpha}}\, |g^{\pm}_{1,k}|^2 \\ &\qquad\leqslant\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{1-\alpha}{1+\alpha}}\, |c^{\pm}_{1,k}|^2 \tfrac{4|k|}{\pi(1+\alpha^3)} \|\Phi_{\alpha,k}\|^4_{L^2(\mathbb{R}^+)} + \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{1-\alpha}{1+\alpha}}\, |c^{\pm}_{0,k}|^2 \tfrac{\pi|k|}{(1+\alpha)} \\ &\qquad\sim\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{2}{1+\alpha}} |c^{\pm}_{1,k}|^2 + \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{3+\alpha}{1+\alpha}} |g^{\pm}_{0,k}|^2 \;<\; +\infty\,, \end{aligned}$$

having used (6.6.26) for the first step, (6.6.25) for the second step, and the a priori bounds (6.5.13) as well as the already proved second condition in (6.6.23) for the last step.

(v) Theorem 6.4.2 states for this case

$$\begin{pmatrix} c^{-}_{1,k} \\ c^{+}_{1,k} \end{pmatrix} \;=\; \begin{pmatrix} \tau_{1,k} & \tau_{2,k} + \mathrm{i}\tau_{3,k} \\ \tau_{2,k} - \mathrm{i}\tau_{3,k} & \tau_{4,k} \end{pmatrix} \begin{pmatrix} c^{-}_{0,k} \\ c^{+}_{0,k} \end{pmatrix}$$

with

$$\begin{aligned}
\gamma_1 &= \tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|^2_{L^2}}{\pi(1+\alpha)}\,\tau_{1,k}-1\Big)\\
\gamma_2+\mathrm{i}\gamma_3 &= (\tau_{2,k}+\mathrm{i}\tau_{3,k})\tfrac{2|k|}{\pi(1+\alpha)^2}\|\Phi_{\alpha,k}\|^2_{L^2}\\
\gamma_4 &= \tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|^2_{L^2}}{\pi(1+\alpha)}\,\tau_{4,k}-1\Big)
\end{aligned}$$

(see (6.4.20) above). Thus,

$$\tau_{1,k}\;\sim\;|k|^{\frac{2}{1+\alpha}}\,,\qquad \tau_{2,k}\pm\mathrm{i}\tau_{3,k}\;\sim\;|k|^{\frac{1-\alpha}{1+\alpha}}\,,\qquad \tau_{4,k}\;\sim\;|k|^{\frac{2}{1+\alpha}}\,,$$

and

$$\begin{pmatrix}c^-_{1,k}\\ c^+_{1,k}\end{pmatrix}\sim\begin{pmatrix}|k|^{\frac{2}{1+\alpha}} & |k|^{\frac{1-\alpha}{1+\alpha}}\\ |k|^{\frac{1-\alpha}{1+\alpha}} & |k|^{\frac{2}{1+\alpha}}\end{pmatrix}\begin{pmatrix}c^-_{0,k}\\ c^+_{0,k}\end{pmatrix}\sim\begin{pmatrix}|k|^{\frac{5+\alpha}{2(1+\alpha)}} & |k|^{\frac{3-\alpha}{2(1+\alpha)}}\\ |k|^{\frac{3-\alpha}{2(1+\alpha)}} & |k|^{\frac{5+\alpha}{2(1+\alpha)}}\end{pmatrix}\begin{pmatrix}g^-_{0,k}\\ g^+_{0,k}\end{pmatrix}$$

at the leading order in k, having used (6.6.25) in the last asymptotics. As the above matrix has determinant of leading order $|k|^{\frac{5+\alpha}{1+\alpha}}$, we obtain

$$\begin{pmatrix}g^-_{0,k}\\ g^+_{0,k}\end{pmatrix}\;\sim\;|k|^{-\frac{5+\alpha}{2(1+\alpha)}}\begin{pmatrix}1 & -|k|^{-1}\\ -|k|^{-1} & 1\end{pmatrix}\begin{pmatrix}c^-_{1,k}\\ c^+_{1,k}\end{pmatrix},$$

whence

$$|g^-_{0,k}|^2+|g^+_{0,k}|^2\;\lesssim\;|k|^{-\frac{5+\alpha}{1+\alpha}}\big(|c^-_{0,k}|^2+|c^+_{0,k}|^2\big)$$

at the leading order in k. Therefore,

$$\sum_{k\in\mathbb{Z}\setminus\{0\}}|k|^{\frac{3+\alpha}{1+\alpha}}\,|g^\pm_{0,k}|^2\;\lesssim\;\sum_{k\in\mathbb{Z}\setminus\{0\}}|k|^{-\frac{2}{1+\alpha}}\,\big(|c^-_{0,k}|^2+|c^+_{0,k}|^2\big)\;<\;+\infty\,,$$

having used the a priori bound (6.5.13) for the last step. This establishes the first condition in (6.6.24). The second condition follows at once from the first by means of the self-adjointness constraints

$$\begin{aligned}
g^-_{1,k} &= \gamma_1 g^-_{0,k}+(\gamma_2+\mathrm{i}\gamma_3)g^+_{0,k}\\
g^+_{1,k} &= (\gamma_2-\mathrm{i}\gamma_3)g^-_{0,k}+\gamma_4 g^+_{0,k}
\end{aligned}$$

from Theorem 6.4.1. □

Remark 6.6.4. In the work [97] it was determined that the deficiency space $\ker(\mathscr{H}_\alpha^*+\mathbb{1}_0)$ of $\mathscr{H}_\alpha$ is isomorphic to $H^{\frac{1}{2}\frac{1-\alpha}{1+\alpha}}(S^1)$. This fact can be easily deduced from the proof of Proposition 6.6.2, in a completely analogous way of part (i). Our analysis thus goes further the Sobolev regularity of the deficiency space, computing higher Sobolev regularities for the domains of self-adjoitness of uniform extensions of $\mathscr{H}_\alpha$.

Remark 6.6.5 (Enhanced summability)**.** Let $(g_k)_{k\in\mathbb{Z}}\in\mathcal{D}(\mathscr{H}_\alpha^*)$. As established in Lemma 6.5.2, the coefficients $c_{0,k}$ given by the representation (6.5.9)-(6.5.10) of g_k satisfy

$$\sum_{k\in\mathbb{Z}\setminus\{0\}}|k|^{-\frac{2}{1+\alpha}}|c^\pm_{0,k}|^2\;<\;+\infty\,.$$

If *in addition* $(g_k)_{k\in\mathbb{Z}}\in\mathcal{D}(\mathscr{H}_\alpha^{\mathrm{u.f.}})$ for some uniformly-fibred extension of $\mathscr{H}_\alpha$, then Prop. 6.6.2 above shows that the coefficients $g_{0,k}$ given by the representation (6.6.14) of g_k satisfy

$$\sum_{k\in\mathbb{Z}\setminus\{0\}}|k|^{\frac{3+\alpha}{1+\alpha}}|g^\pm_{0,k}|^2\;<\;+\infty$$

(this covers also the case when the $g^+_{0,k}$'s or the $g^-_{0,k}$'s are all zero, depending on the considered type of extension). The latter condition, owing to (6.6.25) and hence $g^\pm_{0,k}\sim|k|^{-\frac{1}{2}}c^\pm_{0,k}$, implies

$$\sum_{k\in\mathbb{Z}\setminus\{0\}}|k|^{\frac{2}{1+\alpha}}|c^\pm_{0,k}|^2\;<\;+\infty\,.$$

Thus, the condition of belonging to $\mathcal{D}(\mathscr{H}_\alpha^{\mathrm{u.f.}})$, instead of generically to $\mathcal{D}(\mathscr{H}_\alpha^*)$, enhances the summability of the sequence $(c^\pm_{0,k})_{k\in\mathbb{Z}}$.

6.6.4 Detecting short-scale asymptotics and regularity

As observed with (6.7.41), $\mathcal{F}_2^{-1}$ is applicable to $(\varphi_k)_{k\in\mathbb{Z}}$ and thus (6.6.17) defines a function $\varphi \in L^2(\mathbb{R}\times S^1, \mathrm{d}x\mathrm{d}y)$. The next step in the strategy outlined in Subsect. 6.6.2 is to show convenient short-scale asymptotics as $x \to 0$ for $\varphi(x, y)$ and $\partial_x\varphi(x, y)$.

Evidently, the possibility that $\varphi \notin \mathcal{F}_2^{-1}\mathcal{D}(\mathscr{H}_\alpha^*) = \mathcal{D}(\mathsf{H}_\alpha^*)$ (Lemma 6.7.14) complicates this analysis: no regularity or short-scale asymptotics of the elements of $\mathcal{D}(\mathsf{H}_\alpha^*)$ can be claimed a priori for φ.

For the above purposes we shall make use of the following auxiliary result.

Lemma 6.6.6. *Let $\alpha \in [0, 1)$ and let $R : (0, 1) \times S^1 \to \mathbb{C}$ be a function such that*

(a) $\left\|x^{-(\frac{3}{2}+\frac{\alpha}{2})}R\right\|_{L^2((0,1)\times S^1,\mathrm{d}x\mathrm{d}y)} < +\infty$,

(b) $\left\|\partial_x^2 R\right\|_{L^2((0,1)\times S^1,\mathrm{d}x\mathrm{d}y)} < +\infty$.

Then for almost every $y \in S^1$ the function $(0, 1) \ni x \mapsto R(x, y)$ belongs to $H_0^2((0, 1])$ and as such it satisfies the following properties:

(i) $R(\cdot, y) \in C^1(0, 1)$,

(ii) $R(x, y) \overset{x\downarrow 0}{=} o(x^{3/2})$,

(iii) $\partial_x R(x, y) \overset{x\downarrow 0}{=} o(x^{1/2})$.

Remark 6.6.7. $H_0^2((0, 1])$ in the statement of Lemma 6.6.6 denotes as usual the closure of $C_0^\infty((0, 1])$ in the H^2-norm. The edge $x = 1$ is included so as to mean that there is no vanishing constraint at $x = 1$ for the elements of $H_0^2((0, 1])$ and their derivatives: only vanishing as $x \downarrow 0$ emerges, in the form of conditions (ii) and (iii).

Proof of Lemma 6.6.6. Assumption (a) in Lemma 6.6.6 implies that $R(\cdot, y) \in L^2((0, 1))$, and hence together with (b) it implies that $R(\cdot, y) \in H^2((0, 1))$ for a.e. $y \in S^1$. Therefore $R(\cdot, y) = a_y + b_y x + r_y(x)$ for a.e. $y \in S^1$, for some $a_y, b_y \in \mathbb{C}$ and $r_y \in H_0^2((0, 1])$. For compatibility with assumption (a), necessarily $a_y = b_y = 0$, whence $R(\cdot, y) \in H_0^2((0, 1])$ for a.e. $y \in S^1$. □

Let us discuss the application of Lemma 6.6.6 to our context.

As we are interested in characterising for fixed $y \in S^1$ the behaviour and the regularity of $x \mapsto \varphi(x, y)$ as $x \to 0$ from *each side* of the singular point $x = 0$, it suffices to analyse the case $x > 0$; then completely analogous conclusions are obtained for $x < 0$. Lemma 6.6.6 is thus meant to be applied to the restriction $R(x, y) = \varphi(x, y)\mathbf{1}_{(0,1)}(x)$.

In fact, since in general $\varphi \in L^2(\mathbb{R} \times S^1, \mathrm{d}x\mathrm{d}y) \setminus \mathcal{D}(\mathsf{H}_\alpha^*)$, we are not able to check the assumptions (a) and (b) of Lemma 6.6.6 directly for φ. We opt instead for splitting φ into a component in $\mathcal{D}(\overline{\mathsf{H}_\alpha})$ plus a remainder, the explicit form of which will allow to apply Lemma 6.6.6.

This idea is implicit in the very choice of $(\varphi_k)_{k\in\mathbb{Z}}$ made in (6.6.14). Let us recall that for given $(g_k)_{k\in\mathbb{Z}}$ we could represent

$$g_k^\pm \;=\; \varphi_k^\pm + g_{1,k}^\pm |x|^{1+\frac{\alpha}{2}} P + g_{0,k}^\pm |x|^{-\frac{\alpha}{2}} P$$

and also

$$g_k^\pm \;=\; \widetilde{\varphi}_k^\pm + c_{1,k}^\pm \widetilde{\Psi}_{\alpha,k} + c_{0,k}^\pm \widetilde{\Phi}_{\alpha,k}\,,$$

where

$$(\widetilde{\varphi}_k^\pm)_{k\in\mathbb{Z}} \;\in\; \mathcal{D}\Big(\bigoplus_{k\in\mathbb{Z}} \overline{A_\alpha^\pm(k)}\Big) \;=\; \mathcal{D}\big(\overline{\mathscr{H}_\alpha^\pm}\big) \tag{6.6.27}$$

Moreover, as argued in the proof of Theorem 6.4.3, for each $k \in \mathbb{Z} \setminus \{0\}$ we can split

$$\varphi_k^\pm \;=\; \widetilde{\varphi}_k^\pm + \vartheta_k^\pm\,, \tag{6.6.28}$$

while keeping

$$\widetilde{\varphi}_0^\pm \;\equiv\; \varphi_0^\pm \qquad \text{and} \qquad \vartheta_0^\pm \;\equiv\; 0 \qquad \text{when} \qquad k = 0\,, \tag{6.6.29}$$

where

$$\vartheta_k^\pm \;=\; \vartheta_{0,k}^\pm + \vartheta_{1,k}^\pm \tag{6.6.30}$$

with

$$\vartheta^{\pm}_{0,k} \;:=\; c^{\pm}_{0,k}\Big(\widetilde{\Phi}_{\alpha,k} - \sqrt{\tfrac{\pi(1+\alpha)}{2|k|}}\,|x|^{-\frac{\alpha}{2}}P + \sqrt{\tfrac{\pi|k|}{2(1+\alpha)}}\,|x|^{1+\frac{\alpha}{2}}P\Big) \tag{6.6.31}$$

$$\vartheta^{\pm}_{1,k} \;:=\; c^{\pm}_{1,k}\Big(\widetilde{\Psi}_{\alpha,k} - \sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\,\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)}\,|x|^{1+\frac{\alpha}{2}}P\Big) \tag{6.6.32}$$

and

$$\vartheta^{\pm}_{0,k},\vartheta^{\pm}_{1,k} \;\in\; \mathcal{D}\big(\overline{A^{\pm}_{\alpha}(k)}\big) \;=\; H^2_0(\mathbb{R}^{\pm})\cap L^2(\mathbb{R}^{\pm},\langle x\rangle^{4\alpha}\,\mathrm{d}x)\,. \tag{6.6.33}$$

It is important to remember that for later convenience the zero mode is all cast into $\widetilde{\varphi}^{\pm}_0 \equiv \varphi^{\pm}_0$, hence $(\vartheta_k)_{k\in\mathbb{Z}} \equiv (\vartheta_k)_{k\in\mathbb{Z}\setminus\{0\}}$.

The decomposition (6.6.28)-(6.6.32) induces the splitting

$$(\varphi_k)_{k\in\mathbb{Z}} \;=\; (\widetilde{\varphi}_k)_{k\in\mathbb{Z}} + (\vartheta_k)_{k\in\mathbb{Z}} \tag{6.6.34}$$

as an identity in $\ell^2(\mathbb{Z},L^2(\mathbb{R}^+,\mathrm{d}x))$, where $(\vartheta_k)_{k\in\mathbb{Z}}$ does not necessarily belong to $\mathcal{D}(\mathscr{H}^*_\alpha)$, as $(\varphi_k)_{k\in\mathbb{Z}}$ does not either (Lemma 6.7.14). In turn, owing to (6.7.41) and (6.6.27), the identity (6.6.34) yields the splitting

$$\varphi(x,y) \;=\; \widetilde{\varphi}(x,y) + \vartheta(x,y)\,, \qquad (x,y)\in\mathbb{R}\times S^1\,, \tag{6.6.35}$$

with

$$\widetilde{\varphi} \;:=\; \mathcal{F}_2^{-1}(\widetilde{\varphi}_k)_{k\in\mathbb{Z}} \;\in\; \mathcal{F}_2^{-1}\mathcal{D}\big(\overline{\mathscr{H}^{\pm}_\alpha}\big) \;=\; \mathcal{D}(\overline{\mathsf{H}_\alpha}) \tag{6.6.36}$$

$$\vartheta \;:=\; \mathcal{F}_2^{-1}(\vartheta_k)_{k\in\mathbb{Z}} \;\in\; L^2(\mathbb{R}\times S^1,\mathrm{d}x\mathrm{d}y)\,. \tag{6.6.37}$$

Here ϑ may fail to belong to $\mathcal{D}(\mathsf{H}^*_\alpha)$, precisely as φ.

The explicit information that $\widetilde{\varphi}\in\mathcal{D}(\overline{\mathsf{H}_\alpha})$ and the explicit expression for ϑ will finally allow us to apply Lemma 6.6.6 separately to each of them. This will be the object of Subsect. 6.6.5.

6.6.5 Estimates for $\widetilde{\varphi}$ and ϑ: domain of the closure

In order to undesrtand the behaviour of $\widetilde{\varphi}$, we are first concerned now with the regularity and the behaviour as $x\to 0^{\pm}$ of the functions belonging to the domain of the closure $\mathcal{D}\big(\overline{\mathsf{H}^{\pm}_\alpha}\big)$. This result may be interesting by itself.

Clearly, from (6.2.12),

$$\mathcal{D}\big(\overline{\mathsf{H}^{\pm}_\alpha}\big) \;=\; \overline{C^\infty_0(\mathbb{R}^{\pm}_x\times S^1_y)}^{\|\;\|_{\mathsf{H}_\alpha}}\,, \tag{6.6.38}$$

where $\|h\|_{\mathsf{H}_\alpha} := \big(\|h\|^2_{L^2(\mathbb{R}^{\pm}_x\times S^1_y)} + \|\mathsf{H}^{\pm}_\alpha h\|^2_{L^2(\mathbb{R}^{\pm}_x\times S^1_y)}\big)^{1/2}$.

We also recall, from $\overline{\mathsf{H}^{\pm}_\alpha}\subset(\mathsf{H}^{\pm}_\alpha)^*$ and from (6.2.18), that

$$\overline{\mathsf{H}^{\pm}_\alpha}\,\widetilde{\varphi}^{\pm} \;=\; \Big(-\frac{\partial^2}{\partial x^2} - |x|^{2\alpha}\frac{\partial^2}{\partial y^2} + \frac{C_\alpha}{|x|^2}\Big)\widetilde{\varphi}^{\pm} \qquad \forall\widetilde{\varphi}^{\pm}\in\mathcal{D}\big(\overline{\mathsf{H}^{\pm}_\alpha}\big)\,. \tag{6.6.39}$$

The main result here is the following.

Proposition 6.6.8. *Let $\alpha\in[0,1)$. There exists a constant $K_\alpha>0$ such that for any $\widetilde{\varphi}^{\pm}\in\mathcal{D}(\overline{\mathsf{H}^{\pm}_\alpha})$ one has*

$$\big\|\,|x|^{-2}\widetilde{\varphi}^{\pm}\,\big\|_{L^2(\mathbb{R}^{\pm}_x\times S^1_y)} + \big\|\partial^2_x\widetilde{\varphi}^{\pm}\big\|_{L^2(\mathbb{R}^{\pm}_x\times S^1_y)} \;\leqslant\; K_\alpha\,\big\|\overline{\mathsf{H}^{\pm}_\alpha}\,\widetilde{\varphi}^{\pm}\big\|_{L^2(\mathbb{R}^{\pm}_x\times S^1_y)}\,. \tag{6.6.40}$$

When $\alpha\uparrow 1$, then $K_\alpha\to+\infty$. As a consequence, $\widetilde{\varphi}^{\pm}$ satisfies the assumptions of Lemma 6.6.6 and therefore, for almost every $y\in S^1$,

(i) the function $x\mapsto\widetilde{\varphi}^{\pm}(x,y)$ belongs to $C^1(0,1)$,

(ii) $\widetilde{\varphi}^{\pm}(x,y) = o(|x|^{3/2})$ as $x\to 0^{\pm}$,

(iii) $\partial_x\widetilde{\varphi}^{\pm}(x,y) = o(|x|^{1/2})$ as $x\to 0^{\pm}$.

As we only need information on the limit separately from each side of the singularity, it is enough to consider the '+' case: the same conclusions will apply also to the '-' case. Thus, in the remaining part of this Subsection, we shall simply write $\widetilde{\varphi}$ for $\widetilde{\varphi}^+ \in \mathcal{D}(\overline{\mathsf{H}^+_\alpha})$.

The proof of Proposition 6.6.8 relies on two technical estimates. The first is an iterated version of the standard one-dimensional inequality by Hardy,

$$\|r^{-1}h\|_{L^2(\mathbb{R}^+,\mathrm{d}r)} \leqslant 2\,\|h'\|_{L^2(\mathbb{R}^+,\mathrm{d}r)} \qquad \forall\, h \in C_0^\infty(\mathbb{R}^+)\,. \tag{6.6.41}$$

Lemma 6.6.9 (Double-Hardy inequality)**.** *For any $h \in C_0^\infty(\mathbb{R}^+)$ one has*

$$\|r^{-2}h\|_{L^2(\mathbb{R}^+,\mathrm{d}r)} \leqslant \frac{4}{3}\,\|h''\|_{L^2(\mathbb{R}^+,\mathrm{d}r)}\,. \tag{6.6.42}$$

Corollary 6.6.10. *Let $\widetilde{\varphi} \in C_0^\infty(\mathbb{R}^+_x \times S^1_y)$. Then*

$$\|x^{-2}\widetilde{\varphi}\|_{L^2(\mathbb{R}^+_x\times S^1_y)} \leqslant \frac{4}{3}\|\partial_x^2\widetilde{\varphi}\|_{L^2(\mathbb{R}^+_x\times S^1_y)}\,. \tag{6.6.43}$$

The proof of Lemma 6.6.9 is well-known and we avoid giving details here. The second estimate is meant to control the term $x^{2\alpha}\partial_y^2$ of $\overline{\mathsf{H}_\alpha}$ and reads as follows.

Lemma 6.6.11. *Let $\alpha \in [0,1)$. There exists a constant $D_\alpha > 0$ such that for any $\widetilde{\varphi} \in \mathcal{D}(\overline{\mathsf{H}^+_\alpha})$ one has*

$$\|x^{2\alpha}\partial_y^2\widetilde{\varphi}\|_{L^2(\mathbb{R}^+_x\times S^1_y)} \leqslant D_\alpha\big\|\overline{\mathsf{H}^+_\alpha}\,\widetilde{\varphi}\big\|_{L^2(\mathbb{R}^+_x\times S^1_y)}\,. \tag{6.6.44}$$

Proof. It is enough to prove (6.6.44) for any $\widetilde{\varphi} \in C_0^\infty(\mathbb{R}^+_x \times S^1_y)$; then the general inequality is merely obtained by closure, owing to (6.6.38). To this aim, let $(\widetilde{\varphi}_k)_{k\in\mathbb{Z}} := \mathcal{F}_2^+\widetilde{\varphi} \in \mathcal{H} \cong \ell^2(\mathbb{Z}, L^2(\mathbb{R}^+,\mathrm{d}x))$. One has

$$\begin{aligned}
\big\|x^{2\alpha}\partial_y^2\widetilde{\varphi}\big\|^2_{L^2(\mathbb{R}^+_x\times S^1_y)} &= \sum_{k\in\mathbb{Z}} \|x^{2\alpha}k^2\,\widetilde{\varphi}_k\|^2_{L^2(\mathbb{R}^+)} \\
&= \sum_{k\in\mathbb{Z}\setminus\{0\}} \|x^{2\alpha}k^2\,R_{G_{\alpha,k}}A_{\alpha,F}(k)\widetilde{\varphi}_k\|^2_{L^2(\mathbb{R}^+)} \\
&\leqslant \sum_{k\in\mathbb{Z}\setminus\{0\}} \|x^{2\alpha}k^2\,R_{G_{\alpha,k}}\|^2_{\mathrm{op}}\big\|\overline{A^+_\alpha(k)}\widetilde{\varphi}_k\big\|^2_{L^2(\mathbb{R}^+)}
\end{aligned}$$

where we used Plancherel's formula in the first identity and Proposition 6.3.15 in the second identity. Owing from Lemma 6.3.3(ii), $\|x^{2\alpha}k^2\,R_{G_{\alpha,k}}\|_{\mathrm{op}} \leqslant D_\alpha$ uniformly in k for some $D_\alpha > 0$. Based on this fact, one then has

$$\begin{aligned}
\big\|x^{2\alpha}\partial_y^2\widetilde{\varphi}\big\|^2_{L^2(\mathbb{R}^+_x\times S^1_y)} &\leqslant D_\alpha^2\sum_{k\in\mathbb{Z}}\big\|\overline{A^+_\alpha(k)}\widetilde{\varphi}_k\big\|^2_{L^2(\mathbb{R}^+)} = D_\alpha^2\,\big\|\overline{\mathscr{H}^+_\alpha}(\widetilde{\varphi}_k)_{k\in\mathbb{Z}}\big\|^2_{\mathcal{H}} \\
&= D_\alpha^2\,\big\|\overline{\mathsf{H}^+_\alpha}\,\widetilde{\varphi}\big\|^2_{L^2(\mathbb{R}^+_x\times S^1_y)},
\end{aligned}$$

which completes the proof. □

Remark 6.6.12. A result similar to Lemma 6.6.11 has been obtained in the very recent paper [84, Lemma 2.1] for Baouendi-Grushin-type Laplacians of the form $\partial_x^2 + |x|^{2\alpha}\partial_y^2$, $\alpha \geq 1$, using the ellipticity of the Fourier components. Both our and their estimates are based on the positivity of the Laplacians. Notice that $\partial_x^2 + |x|^{2\alpha}\partial_y^2 = \mathrm{div}_{\mathcal{L}} \circ \nabla_g$, where $\mathcal{L} = dxdy$ is the Lebesgue measure and $g = \mathrm{diag}(1, |x|^{-2\alpha})$.

Based upon the above estimates, we can prove Proposition 6.6.8.

Proof of Proposition 6.6.8. Again, it suffices to establish (6.6.40) when $\widetilde{\varphi} \in C_0^\infty(\mathbb{R}^+_x \times S^1_y)$, and then conclude by density from (6.6.38).

One has

$$\begin{aligned}
\|\partial_x^2\widetilde{\varphi}\|_{L^2(\mathbb{R}_x\times S^1_y)} &\leqslant \big\|\overline{\mathsf{H}^+_\alpha}\,\widetilde{\varphi}\big\|_{L^2(\mathbb{R}_x\times S^1_y)} + \big\|x^{2\alpha}\partial_y^2\widetilde{\varphi}\big\|_{L^2(\mathbb{R}^+_x\times S^1_y)} + C_\alpha\|x^{-2}\widetilde{\varphi}\|_{L^2(\mathbb{R}^+_x\times S^1_y)} \\
&\leqslant \big\|\overline{\mathsf{H}^+_\alpha}\,\widetilde{\varphi}\big\|_{L^2(\mathbb{R}^+_x\times S^1_y)} + D_\alpha\big\|\overline{\mathsf{H}^+_\alpha}\,\widetilde{\varphi}\big\|_{L^2(\mathbb{R}^+_x\times S^1_y)} + \frac{4C_\alpha}{3}\|\partial_x^2\widetilde{\varphi}\|_{L^2(\mathbb{R}^+_x\times S^1_y)},
\end{aligned}$$

where the first inequality is a triangular inequality based on (6.6.39), whereas the second inequality follows directly from Corollary 6.6.10 and Lemma 6.6.11.

Therefore,

$$\|\partial_x^2\widetilde{\varphi}\|_{L^2(\mathbb{R}^+_x\times S^1_y)} \leqslant \frac{1+D_\alpha}{1-\frac{4}{3}C_\alpha}\left\|\overline{\mathsf{H}^+_\alpha}\,\widetilde{\varphi}\right\|_{L^2(\mathbb{R}^+_x\times S^1_y)}.$$

As $C_\alpha = \frac{1}{4}\alpha(2+\alpha)$, the constant $K_\alpha := (1+D_\alpha)(1-\frac{4}{3}C_\alpha)^{-1}$ is strictly positive for any α of interest, namely, $\alpha \in (0,1)$. Moreover, $K_\alpha \to +\infty$ as $\alpha \uparrow 1$ (indeed, tracing back the constant D_α through the proof of Lemma 3.3 where it was imported from in Lemma 6.6.11, it is easy to see that D_α does not diverge when $\alpha \uparrow 1$). The proof is thus completed. □

Let us recall that $\vartheta^\pm$ may well fail to belong to $\mathcal{D}(\overline{\mathsf{H}^\pm_\alpha})$ and therefore cannot be controlled by means of Prop. 6.6.8: a separate analysis is needed, and we base it on the explicit expression and homogeneity properties of ϑ.

We state the needed result here, and postpone the technical proof to the Appendix 6.7.8.

Proposition 6.6.13. *Let $\alpha \in [0,1)$. For almost every $y \in S^1$,*

(i) the function $x \mapsto \vartheta^\pm(x,y)$ belongs to $C^1(0,1)$,

(ii) $\vartheta^\pm(x,y) = o(|x|^{3/2})$ as $x \to 0^\pm$,

(iii) $\partial_x\vartheta^\pm(x,y) = o(|x|^{1/2})$ as $x \to 0^\pm$.

6.6.6 Proof of the classification theorem

Proof of Theorem 6.6.1. Let us characterise the domain $\mathcal{D}(\mathcal{F}_2^{-1}\mathscr{H}_\alpha^{\text{u.f.}}\mathcal{F}_2)$ of the various uniformly fibred extensions of $\mathsf{H}_\alpha = \mathcal{F}_2^{-1}\mathscr{H}_\alpha\mathcal{F}_2$.

The expression (6.6.5) for H^*_α provided in the statement of the theorem was already found in (6.2.18).

Next, let us consider a generic $\phi = \mathcal{F}_2^{-1}(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathcal{F}_2^{-1}\mathscr{H}_\alpha^{\text{u.f.}}\mathcal{F}_2)$, where $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}_\alpha^{\text{u.f.}})$. Owing to the definitions (6.6.16)-(6.6.19) and to Corollary 6.6.3,

$$\phi(x,y) = \varphi(x,y) + g_1(y)|x|^{1+\frac{\alpha}{2}}P(x) + g_0(y)|x|^{-\frac{\alpha}{2}}P(x) \tag{6.6.45}$$

where P is a smooth cut-off which is identically equal to one for $|x| < 1$ and zero for $|x| > 2$, and $g_0, g_1 \in L^2(S^1)$ with further Sobolev regularity as specified therein.

Moreover, upon splitting $\varphi = \widetilde{\varphi} + \vartheta$ as in (6.6.35), and using Prop. 6.6.8 for $\widetilde{\varphi}$ and Prop. 6.6.13 for ϑ, we deduce that for almost every $y \in S^1$

- the function $x \mapsto \varphi^\pm(x,y)$ belongs to $C^1(0,1)$,
- $\varphi^\pm(x,y) = o(|x|^{3/2})$ as $x \to 0^\pm$,
- $\partial_x\varphi^\pm(x,y) = o(|x|^{1/2})$ as $x \to 0^\pm$.

Plugging this information into (6.6.45) yields

$$\begin{aligned}
\lim_{x\to 0^\pm}|x|^{\frac{\alpha}{2}}\,\phi^\pm(x,y) &= g_0^\pm(y)\\
\lim_{x\to 0^\pm}|x|^{-(1+\frac{\alpha}{2})}\big(\phi^\pm(x,y) - g_0^\pm(y)|x|^{-\frac{\alpha}{2}}\big) &= g_1^\pm(y) + \lim_{x\to 0^\pm}|x|^{-(1+\frac{\alpha}{2})}\varphi^\pm(x,y)\\
&= g_1^\pm(y),
\end{aligned}$$

namely

$$g_0 = \phi_0, \qquad g_1 = \phi_1, \tag{6.6.46}$$

proving also that the limits (6.6.6), as well as the limits of the first line of (6.6.7), do exist. Also, the Sobolev regularity stated for ϕ_0 and ϕ_1 follows directly from Corollary 6.6.3.

The second identity in (6.6.7) is obtained as follows. By means of (6.6.45) we compute

$$\begin{aligned}
\pm(1+\alpha)^{-1}\lim_{x\to 0^\pm}|x|^{-\alpha}\partial_x\big(|x|^{\frac{\alpha}{2}}\phi^\pm(x,y)\big) &=\\
&= \pm(1+\alpha)^{-1}\lim_{x\to 0^\pm}|x|^{-\alpha}\partial_x\big(|x|^{\frac{\alpha}{2}}\varphi^\pm(x,y) + g_1^\pm(y)|x|^{1+\alpha} + g_0^\pm(y)\big)\\
&= g_1^\pm(y) \pm (1+\alpha)^{-1}\lim_{x\to 0^\pm}|x|^{-\alpha}\partial_x\big(|x|^{\frac{\alpha}{2}}\varphi^\pm(x,y)\big).
\end{aligned}$$

On the other hand,

$$\lim_{x\to 0^\pm} |x|^{-\alpha}\partial_x\big(|x|^{\frac{\alpha}{2}}\varphi^\pm(x,y)\big) = \lim_{x\to 0^\pm}\big(\tfrac{\alpha}{2}|x|^{-(1+\frac{\alpha}{2})}\varphi^\pm(x,y) + |x|^{-\frac{\alpha}{2}}\partial_x\varphi^\pm(x,y)\big) = 0\,,$$

having used the properties $\varphi^\pm(x,y) = o(|x|^{3/2})$ and $\partial_x\varphi^\pm(x,y) = o(|x|^{1/2})$ as $x \to 0^\pm$. This yields the second identity in (6.6.7).

It remains to show that for each type of extension, the stated boundary conditions of self-adjointness do hold for ϕ_0 and ϕ_1. As, by (6.6.18)-(6.6.19) and by (6.6.46)

$$\begin{aligned}\phi_0^\pm(y) &= \frac{1}{\sqrt{2\pi}}\sum_{k\in\mathbb{Z}} e^{\mathrm{i}ky} g_{0,k}^\pm \\ \phi_1^\pm(y) &= \frac{1}{\sqrt{2\pi}}\sum_{k\in\mathbb{Z}} e^{\mathrm{i}ky} g_{1,k}^\pm\,,\end{aligned}$$

the above series converging in $L^2(S^1)$, and since for each *uniformly fibred* extension $\mathscr{H}_\alpha^{\mathrm{u.f.}}$ the boundary conditions are expressed by *the same linear combinations* of the $g_{0,k}^\pm$'s and $g_{1,k}^\pm$'s for each k, then now the boundary conditions of self-adjointness in terms of ϕ_0 and ϕ_1 are immediately read out from those of the classification Theorem 6.4.1 for bilateral-fibre extensions (see also Table 6.1) in terms of $g_{0,k}^\pm$ and $g_{1,k}^\pm$. □

To conclude, the thesis of Theorem 6.1.1 follows by conjugating back the operator H_α, and its self-adjoint extensions that we found, via the unitary transformation $\phi^\pm = U_\alpha^\pm f^\pm = |x|^{-\frac{\alpha}{2}} f^\pm$.

6.7 Appendix

This appendix aims at furnishing details and proves that have been postponed in order to ease the reading of the chapter. Some of them are original and thus more important than others that are revisited and already known facts. More precisely, Sections 6.7.1, 6.7.2, and 6.7.6 revisit well-known facts about infinite-direct sum of operators, their properties on closure, adjoint and self-adjoint extensions. Sections 6.7.3 and 6.7.8 present the proves of technical yet important results, which are original. Section 6.7.4 contains the proves of three lemmas that are standard and well-known. Section 6.7.5 is a revisitation of some known results about inverse-square potential hamiltonians on the half-line, which correspond to the fibre $k = 0$ of our investigated operator. Section 6.7.7 is original and provides examples of why a particular decomposition of the adjoint operator may present singular factors: that is, the factors may not belong individually to the domain of the adjoint but their sum does due to the cancellation of singular terms.

6.7.1 Orthogonal sum operators

We recall the structure of operators acting on $\mathcal{H}$ (resp., on $\mathcal{H}^\pm$) in the form of infinite orthogonal sum, that is, operators that are reduced by the orthogonal decomposition (6.2.9) (resp., (6.2.7)). By this we mean an operator T for which there is a collection $(T(k))_{k\in\mathbb{Z}}$ of operators on $\mathfrak{h}$ (resp., on $\mathfrak{h}^\pm$) such that

$$\begin{aligned}\mathcal{D}(T) &:= \left\{\psi \equiv (\psi_k)_{k\in\mathbb{Z}} \in \mathcal{H} \;\middle|\; \begin{array}{l}\text{(i)}\quad \psi_k \in \mathcal{D}(T(k))\ \ \forall k\in\mathbb{Z} \\ \text{(ii)}\ \displaystyle\sum_{k\in\mathbb{Z}} \big\|T(k)\psi_k\big\|_{\mathfrak{h}}^2 < +\infty\end{array}\right\} \\ T\psi &:= \big(T(k)\,\psi_k\big)_{k\in\mathbb{Z}}\,,\end{aligned} \tag{6.7.1}$$

(and analogous formulas on each half-fibre), the shorthand for which is

$$T = \bigoplus_{k\in\mathbb{Z}} T(k)\,. \tag{6.7.2}$$

Thus, $T(k) = T \restriction (\mathcal{D}(T)\cap\mathfrak{h}_k)$, where $\mathfrak{h}_k$ is the fibre $\mathfrak{h}$ counted in the k-th position with respect to the sum (6.2.9), and each $\mathfrak{h}_k$ is a reducing subspace for T. A convenient shorthand for the above expression for $\mathcal{D}(T)$ is

$$\mathcal{D}(T) = \boxplus_{k\in\mathbb{Z}} \mathcal{D}(T(k))\,. \tag{6.7.3}$$

As commented already, we write '$\boxplus$' instead of '$\oplus$' to denote that the infinite orthogonal sum involves now non-closed subspaces of $\mathcal{H}$.

Remark 6.7.1. It is crucial to observe that $\mathscr{H}_\alpha$ is *not* decomposable as $\mathscr{H}_\alpha = \bigoplus_{k\in\mathbb{Z}} A_\alpha(k)$ in the sense of formula (6.7.1), and in fact

$$\mathscr{H}_\alpha \subsetneq \bigoplus_{k\in\mathbb{Z}} A_\alpha(k)\,. \tag{6.7.4}$$

Indeed, as seen in (6.2.15),

$$\sum_k \|A_\alpha(k)\psi_k\|_{\mathfrak{h}}^2 = \left\|\Big(-\frac{\partial^2}{\partial x^2} - |x|^{2\alpha}\frac{\partial^2}{\partial y^2} + \frac{\alpha(2+\alpha)}{4x^2}\Big)\phi\right\|^2_{L^2(\mathbb{R}^\pm_x\times S^1_y)},$$

where $\psi = \mathcal{F}_2\phi$, the finiteness of which is guaranteed by $\phi \in C_0^\infty(\mathbb{R}^\pm_x \times S^1_y)$ in the case when $\psi \in \mathcal{D}(\mathscr{H}_\alpha)$, but of course is also guaranteed by a much larger class of ϕ's that are still smooth and compactly supported in x, but are not smooth in y – thus corresponding to ψ's that do not belong to $\mathcal{D}(\mathscr{H}_\alpha)$.

Most relevantly for our purposes, the closure and the adjoint pass through the orthogonal sum of operators.

Lemma 6.7.2. *If $T = \bigoplus_{k\in\mathbb{Z}} T(k)$, then*

$$T^* = \bigoplus_{k\in\mathbb{Z}} T(k)^* \tag{6.7.5}$$

$$\overline{T} = \bigoplus_{k\in\mathbb{Z}} \overline{T(k)}, \tag{6.7.6}$$

where the symbol of operator closure and adjoint clearly refers to the corresponding Hilbert spaces where the considered operators act on. Moreover,

$$\ker T^* = \bigoplus_{k\in\mathbb{Z}} \ker T(k)^*\,. \tag{6.7.7}$$

Proof. Let $\psi \in \mathcal{D}(T^*)$: then there exists $\eta \in \mathcal{H}$ such that

$$\sum_{k\in\mathbb{Z}} \langle \eta_k, \xi_k\rangle_{\mathfrak{h}} = \langle \eta, \xi\rangle_{\mathcal{H}} = \langle \psi, T\,\xi\rangle_{\mathcal{H}} = \sum_{k\in\mathbb{Z}} \langle \psi_k, T(k)\,\xi_k\rangle_{\mathfrak{h}} \qquad \forall \xi \in \mathcal{D}(T)\,.$$

By localising ξ separately in each fibre $\mathfrak{h}_k$ one then deduces that for each $k \in \mathbb{Z}$ $\psi_k \in \mathcal{D}(T(k)^*)$ and $\eta_k = T(k)^*\psi_k$, whence also $\sum_{k\in\mathbb{Z}} \left\|T(k)^*\psi_k\right\|_{\mathfrak{h}}^2 = \|\eta\|_{\mathcal{H}}^2 < +\infty$. This means precisely that $\psi \in \mathcal{D}(\bigoplus_{k\in\mathbb{Z}} T(k)^*)$ and $T^*\psi = (T(k)^*\psi_k)_{k\in\mathbb{Z}} = (\bigoplus_{k\in\mathbb{Z}} T(k)^*)\psi$, i.e., $T^* \subset \bigoplus_{k\in\mathbb{Z}} T(k)^*$.

Conversely, if $\psi \in \mathcal{D}(\bigoplus_{k\in\mathbb{Z}} T(k)^*)$, then for each $k \in \mathbb{Z}$ one has $\langle T(k)^*\psi_k, \xi_k\rangle_{\mathfrak{h}} = \langle \psi_k, T(k)\,\xi_k\rangle_{\mathfrak{h}}$ $\forall \xi_k \in \mathcal{D}(T(k))$ and $\sum_{k\in\mathbb{Z}} \|T^*(k)\psi_k\|_{\mathfrak{h}}^2 < +\infty$. Setting $\eta_k := T^*(k)\psi_k$ and $\eta := (\eta_k)_{k\in\mathbb{Z}}$ one then has that $\eta \in \mathcal{H}$ and

$$\langle \eta, \xi\rangle_{\mathcal{H}} = \sum_{k\in\mathbb{Z}} \langle \eta_k, \xi_k\rangle_{\mathfrak{h}} = \sum_{k\in\mathbb{Z}} \langle \psi_k, T(k)\xi_k\rangle_{\mathfrak{h}} = \langle \psi, T\,\xi\rangle_{\mathcal{H}} \qquad \forall \xi \in \mathcal{D}(T)\,.$$

This means that $\psi \in \mathcal{D}(T^*)$ and $T^*\psi = \eta = (T(k)^*\psi_k)_{k\in\mathbb{Z}} = (\bigoplus_{k\in\mathbb{Z}} T(k)^*)\psi$, i.e., $T^* \supset \bigoplus_{k\in\mathbb{Z}} T(k)^*$.

Identity (6.7.5) is thus established, and (6.7.6) follows from applying (6.7.5) to the operator T^* instead of T. Identity (6.7.7) is another straightforward consequence of (6.7.5). □

Now, although $\mathscr{H}_\alpha \subsetneq \bigoplus_{k\in\mathbb{Z}} A_\alpha(k)$ (Remark 6.7.1), the two operators have actually the same adjoint and the same closure.

Lemma 6.7.3. *One has*

$$\mathscr{H}_\alpha^* = \bigoplus_{k\in\mathbb{Z}} A_\alpha(k)^* \tag{6.7.8}$$

and

$$\overline{\mathscr{H}_\alpha} = \bigoplus_{k\in\mathbb{Z}} \overline{A_\alpha(k)}, \tag{6.7.9}$$

i.e.,

$$\begin{aligned} \mathcal{D}(\mathscr{H}_\alpha^*) &:= \left\{ \psi \equiv (\psi_k)_{k\in\mathbb{Z}} \in \mathcal{H} \;\middle|\; \begin{array}{l} \text{(i)}\quad \psi_k \in \mathcal{D}(A_\alpha(k)^*)\ \ \forall k \in \mathbb{Z} \\ \text{(ii)}\ \sum_{k\in\mathbb{Z}} \left\|A_\alpha(k)^*\psi_k\right\|_{\mathfrak{h}}^2 < +\infty \end{array} \right\} \\ \mathscr{H}_\alpha^*\psi &:= \big(A_\alpha(k)^*\,\psi_k\big)_{k\in\mathbb{Z}} \end{aligned} \tag{6.7.10}$$

and

$$\mathcal{D}(\overline{\mathscr{H}_\alpha}) \;:=\; \left\{ \psi \equiv (\psi_k)_{k\in\mathbb{Z}} \in \mathcal{H} \;\middle|\; \begin{array}{l} \text{(i)} \quad \psi_k \in \mathcal{D}(\overline{A_\alpha(k)}) \;\; \forall k \in \mathbb{Z} \\ \text{(ii)} \; \sum_{k\in\mathbb{Z}} \big\|\overline{A_\alpha(k)}\psi_k\big\|_{\mathfrak{h}}^2 < +\infty \end{array} \right\} \tag{6.7.11}$$

$$\overline{\mathscr{H}_\alpha}\psi \;:=\; \big(\overline{A_\alpha(k)}\,\psi_k\big)_{k\in\mathbb{Z}}\,.$$

Analogously,

$$(\mathscr{H}_\alpha^{\pm})^* \;=\; \bigoplus_{k\in\mathbb{Z}} A_\alpha^{\pm}(k)^*\,, \qquad \overline{\mathscr{H}_\alpha^{\pm}} \;=\; \bigoplus_{k\in\mathbb{Z}} \overline{A_\alpha^{\pm}(k)}\,. \tag{6.7.12}$$

Moreover,

$$\ker \mathscr{H}_\alpha^* \;=\; \bigoplus_{k\in\mathbb{Z}} \ker A_\alpha(k)^*\,. \tag{6.7.13}$$

Proof. On the one hand, $\mathscr{H}_\alpha^* \supset (\bigoplus_{k\in\mathbb{Z}} A_\alpha(k))^* = \bigoplus_{k\in\mathbb{Z}} A_\alpha(k)^*$ (owing to (6.7.4) and (6.7.5) above).

On the other hand, one proves the opposite inclusion, namely $\mathscr{H}_\alpha^* \subset \bigoplus_{k\in\mathbb{Z}} A_\alpha(k)^*$, following the very same argument used for the proof of $T^* \subset \bigoplus_{k\in\mathbb{Z}} T(k)^*$ in Lemma 6.7.2. This is possible because for $\xi \in \mathcal{D}(\mathscr{H}_\alpha)$, one has $\xi_k \in C_0^\infty(\mathbb{R}\setminus\{0\}) = \mathcal{D}(A_\alpha(k))$.

Thus, explicitly, if $\psi \in \mathcal{D}(\mathscr{H}_\alpha^*)$, then there exists $\eta \in \mathcal{H}$ such that

$$\sum_{k\in\mathbb{Z}} \langle \eta_k, \xi_k\rangle_{\mathfrak{h}} \;=\; \langle \eta, \xi\rangle_{\mathcal{H}} \;=\; \langle \psi, \mathscr{H}_\alpha\,\xi\rangle_{\mathcal{H}} \;=\; \sum_{k\in\mathbb{Z}} \langle \psi_k, A_\alpha(k)\,\xi_k\rangle_{\mathfrak{h}} \qquad \forall \xi \in \mathcal{D}(\mathscr{H}_\alpha)\,.$$

By localising ξ separately in each fibre $\mathfrak{h}_k$ one then deduces that for each $k \in \mathbb{Z}$ $\psi_k \in \mathcal{D}(A_\alpha(k)^*)$ and $\eta_k = A_\alpha(k)^*\psi_k$, whence also $\sum_{k\in\mathbb{Z}} \big\|A_\alpha(k)^*\psi_k\big\|_{\mathfrak{h}}^2 = \|\eta\|_{\mathcal{H}}^2 < +\infty$. This means that $\psi \in \mathcal{D}(\bigoplus_{k\in\mathbb{Z}} A_\alpha(k)^*)$ and $\mathscr{H}_\alpha^*\psi = (A_\alpha(k)^*\psi_k)_{k\in\mathbb{Z}} = (\bigoplus_{k\in\mathbb{Z}} A_\alpha(k)^*)\psi$.

Thus, (6.7.8) is proved. Applying (6.7.5) to (6.7.8) then yields (6.7.9). □

6.7.2 Momentum-fibred extensions. Local and non-local extensions.

The technical point that is going to be crucial for us in studying the self-adjoint extensions of $\mathscr{H}_\alpha^{\pm}$ and $\mathscr{H}_\alpha$ is the following.

Proposition 6.7.4. *Let $\{B(k)\,|\,k \in \mathbb{Z}\}$ be a collection of operators on the fibre space $\mathfrak{h}$ (resp., $\mathfrak{h}^{\pm}$) such that, for each k, $B(k)$ is a self-adjoint extension of $A_\alpha(k)$ (resp., $A_\alpha^{\pm}(k)$), and let*

$$B \;=\; \bigoplus_{k\in\mathbb{Z}} B(k)\,. \tag{6.7.14}$$

Then B is a self-adjoint extension of $\mathscr{H}_\alpha$ (resp., $\mathscr{H}_\alpha^{\pm}$).

The proof goes through reasonings that are somewhat standard, but for completeness and later discussion we sketch it here.

Proof of Proposition 6.7.4. B is an actual extension of $\mathscr{H}_\alpha$, because

$$\mathscr{H}_\alpha \;\subset\; \bigoplus_{k\in\mathbb{Z}} A_\alpha(k) \;\subset\; \bigoplus_{k\in\mathbb{Z}} B(k)\,.$$

It is straightforward to see that B is symmetric, so in order to establish the self-adjointness of B one only needs to prove that $\mathrm{ran}(B \pm \mathrm{i}\mathbb{1}) = \mathcal{H}$.

For generic $\eta \equiv (\eta_k)_{k\in\mathbb{Z}} \in \mathcal{H}$ let us then set $\psi_k := (B(k) + \mathrm{i}\mathbb{1})^{-1}\eta_k$ $\forall k \in \mathbb{Z}$. By construction $\psi_k \in \mathcal{D}(B(k))$, $\|\psi_k\|_{\mathfrak{h}} \leqslant \|\eta_k\|_{\mathfrak{h}}$, and $\|B(k)\psi_k\|_{\mathfrak{h}} \leqslant \|\eta_k\|_{\mathfrak{h}}$, whence also $\sum_{k\in\mathbb{Z}} \|\psi_k\|_{\mathfrak{h}}^2 < +\infty$ and $\sum_{k\in\mathbb{Z}} \|B(k)\psi_k\|_{\mathfrak{h}}^2 < +\infty$. Therefore, $\psi \equiv (\psi_k)_{k\in\mathbb{Z}} \in \mathcal{D}(B)$. Moreover, $(B+\mathrm{i}\mathbb{1})\psi = ((B(k)+\mathrm{i}\mathbb{1})\psi_k)_{k\in\mathbb{Z}} = (\eta_k)_{k\in\mathbb{Z}} = \eta$. This proves that $\mathrm{ran}(B+\mathrm{i}\mathbb{1}) = \mathcal{H}$. Analogously, $\mathrm{ran}(B - \mathrm{i}\mathbb{1}) = \mathcal{H}$. □

Proposition 6.7.4 provides a mechanism for constructing self-adjoint operators B of the form (6.7.14) by re-assembling, fibre by fibre in the momentum number k conjugate to y, self-adjoint extensions of the fibre operators $A_\alpha(k)$; by further exploiting the canonical unitary equivalence

$$B \overset{\cong}{\longmapsto} (\mathcal{F}_2^- U_\alpha^- \oplus \mathcal{F}_2^+ U_\alpha^+)^* \, B \, (\mathcal{F}_2^- U_\alpha^- \oplus \mathcal{F}_2^+ U_\alpha^+) \tag{6.7.15}$$

this yields actual self-adjoint extensions of H_α. With self-explanatory meaning, we shall refer to such extensions as '*momentum-fibred extensions*', or simply '*fibred extensions*'.

Thus, fibred extensions have the distinctive feature of being characterised, in position-momentum coordinates (x, k), by boundary conditions on the elements ψ of their domain which connect the behaviour of *each* mode $\psi_k(x)$ as $x \to 0^+$ and $x \to 0^-$, with no crossing conditions between different modes. In other words, such extensions are *local* in momentum – which is another way we shall refer to them in the following – whence their primary physical and conceptual relevance.

Evidently, $\mathscr{H}_\alpha$ (and hence H_α) admits plenty of extensions that are *non-local* in momentum, namely with boundary condition as $x \to 0^\pm$ that mixes different k-modes.

It is also clear that a generic fibred extension of $\mathscr{H}_\alpha$ may or may not be reduced into a 'left' and 'right' component by the Hilbert space direct sum (6.2.9), whereas $\mathscr{H}_\alpha$ itself certainly is. Indeed, at the level of each fibre, the extension $B(k)$ may or may not be reduced by the sum $\mathfrak{h} = \mathfrak{h}^- \oplus \mathfrak{h}^+$ as is instead $A_\alpha(k)$ by construction (see (6.2.17) above).

In fact, the decoupling between left and right half-cylinder may hold for *all* modes $k \in \mathbb{Z}$ or only for some sub-domains of k. In the former case, the resulting extension of $\mathscr{H}_\alpha$ is in fact a mere 'juxtaposition' of two separate extensions for $\mathscr{H}_\alpha^\pm$ in the left/right half-cylinder.

We shall apply the above formalism and the latter considerations in Section 6.5, where the actual classification of the self-adjoint extensions of $\mathscr{H}_\alpha$ is discussed.

6.7.3 Proof of Lemma 6.3.3

For the proof of Lemma 6.3.3 it is convenient to re-write, by means of (6.3.13) and (6.3.21), for any $k \in \mathbb{Z}\backslash\{0\}$,

$$\mathscr{G}^{(a)}_{\alpha,k}(x,\rho) \;=\; \begin{cases} |k|\, x^{a-\frac{\alpha}{2}}\, \rho^{-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}}\, \sinh\big(\frac{|k|}{1+\alpha}\rho^{1+\alpha}\big) & \text{if } 0<\rho<x \\ |k|\, x^{a-\frac{\alpha}{2}}\, \rho^{-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}}\, \sinh\big(\frac{|k|}{1+\alpha}x^{1+\alpha}\big) & \text{if } 0<x<\rho\,. \end{cases} \tag{6.7.16}$$

It is also convenient to use the bound

$$\mathscr{G}^{(a)}_{\alpha,k}(x,\rho) \;\leqslant\; \widetilde{\mathscr{G}^{(a)}_{\alpha,k}}(x,\rho) \tag{6.7.17}$$

with

$$\widetilde{\mathscr{G}^{(a)}_{\alpha,k}}(x,\rho) \;:=\; \begin{cases} |k|\, x^{a-\frac{\alpha}{2}}\, \rho^{-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}}\, e^{\frac{|k|}{1+\alpha}\rho^{1+\alpha}} & \text{if } 0<\rho<x \\ |k|\, x^{a-\frac{\alpha}{2}}\, \rho^{-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}}\, e^{\frac{|k|}{1+\alpha}x^{1+\alpha}} & \text{if } 0<x<\rho\,. \end{cases} \tag{6.7.18}$$

Proof of Lemma 6.3.3. $R^{(a)}_{G_{\alpha,k}}$ splits into the sum of four integral operators with non-negative kernels given by

$$\begin{aligned} \mathscr{G}^{++}_{\alpha,k,a}(x,\rho) \;&:=\; \mathscr{G}^{(a)}_{\alpha,k}(x,\rho)\, \mathbf{1}_{(M,+\infty)}(x)\, \mathbf{1}_{(M,+\infty)}(\rho) \\ \mathscr{G}^{+-}_{\alpha,k,a}(x,\rho) \;&:=\; \mathscr{G}^{(a)}_{\alpha,k}(x,\rho)\, \mathbf{1}_{(M,+\infty)}(x)\, \mathbf{1}_{(0,M)}(\rho) \\ \mathscr{G}^{-+}_{\alpha,k,a}(x,\rho) \;&:=\; \mathscr{G}^{(a)}_{\alpha,k}(x,\rho)\, \mathbf{1}_{(0,M)}(x)\, \mathbf{1}_{(M,+\infty)}(\rho) \\ \mathscr{G}^{--}_{\alpha,k,a}(x,\rho) \;&:=\; \mathscr{G}^{(a)}_{\alpha,k}(x,\rho)\, \mathbf{1}_{(0,M)}(x)\, \mathbf{1}_{(0,M)}(\rho) \end{aligned}$$

for some cut-off $M > 0$.

The $(-,-)$ operator is a Hilbert-Schmidt operator on $L^2(\mathbb{R}^+)$. Indeed, owing to (6.7.17)-(6.7.18),

$$\begin{aligned} \mathscr{G}^{--}_{\alpha,k,a}(x,\rho) \;&\leqslant\; |k| x^{a-\frac{\alpha}{2}}\, \rho^{-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}|x^{1+\alpha}-\rho^{1+\alpha}|}\, \mathbf{1}_{(0,M)}(x)\, \mathbf{1}_{(0,M)}(\rho) \\ &\leqslant\; |k| x^{a-\frac{\alpha}{2}}\, \rho^{-\frac{\alpha}{2}}\, \mathbf{1}_{(0,M)}(x)\, \mathbf{1}_{(0,M)}(\rho)\,, \end{aligned}$$

whence, for $a > -\frac{1}{2}(1-\alpha)$,

$$\begin{aligned} \iint_{\mathbb{R}^+\times\mathbb{R}^+} \mathrm{d}x\, \mathrm{d}\rho\, \big|\mathscr{G}^{--}_{\alpha,k,a}(x,\rho)\big|^2 \;&\leqslant\; k^2 \int_0^M \mathrm{d}x\, x^{2a-\alpha} \int_0^M \mathrm{d}\rho\, \rho^{-\alpha} \\ &=\; \frac{k^2\, M^{2(a+1-\alpha)}}{(2a+1-\alpha)(1-\alpha)}\,. \end{aligned}$$

Also the $(-,+)$ operator is a Hilbert-Schmidt operator on $L^2(\mathbb{R}^+)$. Indeed,

$$\mathscr{G}^{-+}_{\alpha,k,a}(x,\rho) \;\leqslant\; |k|\, e^{\frac{|k|}{1+\alpha}M^{1+\alpha}}\, x^{a-\frac{\alpha}{2}}\, \rho^{-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}}\, \mathbf{1}_{(0,M)}(x)\, \mathbf{1}_{(M,+\infty)}(\rho)\,,$$

whence, for $a > -\frac{1}{2}(1-\alpha)$,

$$\begin{aligned}
&\iint_{\mathbb{R}^+\times\mathbb{R}^+} \mathrm{d}x\, \mathrm{d}\rho\, \left|\mathscr{G}^{-+}_{\alpha,k,a}(x,\rho)\right|^2 \\
&\qquad \leqslant\; k^2\, e^{\frac{2|k|}{1+\alpha}M^{1+\alpha}} \int_0^M \mathrm{d}x\, x^{2a-\alpha} \int_M^{+\infty} \mathrm{d}\rho\, \rho^{-\alpha}\, e^{-\frac{2|k|}{1+\alpha}\rho^{1+\alpha}} \\
&\qquad \leqslant\; k^2\, M^{-2\alpha}\, e^{\frac{2|k|}{1+\alpha}M^{1+\alpha}} \int_0^M \mathrm{d}x\, x^{2a-\alpha} \int_M^{+\infty} \mathrm{d}\rho\, \rho^{\alpha}\, e^{-\frac{2|k|}{1+\alpha}\rho^{1+\alpha}} \\
&\qquad =\; \frac{|k|}{2}\, M^{-2\alpha}\, e^{\frac{2|k|}{1+\alpha}M^{1+\alpha}} \int_0^M \mathrm{d}x\, x^{2a-\alpha} \int_{\frac{2|k|}{1+\alpha}M^{1+\alpha}}^{+\infty} \mathrm{d}y\, e^{-y} \\
&\qquad =\; \frac{|k|\, M^{2a+1-3\alpha}}{2(2a+1-\alpha)}\,.
\end{aligned}$$

With analogous reasoning,

$$\mathscr{G}^{+-}_{\alpha,k,a}(x,\rho) \;\leqslant\; |k|\, e^{\frac{|k|}{1+\alpha}M^{1+\alpha}}\, \rho^{-\frac{\alpha}{2}}\, x^{a-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}}\, \mathbf{1}_{(M,+\infty)}(x)\, \mathbf{1}_{(0,M)}(\rho)\,,$$

whence

$$\begin{aligned}
\iint_{\mathbb{R}^+\times\mathbb{R}^+} \mathrm{d}x\, \mathrm{d}\rho\, \left|\mathscr{G}^{+-}_{\alpha,k,a}(x,\rho)\right|^2 \;&\leqslant\; k^2\, e^{\frac{2|k|}{1+\alpha}M^{1+\alpha}} \int_0^M \mathrm{d}\rho\, \rho^{-\alpha} \int_M^{+\infty} \mathrm{d}x\, x^{2a-\alpha}\, e^{-\frac{2|k|}{1+\alpha}x^{1+\alpha}} \\
&=\; \frac{k^2 M^{1-\alpha}}{1-\alpha}\, e^{\frac{2|k|}{1+\alpha}M^{1+\alpha}} \int_M^{+\infty} \mathrm{d}x\, x^{2a-\alpha}\, e^{-\frac{2|k|}{1+\alpha}x^{1+\alpha}}\,.
\end{aligned}$$

In turn, integrating by parts, and for $a \leqslant \frac{1}{2} + \frac{3}{2}\alpha$,

$$\begin{aligned}
&\int_M^{+\infty} \mathrm{d}x\, x^{2a-\alpha}\, e^{-\frac{2|k|}{1+\alpha}x^{1+\alpha}} \\
&\qquad =\; \frac{M^{2a-2\alpha}}{2|k|}\, e^{-\frac{2|k|}{1+\alpha}M^{1+\alpha}} + \frac{a-\alpha}{|k|} \int_M^{+\infty} \mathrm{d}x\, x^{2a-1-3\alpha}\, x^{\alpha}\, e^{-\frac{2|k|}{1+\alpha}x^{1+\alpha}} \\
&\qquad \leqslant\; \frac{M^{2a-2\alpha}}{2|k|}\, e^{-\frac{2|k|}{1+\alpha}M^{1+\alpha}} + \frac{(a-\alpha)M^{2a-1-3\alpha}}{2k^2} \int_{\frac{2|k|}{1+\alpha}M^{1+\alpha}}^{+\infty} \mathrm{d}y\, e^{-y} \\
&\qquad =\; e^{-\frac{2|k|}{1+\alpha}M^{1+\alpha}} \Big(\frac{M^{2a-2\alpha}}{2|k|} + \frac{(a-\alpha)M^{2a-1-3\alpha}}{2k^2} \Big)\,.
\end{aligned}$$

Thus,

$$\iint_{\mathbb{R}^+\times\mathbb{R}^+} \mathrm{d}x\, \mathrm{d}\rho\, \left|\mathscr{G}^{+-}_{\alpha,k,a}(x,\rho)\right|^2 \;\leqslant\; \frac{1}{2(1-\alpha)} \left(2|k|M^{2a+1-3\alpha} + (a-\alpha)M^{2(a-2\alpha)}\right),$$

which shows that the $(+,-)$ operator is a Hilbert-Schmidt operator on $L^2(\mathbb{R}^+)$.

Last, let us show by means of a standard Schur test that the norm of the $(+,+)$ operator is bounded by $\sqrt{AB}$, where

$$\begin{aligned}
A \;&:=\; \sup_{x\in(M,+\infty)} \int_M^{+\infty} \mathrm{d}\rho\, \mathscr{G}^{(a)}_{\alpha,k}(x,\rho) \\
B \;&:=\; \sup_{\rho\in(M,+\infty)} \int_M^{+\infty} \mathrm{d}x\, \mathscr{G}^{(a)}_{\alpha,k}(x,\rho)\,.
\end{aligned}$$

Owing to (6.7.17)-(6.7.18),

$$\begin{aligned}
A \;&\leqslant\; A_1 + A_2 \\
B \;&\leqslant\; B_1 + B_2
\end{aligned}$$

with

$$
\begin{aligned}
A_1 &:= \sup_{x\in(M,+\infty)} |k|\, x^{a-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}} \int_M^x \mathrm{d}\rho\, \rho^{-\frac{\alpha}{2}}\, e^{\frac{|k|}{1+\alpha}\rho^{1+\alpha}} \\
A_2 &:= \sup_{x\in(M,+\infty)} |k|\, x^{a-\frac{\alpha}{2}}\, e^{\frac{|k|}{1+\alpha}x^{1+\alpha}} \int_x^{+\infty} \mathrm{d}\rho\, \rho^{-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}} \\
B_1 &:= \sup_{\rho\in(M,+\infty)} |k|\, \rho^{-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}} \int_M^\rho \mathrm{d}x\, x^{a-\frac{\alpha}{2}}\, e^{\frac{|k|}{1+\alpha}x^{1+\alpha}} \\
B_2 &:= \sup_{\rho\in(M,+\infty)} |k|\, \rho^{-\frac{\alpha}{2}}\, e^{\frac{|k|}{1+\alpha}\rho^{1+\alpha}} \int_\rho^{+\infty} \mathrm{d}x\, x^{a-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}} .
\end{aligned}
$$

Concerning A_1, integration by parts yields

$$
\begin{aligned}
|k| \int_M^x \mathrm{d}\rho\, \rho^{-\frac{\alpha}{2}}\, e^{\frac{|k|}{1+\alpha}\rho^{1+\alpha}} &= x^{-\frac{3}{2}\alpha}\, e^{\frac{|k|}{1+\alpha}x^{1+\alpha}} - M^{-\frac{3}{2}\alpha}\, e^{\frac{|k|}{1+\alpha}M^{1+\alpha}} \\
&\quad + \frac{3\alpha}{2} \int_M^x \mathrm{d}\rho\, \rho^{-(1+\frac{3}{2}\alpha)}\, e^{\frac{|k|}{1+\alpha}\rho^{1+\alpha}}
\end{aligned}
$$

and choosing $M \geqslant M_\circ$, where

$$
M_\circ := \left(\frac{2+3\alpha}{2|k|}\right)^{\frac{1}{1+\alpha}}
$$

is the point of absolute minimum of the function $\rho \mapsto \rho^{-(1+\frac{3}{2}\alpha)}\, e^{\frac{|k|}{1+\alpha}\rho^{1+\alpha}}$, yields

$$
\begin{aligned}
|k| \int_M^x \mathrm{d}\rho\, \rho^{-\frac{\alpha}{2}}\, e^{\frac{|k|}{1+\alpha}\rho^{1+\alpha}} &\leqslant x^{-\frac{3}{2}\alpha}\, e^{\frac{|k|}{1+\alpha}x^{1+\alpha}} + \frac{3\alpha}{2}\, x^{-(1+\frac{3}{2}\alpha)}\, e^{\frac{|k|}{1+\alpha}x^{1+\alpha}} \int_0^x \mathrm{d}\rho \\
&= \big(1+\tfrac{3}{2}\alpha\big) x^{-\frac{3}{2}\alpha}\, e^{\frac{|k|}{1+\alpha}x^{1+\alpha}} .
\end{aligned}
$$

Therefore,

$$
A_1 \leqslant \sup_{x\in(M,+\infty)} \big(1+\tfrac{3}{2}\alpha\big) x^{a-2\alpha} = \big(1+\tfrac{3}{2}\alpha\big) M^{a-2\alpha},
$$

the last identity being valid for $a \leqslant 2\alpha$.

Concerning A_2,

$$
\begin{aligned}
|k| \int_x^{+\infty} \mathrm{d}\rho\, \rho^{-\frac{\alpha}{2}}\, e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}} &\leqslant |k|\, x^{-\frac{3}{2}\alpha} \int_x^{+\infty} \mathrm{d}\rho\, \rho^{\alpha}\, e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}} \\
&= x^{-\frac{3}{2}\alpha} \int_{\frac{|k|}{1+\alpha}x^{1+\alpha}}^{+\infty} \mathrm{d}y\, e^{-y} = x^{-\frac{3}{2}\alpha}\, e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}},
\end{aligned}
$$

whence, when $a \leqslant 2\alpha$,

$$
A_2 \leqslant \sup_{x\in(M,+\infty)} x^{a-2\alpha} = M^{a-2\alpha} .
$$

Concerning B_1,

$$
\begin{aligned}
|k| \int_M^\rho \mathrm{d}x\, x^{a-\frac{\alpha}{2}}\, e^{\frac{|k|}{1+\alpha}x^{1+\alpha}} &= |k| \int_M^\rho \mathrm{d}x\, x^{a-\frac{3}{2}\alpha}\, x^{\alpha}\, e^{\frac{|k|}{1+\alpha}x^{1+\alpha}} \\
&\leqslant |k| \int_M^\rho \mathrm{d}x\, x^{\alpha}\, e^{\frac{|k|}{1+\alpha}x^{1+\alpha}} \times \begin{cases} \rho^{a-\frac{3}{2}\alpha} & \text{if } a \geqslant \frac{3}{2}\alpha \\ M^{a-\frac{3}{2}\alpha} & \text{if } a < \frac{3}{2}\alpha \end{cases} \\
&\leqslant \int_0^{\frac{|k|}{1+\alpha}\rho^{1+\alpha}} \mathrm{d}y\, e^{y} \times \begin{cases} \rho^{a-\frac{3}{2}\alpha} & \text{if } a \geqslant \frac{3}{2}\alpha \\ M^{a-\frac{3}{2}\alpha} & \text{if } a < \frac{3}{2}\alpha \end{cases} \\
&\leqslant e^{\frac{|k|}{1+\alpha}\rho^{1+\alpha}} \times \begin{cases} \rho^{a-\frac{3}{2}\alpha} & \text{if } a \geqslant \frac{3}{2}\alpha \\ M^{a-\frac{3}{2}\alpha} & \text{if } a < \frac{3}{2}\alpha , \end{cases}
\end{aligned}
$$

whence

$$
B_1 \leqslant \sup_{\rho\in(M,+\infty)} \begin{cases} \rho^{a-2\alpha} & \text{if } a \geqslant \frac{3}{2}\alpha \\ \rho^{-\frac{\alpha}{2}}\, M^{a-\frac{3}{2}\alpha} & \text{if } a < \frac{3}{2}\alpha . \end{cases}
$$

In either case, as long as $a \leqslant 2\alpha$,

$$B_1 \;\leqslant\; M^{a-2\alpha}\,.$$

Concerning B_2, let us split the analysis between $a \leqslant \frac{3}{2}\alpha$ and $a > \frac{3}{2}\alpha$. In the former case,

$$\begin{aligned}|k|\int_\rho^{+\infty}\mathrm{d}x\,x^{a-\frac{\alpha}{2}}\,e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}} \;&\leqslant\; \rho^{a-\frac{3}{2}\alpha}|k|\int_\rho^{+\infty}\mathrm{d}x\,x^{\alpha}\,e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}}\\ &=\; \rho^{a-\frac{3}{2}\alpha}\int_{\frac{|k|}{1+\alpha}}^{+\infty}\mathrm{d}y\,e^{-y} \;=\; \rho^{a-\frac{3}{2}\alpha}\,e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}}\,,\end{aligned}$$

whence, as long as $a \leqslant 2\alpha$,

$$B_2 \;\leqslant\; \sup_{\rho\in(M,+\infty)}\rho^{a-2\alpha} \;\leqslant\; M^{a-2\alpha}\,.$$

When instead $a > \frac{3}{2}\alpha$, then, integrating by parts and using $a \leqslant 1+\frac{5}{2}\alpha$,

$$\begin{aligned}&|k|\int_\rho^{+\infty}\mathrm{d}x\,x^{a-\frac{\alpha}{2}}\,e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}}\\ &\qquad=\; \rho^{a-\frac{3}{2}\alpha}\,e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}} + \big(a-\tfrac{3\alpha}{2}\big)\int_\rho^{+\infty}\mathrm{d}x\,x^{a-\frac{3}{2}\alpha-1}\,e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}}\\ &\qquad\leqslant\; \rho^{a-\frac{3}{2}\alpha}\,e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}} + \big(a-\tfrac{3\alpha}{2}\big)\rho^{a-\frac{5}{2}\alpha-1}\int_\rho^{+\infty}\mathrm{d}x\,x^{\alpha}\,e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}}\\ &\qquad=\; \rho^{a-\frac{3}{2}\alpha}\,e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}} + \big(a-\tfrac{3\alpha}{2}\big)\rho^{a-\frac{5}{2}\alpha-1}|k|^{-1}\int_{\frac{|k|}{1+\alpha}\rho^{1+\alpha}}^{+\infty}\mathrm{d}y\,e^{-y}\\ &\qquad=\; e^{-\frac{|k|}{1+\alpha}\rho^{1+\alpha}}\big(\rho^{a-\frac{3}{2}\alpha} + (a-\tfrac{3\alpha}{2})\,|k|^{-1}\rho^{a-\frac{5}{2}\alpha-1}\big)\,,\end{aligned}$$

whence

$$\begin{aligned}B_2 \;&\leqslant\; \sup_{\rho\in(M,+\infty)}\big(\rho^{a-2\alpha} + (a-\tfrac{3\alpha}{2})\,|k|^{-1}\rho^{a-3\alpha-1}\big)\\ &\leqslant\; M^{a-2\alpha}\big(1+(a-\tfrac{3\alpha}{2})\,(|k|M^{1+\alpha})^{-1}\big)\,.\end{aligned}$$

This completes the proof of the boundedness, via a Schur test, of the $(+,+)$ operator.

Summarising, with the above choice of the cut-off $M \geqslant M_\circ$, and under the intersection of all the above restrictions of a in terms of α, that is, $-\frac{1}{2}(1-\alpha) \leqslant a \leqslant 2\alpha$, we have found that there is an overall constant $Z_{a,\alpha} > 0$ such that

$$\begin{aligned}\big\|R^{(a)}_{G_{\alpha,k}}\big\|^2_{\mathrm{op}} \;\leqslant\; Z_{a,\alpha}\Big(&k^2M^{2(a+1-\alpha)} + |k|\,M^{2a+1-3\alpha} + M^{2a-4\alpha}\\ &+ M^{2a-4\alpha}(|k|\,M^{1+\alpha})^{-1}\Big)\,.\end{aligned}$$

This yields the statement of boundedness of part (i). The self-adjointness of $R_{G_{\alpha,k}} = |k|^{-2}\,R^{(0)}_{G_{\alpha,k}}$ is clear from (6.3.23): the adjoint $R^*_{G_{\alpha,k}}$ has kernel $\overline{G_{\alpha,k}(\rho,r)}$, but G is real-valued and $G_{\alpha,k}(\rho,r) = G_{\alpha,k}(r,\rho)$, whence indeed $R^*_{G_{\alpha,k}} = R_{G_{\alpha,k}}$. Thus, part (i) is proved.

As for part (ii), for the cut-off we make the special choice $M = M_\circ$ when $a = 2\alpha$. In this case,

$$\begin{aligned}|k|\,M^{1+\alpha} \;&=\; 1+\tfrac{3}{2}\alpha\\ |k|\,M^{2a+1-3\alpha} \;&=\; |k|\,M^{1+\alpha} \;=\; 1+\tfrac{3}{2}\alpha\\ k^2M^{2(a+1-\alpha)} \;&=\; \big(|k|\,M^{1+\alpha}\big)^2 \;=\; \big(1+\tfrac{3}{2}\alpha\big)^2,\end{aligned}$$

implying that there is an updated constant $\widetilde{Z}_{a,\alpha} > 0$ such that

$$\big\|R^{(2\alpha)}_{G_{\alpha,k}}\big\|_{\mathrm{op}} \;\leqslant\; \widetilde{Z}_{a,\alpha}$$

uniformly in k. Thus, also part (ii) is proved. □

6.7.4 Proves of some ODE lemmas

Proof of Lemma 6.3.9. (i) Let $h := A_\alpha(k)^* g = S_{\alpha,k}\, g$. As already observed at the beginning of Sect. 6.3.2, g can be expressed in terms of h by the standard representation

$$g = A_0 F_{\alpha,k} + A_\infty \Phi_{\alpha,k} + \Theta_\infty^{(h)} F_{\alpha,k} + \Theta_0^{(h)} \Phi_{\alpha,k}$$

for some constants $A_0, A_\infty \in \mathbb{C}$ determined by h and some h-dependent functions explicitly given, as follows from (6.3.19), (6.3.22), and (6.3.23), by

$$\begin{aligned} \Theta_0^{(h)}(x) &:= \frac{1}{W}\int_0^x F_{\alpha,k}(\rho) h(\rho)\,\mathrm{d}\rho \\ \Theta_\infty^{(h)}(x) &:= \frac{1}{W}\int_x^{+\infty} \Phi_{\alpha,k}(\rho) h(\rho)\,\mathrm{d}\rho\,. \end{aligned}$$

Comparing the latter formulas with (6.3.35)-(6.3.36), we deduce that

$$\begin{aligned} \Theta_0^{(h)}(x) &= b_0^{(g)}(x) \\ \Theta_\infty^{(h)}(x) &= \frac{1}{W}\int_x^{+\infty} \Phi_{\alpha,k}(\rho)(A_\alpha(k)^* g)(\rho)\,\mathrm{d}\rho \\ &= W^{-1}\,\langle \Phi_{\alpha,k}, A_\alpha(k)^* g\rangle_{L^2(\mathbb{R}^+)} + b_\infty^{(g)}(x)\,. \end{aligned}$$

So (6.3.36) is proved upon setting

$$\begin{aligned} a_0^{(g)} &:= A_0 + W^{-1}\,\langle \Phi_{\alpha,k}, A_\alpha(k)^* g\rangle_{L^2(\mathbb{R}^+)} \\ a_\infty^{(g)} &:= A_\infty\,. \end{aligned}$$

(ii) Since $\Phi_{\alpha,k}$, $F_{\alpha,k}$ and $A_\alpha(k)^* g$ are all square-integrable on the interval $[0,x]$, the integrand functions in (6.3.35) are L^1-functions on $[0,x]$: this proves (6.3.37) and justifies the simple estimates

$$\begin{aligned} |b_0^{(g)}(x)| &\lesssim \|F_{\alpha,k}\|_{L^2((0,x))}\|A_\alpha^*(k) g\|_{L^2((0,x))} \overset{x\downarrow 0}{=} o(1) \\ |b_\infty^{(g)}(x)| &\lesssim \|\Phi_{\alpha,k}\|_{L^2((0,x))}\|A_\alpha^*(k) g\|_{L^2((0,x))} \overset{x\downarrow 0}{=} o(1), \end{aligned}$$

so (6.3.38) is proved too. Last, we find

$$\begin{aligned} |b_\infty^{(g)}(x) F_{\alpha,k}(x)| &\lesssim x^{1+\frac{\alpha}{2}}\Big(\int_0^x \rho^{-\alpha}\,\mathrm{d}\rho\Big)^{\frac{1}{2}}\|h\|_{L^2((0,x))} \lesssim x^{3/2} o(1) = o(x^{3/2}) \\ |b_0^{(g)}(x)\Phi_{\alpha,k}(x)| &\lesssim x^{-\frac{\alpha}{2}}\int_0^x \rho^{1+\frac{\alpha}{2}}|h(\rho)|\mathrm{d}\rho \leqslant x\|h\|_{L^2((0,x))} x^{1/2} = o(x^{3/2}), \end{aligned}$$

and (6.3.39) follows. □

Proof of Lemma 6.3.10. The linearity of L_u is obvious.

We check the finiteness of $L_u(g)$ as follows. Let us decompose (according to (6.3.36) and using the basis of $\mathcal{L}$)

$$\begin{aligned} g &= a_0^{(g)} F_{\alpha,k} + a_\infty^{(g)}\Phi_{\alpha,k} + b_\infty^{(g)} F_{\alpha,k} + b_0^{(g)}\Phi_{\alpha,k} \\ u &= c_0 F_{\alpha,k} + c_\infty \Phi_{\alpha,k}\,. \end{aligned}$$

Owing to (6.3.45) it suffices to control the finiteness of $L_{F_{\alpha,k}}(g)$ and $L_{\Phi_{\alpha,k}}(g)$. By linearity

(i)
$$\begin{aligned} L_{F_{\alpha,k}}(g) &= a_0^{(g)} L_{F_{\alpha,k}}(F_{\alpha,k}) + a_\infty^{(g)} L_{F_{\alpha,k}}(\Phi_{\alpha,k}) + L_{F_{\alpha,k}}(b_\infty^{(g)} F_{\alpha,k} + b_0^{(g)}\Phi_{\alpha,k}) \\ L_{\Phi_{\alpha,k}}(g) &= a_0^{(g)} L_{\Phi_{\alpha,k}}(F_{\alpha,k}) + a_\infty^{(g)} L_{\Phi_{\alpha,k}}(\Phi_{\alpha,k}) + L_{\Phi_{\alpha,k}}(b_\infty^{(g)} F_{\alpha,k} + b_0^{(g)}\Phi_{\alpha,k})\,. \end{aligned}$$

Moreover, obviously,

(ii)
$$\begin{aligned} L_{F_{\alpha,k}}(F_{\alpha,k}) &= L_{\Phi_{\alpha,k}}(\Phi_{\alpha,k}) = 0 \\ L_{F_{\alpha,k}}(\Phi_{\alpha,k}) &= -W = -L_{\Phi_{\alpha,k}}(F_{\alpha,k}), \end{aligned}$$

and we also claim that

(iii)
$$L_{F_{\alpha,k}}\big(b_\infty^{(g)} F_{\alpha,k} + b_0^{(g)}\Phi_{\alpha,k}\big) = 0 = L_{\Phi_{\alpha,k}}\big(b_\infty^{(g)} F_{\alpha,k} + b_0^{(g)}\Phi_{\alpha,k}\big)\,.$$

Plugging (ii) and (iii) into (i) the finiteness

$$L_{F_{\alpha,k}}(g) \;=\; -Wa_\infty^{(g)}, \qquad L_{\Phi_{\alpha,k}}(g) \;=\; Wa_0^{(g)}$$

follows.

To prove (iii) we compute

$$\begin{aligned}
&\det\begin{pmatrix} F_{\alpha,k} & b_\infty^{(g)}F_{\alpha,k} + b_0^{(g)}\Phi_{\alpha,k} \\ F'_{\alpha,k} & (b_\infty^{(g)}F_{\alpha,k} + b_0^{(g)}\Phi_{\alpha,k})' \end{pmatrix} = \\
&\quad = F_{\alpha,k}^2(b_\infty^{(g)})' + F_{\alpha,k}(b_0^{(g)})'\Phi_{\alpha,k} + F_{\alpha,k}b_\infty^{(g)}F'_{\alpha,k} - F'_{\alpha,k}b_0^{(g)}\Phi_{\alpha,k} \\
&\quad = F_{\alpha,k}b_\infty^{(g)}F'_{\alpha,k} - F'_{\alpha,k}b_0^{(g)}\Phi_{\alpha,k}\,,
\end{aligned}$$

having used the cancellation

$$F_{\alpha,k}^2(b_\infty^{(g)})' + F_{\alpha,k}(b_0^{(g)})'\Phi_{\alpha,k} \;=\; 0\,,$$

that follows from (6.3.35). Therefore, by means of the asymptotics (6.3.14) and (6.3.38) as $x \downarrow 0$, namely,

$$\begin{aligned}
&F_{\alpha,k}(x) \;=\; O(x^{1+\frac{\alpha}{2}}), \qquad F'_{\alpha,k}(x) = O(x^{\frac{\alpha}{2}}), \qquad \Phi_{\alpha,k}(x) \;=\; O(x^{-\frac{\alpha}{2}}), \\
&b_0^{(g)}(x) \;=\; o(1), \qquad b_\infty^{(g)}(x) \;=\; o(1),
\end{aligned}$$

we conclude

$$L_{F_{\alpha,k}}\big(b_\infty^{(g)}F_{\alpha,k} + b_0^{(g)}\Phi_{\alpha,k}\big) \;=\; \lim_{x\downarrow 0}\big(F_{\alpha,k}b_\infty^{(g)}F'_{\alpha,k} - F'_{\alpha,k}b_0^{(g)}\Phi_{\alpha,k}\big) \;=\; 0\,.$$

The proof of the second identity in (iii) is completely analogous.

Last, let us prove that $L_u(\varphi) = 0$ for $\varphi \in \mathcal{D}(\overline{A_\alpha(k)})$ and $u \in \mathcal{L}$. Although u does not necessarily belong to $\mathcal{D}(A_\alpha(k)^*)$ (it might fail to be square-integrable at infinity), the function χu surely does for $\chi \in C_0^\infty([0,+\infty))$ with $\chi(x) = 1$ on $x \in [0, \frac{1}{2}]$ and $\chi(x) = 0$ on $x \in [1, +\infty)$. This fact follows from (6.2.21) observing that $\chi u \in L^2(\mathbb{R}^+)$ and also

$$S_{\alpha,k}(u\chi) \;=\; \chi S_{\alpha,k}\,u - 2u'\chi' - u\chi'' \;=\; -2u'\chi' - u\chi'' \in L^2(\mathbb{R}^+)\,.$$

The choice of χ guarantees that the Wronskians $W_x(\overline{u\chi}, g)$ and $W_x(\overline{u}, g)$ coincide in a neighbourhood of $x = 0$, that is, $L_{u\chi} = L_u$. Therefore, by means of (6.3.41), (6.3.43), and (6.3.45) we deduce

$$\begin{aligned}
L_u(\varphi) \;&=\; L_{u\chi}(\varphi) \;=\; \lim_{x\downarrow 0} W_x(\overline{u\chi}, \varphi) \;=\; -\omega(u\chi, \varphi) \\
&=\; \langle u\chi, A_\alpha(k)^*\varphi\rangle - \langle A_\alpha(k)^*u\chi, \varphi\rangle \;=\; \langle u\chi, \overline{A_\alpha(k)}\varphi\rangle - \langle u\chi, \overline{A_\alpha(k)}\varphi\rangle \;=\; 0,
\end{aligned}$$

which completes the proof. □

Proof of Lemma 6.3.11. The implication (i) ⇒ (ii) follows at once from

$$\omega(\varphi, g) \;=\; \langle A_\alpha(k)^*\varphi, g\rangle - \langle \varphi, A_\alpha(k)^*g\rangle \;=\; \langle \overline{A_\alpha(k)}\varphi, g\rangle - \langle \overline{A_\alpha(k)}\varphi, g\rangle \;=\; 0\,.$$

For the converse implication (i) ⇐ (ii), we observe that the property

$$0 \;=\; \omega(\varphi, g) \;=\; \langle A_\alpha(k)^*\varphi, g\rangle - \langle \varphi, A_\alpha(k)^*g\rangle \qquad \forall g \in \mathcal{D}(A_\alpha(k)^*)$$

is equivalent to $\langle A_\alpha(k)^*\varphi, g\rangle = \langle \varphi, A_\alpha(k)^*g\rangle$ $\forall g \in \mathcal{D}(S^*)$, which implies that $\varphi \in \mathcal{D}(A_\alpha(k)^{**}) = \mathcal{D}(\overline{A_\alpha(k)})$.

The implication (i) ⇒ (iii) is given by Lemma 6.3.10. Let us now prove that (iii) ⇒ (ii): thus, now $L_u(\varphi) = 0$ for all $u \in \mathcal{L}$ and we want to prove that for such φ one has $\omega(\varphi, g) = 0$ for all $g \in \mathcal{D}(A_\alpha(k)^*)$. Owing to the decomposition (6.3.36) for g,

$$\omega(\varphi, g) \;=\; a_0^{(g)}\omega(\varphi, F_{\alpha,k}) + a_\infty^{(g)}\omega(\varphi, \Phi_{\alpha,k}) + \omega(\varphi, b_\infty^{(g)}F_{\alpha,k}) + \omega(\varphi, b_0^{(g)}\Phi_{\alpha,k})\,.$$

The first two summands in the r.h.s. above are zero: indeed,

$$\overline{\omega(\varphi, F_{\alpha,k})} \;=\; -\omega(F_{\alpha,k}, \varphi) \;=\; \lim_{x\downarrow 0} W_x(\overline{F_{\alpha,k}}, \varphi) \;=\; L_{F_{\alpha,k}}(\varphi) \;=\; 0$$

having used in the last step the assumption that $L_u(\varphi) = 0$ for all $u \in \mathcal{L}$, and analogously, $\overline{\omega(\varphi, \Phi_{\alpha,k})} = L_{\Phi_{\alpha,k}}(\varphi) = 0$. Therefore,

$$\begin{aligned}
\overline{\omega(\varphi, g)} &= \overline{\omega(\varphi, b_\infty^{(g)} F_{\alpha,k})} + \overline{\omega(\varphi, b_0^{(g)} \Phi_{\alpha,k})} \\
&= -\omega(b_\infty^{(g)} F_{\alpha,k}, \varphi) - \omega(b_0^{(g)} \Phi_{\alpha,k}, \varphi) \\
&= \lim_{x\downarrow 0} \big(W_x(b_\infty^{(g)} F_{\alpha,k}, \varphi) + W_x(b_0^{(g)} \Phi_{\alpha,k}, \varphi) \big) \\
&= \lim_{x\downarrow 0} \big(b_\infty^{(g)} W_x(F_{\alpha,k}, \varphi) + b_0^{(g)} W_x(\Phi_{\alpha,k}, \varphi) \big) \\
&= b_\infty^{(g)} L_{F_{\alpha,k}}(\varphi) + b_0^{(g)} L_{\Phi_{\alpha,k}}(\varphi) \;=\; 0 ,
\end{aligned}$$

having used again the assumption (ii) in the last step (observe also that helpful cancellation $(b_\infty^{(g)})' F_{\alpha,k}\varphi + (b_0^{(g)})' \Phi_{\alpha,k}\varphi = 0$ occurred in computing the determinants in the fourth step).

Properties (i), (ii), and (iii) are thus equivalent. Last, let us establish the equivalence (i) $\Leftrightarrow$ (iv). Representing φ according to (6.3.36) as

$$\varphi \;=\; a_0^{(\varphi)} F_{\alpha,k} + a_\infty^{(\varphi)} \Phi_{\alpha,k} + b_\infty^{(\varphi)} F_{\alpha,k} + b_0^{(\varphi)} \Phi_{\alpha,k} ,$$

and using the identities $W_x(F_{\alpha,k}, F_{\alpha,k}) = 0$ and $W_x(F_{\alpha,k}, \Phi_{\alpha,k}) = -W$, one has

$$L_{F_{\alpha,k}}(\varphi) \;=\; \lim_{x\downarrow 0} W_x(F_{\alpha,k}, \varphi) \;=\; -W a_\infty^{(\varphi)} + \lim_{x\downarrow 0} W_x(F_{\alpha,k}, b_\infty^{(\varphi)} F_{\alpha,k} + b_0^{(\varphi)} \Phi_{\alpha,k}) .$$

The determinant in the latter Wronskian has the very same form of the determinant computed in the proof of Lemma 6.3.10: using the same cancellation $F_{\alpha,k}^2 (b_\infty^{(\varphi)})' + F_{\alpha,k} (b_0^{(\varphi)})' \Phi_{\alpha,k} = 0$ and the usual short-distance asymptotics we find

$$L_{F_{\alpha,k}}(\varphi) \;=\; -W a_\infty^{(\varphi)} .$$

In a completely analogous fashion,

$$L_{\Phi_{\alpha,k}}(\varphi) \;=\; W a_0^{(\varphi)} .$$

Therefore, $\varphi \in \mathcal{D}(\overline{A_\alpha(k)})$ if and only if $L_u(\varphi) = 0$ for all $u \in \mathcal{L}$ (because (i) $\Leftrightarrow$ (iii)), and the latter property is equivalent to $a_0^{(\varphi)} = a_\infty^{(\varphi)} = 0$. □

6.7.5 The mode $k = 0$

We discuss here how the analysis of the previous Section is to be modified when $k = 0$. It is straightforward, but for completeness we present it in the appendix. In fact, by other means and from a different perspective, the extensions of $A_\alpha(0)$ were also determined in [38]: we shall therefore omit an amount of details that can be either worked out in the very same manner of Sect. 6.3, or can be found in [38].

We follow the same conceptual scheme, but applying it now to the *shifted* operator $A_\alpha(0) + \mathbb{1}$: owing to (6.3.2), such a (densely defined, symmetric) operator has strictly positive bottom.

Thus, whereas for $k \neq 0$ self-adjoint extensions were determined a la KVB by implementing the self-adjointness condition between regular and singular part of the domain of the adjoint

$$\mathcal{D}(A_\alpha(k)^*) \;=\; \mathcal{D}(\overline{A_\alpha(k)}) \dotplus (A_{\alpha,F}(k))^{-1} \ker A_\alpha(k)^* \dotplus \ker A_\alpha(k)^* ,$$

when $k = 0$ the self-adjointness condition is implemented as a restriction in the formula

$$\begin{aligned}
\mathcal{D}(A_\alpha(0)^* + \mathbb{1}) \;=\; & \mathcal{D}(\overline{A_\alpha(0)} + \mathbb{1}) \dotplus \\
& \dotplus (A_{\alpha,F}(0) + \mathbb{1})^{-1} \ker(A_\alpha(0)^* + \mathbb{1}) \dotplus \ker(A_\alpha(0)^* + \mathbb{1}) ,
\end{aligned}$$

where obviously $\mathcal{D}(A_\alpha(0)^* + \mathbb{1}) = \mathcal{D}(A_\alpha(0)^*)$ and $\mathcal{D}(\overline{A_\alpha(0)} + \mathbb{1}) = \mathcal{D}(\overline{A_\alpha(0)})$, and analogously the domain of each extension is insensitive to the shift by $\mathbb{1}$. The main result is Theorem 6.7.11 below.

Let us start with the homogeneous problem

$$0 \;=\; (S_{\alpha,0} + \mathbb{1})h \;=\; -h'' + C_\alpha x^{-2} h + h . \tag{6.7.19}$$

Setting

$$w(z) \;:=\; \frac{h(x)}{\sqrt{x}} , \qquad \nu \;:=\; \sqrt{\frac{1 + 4C_\alpha}{4}} \;=\; \frac{1+\alpha}{2} ,$$

(6.7.19) takes the form of the modified Bessel equation

$$x^2 w'' + x w' - (z^2 + \nu^2) w \;=\; 0\,, \qquad x \in \mathbb{R}^+\,. \tag{6.7.20}$$

From the two linearly independent solutions K_ν and I_ν to the latter [2, Sect. 9.6] we therefore have that

$$\begin{aligned} \Phi_{\alpha,0}(x) \;&:=\; \sqrt{x}\, K_{\frac{1+\alpha}{2}}(x) \\ F_{\alpha,0}(x) \;&:=\; \sqrt{x}\, I_{\frac{1+\alpha}{2}}(x) \end{aligned} \tag{6.7.21}$$

are two linearly independent solutions to (6.7.19). In fact, only $\Phi_{\alpha,0}$ is square-integrable, as is seen from the short-distance asymptotics [2, Eq. (9.6.2) and (9.6.10)]

$$\begin{aligned} \Phi_{\alpha,0} \;&\overset{x\downarrow 0}{=}\; 2^{\frac{\alpha-1}{2}} \Gamma\left(\tfrac{1+\alpha}{2}\right) x^{-\frac{\alpha}{2}} - \frac{\Gamma\left(\frac{1-\alpha}{2}\right)}{2^{\frac{1+\alpha}{2}}(1+\alpha)} x^{1+\frac{\alpha}{2}} + O(x^{2-\frac{\alpha}{2}}) \\ F_{\alpha,0}(x) \;&\overset{x\downarrow 0}{=}\; \left(2^{\frac{1+\alpha}{2}} \Gamma\left(\tfrac{3+\alpha}{2}\right)\right)^{-1} x^{1+\frac{\alpha}{2}} + O(x^{3+\frac{\alpha}{2}}) \end{aligned} \tag{6.7.22}$$

and from the large-distance asymptotics [2, Eq. (9.7.1) and (9.7.2)]

$$\begin{aligned} \Phi_{\alpha,0}(x) \;&\overset{x\to+\infty}{=}\; \sqrt{\tfrac{\pi}{2}}\, e^{-x}\,(1 + O(x^{-1})) \\ F_{\alpha,0}(x) \;&\overset{x\to+\infty}{=}\; \tfrac{1}{\sqrt{2\pi}}\, e^{x}\,(1 + O(x^{-1}))\,. \end{aligned} \tag{6.7.23}$$

Thus, in analogy to Lemma 6.3.2, we find:

Lemma 6.7.5. *For $\alpha \in (0,1)$,*

$$\ker(A_\alpha(0)^* + \mathbb{1}) \;=\; \mathrm{span}\{\Phi_{\alpha,0}\}\,. \tag{6.7.24}$$

Next, concerning the non-homogeneous problem

$$S_{\alpha,0} u + u \;=\; g \tag{6.7.25}$$

in the unknown u for given g, the Wronskian relative to the fundamental system $\{\Phi_{\alpha,0}, F_{\alpha,0}\}$ is constant in r and explicitly given by

$$W(\Phi_{\alpha,0}, F_{\alpha,0}) \;=\; \det\begin{pmatrix} \Phi_{\alpha,0}(r) & F_{\alpha,0}(r) \\ \Phi'_{\alpha,0}(r) & F'_{\alpha,0}(r) \end{pmatrix} \;=\; 1\,, \tag{6.7.26}$$

as one computes based on the asymptotics (6.7.22) or (6.7.23). By standard variation of constants, a particular solution to (6.7.25) is

$$u_{\mathrm{part}}(r) \;=\; \int_0^{+\infty} G_{\alpha,0}(r,\rho) g(\rho)\, \mathrm{d}\rho \tag{6.7.27}$$

with

$$G_{\alpha,0}(r,\rho) \;:=\; \begin{cases} \Phi_{\alpha,0}(r) F_{\alpha,0}(\rho) & \text{if } 0 < \rho < r \\ F_{\alpha,0}(r) \Phi_{\alpha,0}(\rho) & \text{if } 0 < r < \rho\,. \end{cases} \tag{6.7.28}$$

With the same arguments used for Lemma 6.3.3, using now the asymptotics (6.7.22)-(6.7.23), we find the following analogue (an explicit proof of which can be found also in [38, Lemma 4.4]).

Lemma 6.7.6. *Let $\alpha \in (0,1)$. Let $R_{G_{\alpha,0}}$ be the operator associated with the integral kernel* (6.7.28)*. $R_{G_{\alpha,0}}$ can be realised as an everywhere defined, bounded, and self-adjoint operator on $L^2(\mathbb{R}^+, \mathrm{d}r)$.*

Analogously to (6.3.28) we set

$$\Psi_{\alpha,0}(x) \;:=\; R_{G_{\alpha,0}} \Phi_{\alpha,0}\,. \tag{6.7.29}$$

The proof of Lemma 6.3.7 can be then repeated verbatim, with $\Phi_{\alpha,0}$ and $F_{\alpha,0}$ in place of $\Phi_{\alpha,k}$ and $F_{\alpha,k}$, so as to obtain:

Lemma 6.7.7. *For $\alpha \in (0,1)$,*

$$\Psi_{\alpha,0}(x) \overset{x\downarrow 0}{=} \left(2^{\frac{1+\alpha}{2}}\Gamma\left(\tfrac{3+\alpha}{2}\right)\right)^{-1} \|\Phi_{\alpha,0}\|^2_{L^2}\, x^{1+\frac{\alpha}{2}} + o(x^{3/2})\,. \tag{6.7.30}$$

Concerning $\overline{A_\alpha(0)}$, it suffices for our purposes to import from the literature the following analogue of Lemma 6.3.12.

Lemma 6.7.8. *Let $\alpha \in (0,1)$. If $\varphi \in \mathcal{D}(\overline{A_\alpha(0)})$, then $\varphi(x) = o(x^{3/2})$ and $\varphi'(x) = o(x^{1/2})$ as $x \downarrow 0$.*

Proof. A direct consequence of [38, Prop. 4.11(i)]: in the notation therein $\overline{A_\alpha(0)}$ is the operator $L^{\min}_m$ with $m^2 - \frac{1}{4} = C_\alpha$, that is, $m = \frac{1+\alpha}{2}$, and their requirement $m \in (0,1)$ is therefore satisfied. □

As a further step, repeating the argument for Lemma 6.3.6 one concludes that $R^{-1}_{G_{\alpha,0}}$ is a self-adjoint extension of $A_\alpha(0) + \mathbb{1}$ with everywhere defined and bounded inverse, whose domain clearly contains $\Psi_{\alpha,0}$. Such a reference extension induces a classification of all other self-adjoint extensions in complete analogy to what discussed in Subsect. 6.3.5. Thus, (6.3.48) and (6.3.49) are valid in the identical form also when $k = 0$, and the short-range asymptotics for $\Phi_{\alpha,0}$ (formula (6.7.22)), for $\Psi_{\alpha,0}$ (Lemma 6.7.7), and for the elements of $\mathcal{D}(\overline{A_\alpha(0)})$ (Lemma 6.7.8) imply that for a generic

$$g \;=\; \varphi + c_1\Psi_{\alpha,0} + c_0\Phi_{\alpha,0} \;\in\; \mathcal{D}(A_\alpha(0)^*) \tag{6.7.31}$$

(with $\varphi \in \mathcal{D}(\overline{A_\alpha(0)})$ and $c_0, c_1 \in \mathbb{C}$) the limits

$$\begin{aligned} g_0 \;&:=\; \lim_{x\downarrow 0} x^{\frac{\alpha}{2}} g(x) \;=\; c_0\, 2^{-\frac{1-\alpha}{2}}\Gamma\left(\tfrac{1+\alpha}{2}\right) \\ g_1 \;&:=\; \lim_{x\downarrow 0} x^{-(1+\frac{\alpha}{2})}(g(x) - g_0 x^{-\frac{\alpha}{2}}) \\ &= c_1\big(2^{\frac{1+\alpha}{2}}\Gamma(\tfrac{3+\alpha}{2})\big)^{-1}\|\Phi_{\alpha,0}\|^2_{L^2(\mathbb{R}^+)} - c_0\big(2^{\frac{1+\alpha}{2}}(1+\alpha)\big)^{-1}\Gamma(\tfrac{1-\alpha}{2}) \end{aligned} \tag{6.7.32}$$

exist and are finite, and one has the asymptotics

$$g(x) \overset{x\downarrow 0}{=} g_0 x^{-\frac{\alpha}{2}} + g_1 x^{1+\frac{\alpha}{2}} + o(x^{3/2})\,. \tag{6.7.33}$$

Then, analogously to (6.3.53)-(6.3.54), the condition of self-adjointness reads again as $c_1 = \beta c_0$ for some $\beta \in \mathbb{R}$, or equivalently as

$$g_1 \;=\; \gamma g_0\,, \qquad \gamma \;:=\; \frac{\|\Phi_{\alpha,0}\|^2_{L^2}}{2^\alpha\Gamma(\frac{1+\alpha}{2})\Gamma(\frac{3+\alpha}{2})}\left(\beta - \frac{\Gamma(\frac{1-\alpha}{2})\Gamma(\frac{3+\alpha}{2})}{(1+\alpha)\|\Phi_{\alpha,0}\|^2_{L^2}}\right). \tag{6.7.34}$$

This yields an obvious analogue of the 'temporary' classification of Prop. 6.3.14, where if $A^{[\gamma]}_\alpha(0)+\mathbb{1}$ is a self-adjoint extension of $A_\alpha(0) + \mathbb{1}$, so is $A^{[\gamma]}_\alpha(0)$ for $A_\alpha(0)$, with $\mathcal{D}(A^{[\gamma]}_\alpha(0) + \mathbb{1}) = \mathcal{D}(A^{[\gamma]}_\alpha(0))$.

In fact, based on the very same argument of Lemma 6.3.16, repeated now for the characterisation of the form domain of $A_{\alpha,F}(0)$, one can also reproduce the argument of Prop. 6.3.15, establishing the following analogue.

Proposition 6.7.9. *For $\alpha \in (0,1)$, one has $A_{\alpha,F}(0) + \mathbb{1} = R^{-1}_{G_{\alpha,0}}$ and $\Psi_{\alpha,0} = (A_{\alpha,F}(0) + \mathbb{1})^{-1}\Phi_{\alpha,0}$.*

Noticeably, the following useful characterisation of the domain of the Friedrichs extension of $A_\alpha(0)$ is available in the literature.

Proposition 6.7.10. *For $\alpha \in (0,1)$,*

$$\mathcal{D}(A_{\alpha,F}(0)) = \mathcal{D}(\overline{A_\alpha(0)}) + \mathrm{span}\{x^{1+\frac{\alpha}{2}}P\}\,, \tag{6.7.35}$$

where $P \in C^\infty_0([0,+\infty))$ with $P(0) = 1$.

Proof. In the notation of [38], the Friedrichs extension is the operator H^θ_m with $m^2 - \frac{1}{4} = C_\alpha$, hence $m = \frac{1+\alpha}{2} \in (0,1)$, and with $\theta = \frac{\pi}{2}$ ([38, Prop. 4.19]), whereas $\overline{A_\alpha(0)}$ is the operator $L^{\min}_m$. In turn, such H^θ_m is recognised to be the operator $L^{u_\theta}_m$, where u_θ is the function that for $\theta = \frac{\pi}{2}$ has the form $u_{\pi/2}(x) = x^{1+\alpha/2}$ ([38, Prop. 4.17(1)]). With this correspondence, the formula $\mathcal{D}(L^{u_\theta}_m) = \mathcal{D}(L^{\min}_m) + \mathrm{span}\{u_\theta P\}$ ([38, Prop. A.5]) then yields precisely (6.7.35). □

With all the ingredients collected so far, and based on a straightforward adaptation of the arguments of Subsect. 6.3.6, the above 'temporary' classification then takes the following final form.

Theorem 6.7.11. *Let $\alpha \in [0,1)$.*

(i) The adjoint of $A_\alpha(0)$ has domain

$$\begin{aligned} \mathcal{D}(A_\alpha(0)^*) &= \left\{ \begin{array}{c} g \in L^2(\mathbb{R}^+) \ \text{ such that} \\ \big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\alpha(2+\alpha)}{4x^2}\big) g \in L^2(\mathbb{R}^+) \end{array} \right\} \\ &= \mathcal{D}(\overline{A_\alpha(0)}) \dotplus \mathrm{span}\{\Psi_{\alpha,0}\} \dotplus \mathrm{span}\{\Phi_{\alpha,0}\}\,, \end{aligned} \tag{6.7.36}$$

where $\Phi_{\alpha,0}$ and $\Psi_{\alpha,0}$ are two smooth functions on $\mathbb{R}^+$ explicitly defined, in terms of modified Bessel functions, respectively by formulas (6.7.21)*,* (6.7.28)*, and* (6.7.29)*. Moreover,*

$$\ker(A_\alpha(0)^* + \mathbb{1}) = \mathrm{span}\{\Phi_{\alpha,0}\}\,. \tag{6.7.37}$$

(ii) The self-adjoint extensions of $A_\alpha(0)$ in $L^2(\mathbb{R}^+)$ form the family

$$\{A_\alpha^{[\gamma]}(0) \,|\, \gamma \in \mathbb{R} \cup \{\infty\}\}\,.$$

The extension with $\gamma = \infty$ is the Friedrichs extension $A_{\alpha,F}(0)$, whose domain is given by (6.7.35)*, and moreover $(A_{\alpha,F}(0) + \mathbb{1})^{-1} = R_{G_{\alpha,0}}$, the everywhere defined and bounded operator with integral kernel given by* (6.7.28)*. For generic $\gamma \in \mathbb{R}$ one has*

$$\mathcal{D}(A_\alpha^{[\gamma]}(0)) = \big\{ g \in \mathcal{D}(A_\alpha(0)^*) \,\big|\, g(x) \overset{x\downarrow 0}{=} g_0 x^{-\frac{\alpha}{2}} + \gamma g_0 x^{1+\frac{\alpha}{2}} + o(x^{\frac{3}{2}}),\ g_0 \in \mathbb{C} \big\}\,. \tag{6.7.38}$$

6.7.6 Friedrichs extension for infinite sum operators

Lemma 6.7.12. *Let $\alpha \in [0,1)$. One has*

$$\mathscr{H}_{\alpha,F} = \bigoplus_{k\in\mathbb{Z}} A_{\alpha,F}(k)\,. \tag{6.7.39}$$

Lemma 6.7.12 is an application of a general fact that for completeness we revisit here.

Lemma 6.7.13. *Let $T = \bigoplus_{k\in\mathbb{Z}} T(k)$ be a direct sum operator acting on the Hilbert space $\mathcal{H} = \bigoplus_{k\in\mathbb{Z}} \mathfrak{h}_k$, where each $T(k)$ is densely defined, symmetric, and semi-bounded from below on $\mathfrak{h}_k$, with uniform lower bound*

$$m := \inf_{k\in\mathbb{Z}} \inf_{\substack{u\in\mathcal{D}(T(k)) \\ u\neq 0}} \frac{\langle u, T(k)u\rangle_{\mathfrak{h}_k}}{\|u\|^2_{\mathfrak{h}_k}} > -\infty\,.$$

Denote by T_F, resp. $T_F(k)$, the Friedrichs extension of T, resp. $T(k)$. Then

$$T_F = \bigoplus_{k\in\mathbb{Z}} T_F(k)\,.$$

Proof. It is clear that $\bigoplus_{k\in\mathbb{Z}} T_F(k)$ is a self-adjoint extension of T. To recognise it as the Friedrichs extension, it suffices to check that the *operator* domain $\mathcal{D}(\bigoplus_{k\in\mathbb{Z}} T_F(k))$ is an actual subspace of the *form* domain $\mathcal{D}[T]$. To this aim, let us observe that

$$\mathcal{D}(\bigoplus_{k\in\mathbb{Z}} T_F(k)) = \boxplus_{k\in\mathbb{Z}} \mathcal{D}(T_F(k)) \subset \boxplus_{k\in\mathbb{Z}} \mathcal{D}[T(k)]$$

(the first identity is precisely (6.7.3) discussed previously, and the inclusion is due to the fact that for each k the Friedrichs-extension characterising property $\mathcal{D}(T_F(k)) \subset \mathcal{D}[T(k)]$ holds). On the other hand, $\mathcal{D}[T] = \mathcal{D}((T - m\mathbb{1})^{1/2})$ and $\mathcal{D}[T(k)] = \mathcal{D}((T(k) - m\mathbb{1}_k)^{1/2})$, whence

$$\begin{aligned} \mathcal{D}[T] &= \mathcal{D}\Big[\bigoplus_{k\in\mathbb{Z}} T(k)\Big] = \mathcal{D}\Big(\Big(\bigoplus_{k\in\mathbb{Z}} (T(k) - m\mathbb{1}_k)\Big)^{1/2}\Big) \\ &= \mathcal{D}\Big(\bigoplus_{k\in\mathbb{Z}} (T(k) - m\mathbb{1}_k)^{1/2}\Big) = \boxplus_{k\in\mathbb{Z}} \mathcal{D}\big((T(k) - m\mathbb{1}_k)^{1/2}\big) = \boxplus_{k\in\mathbb{Z}} \mathcal{D}[T(k)]\,. \end{aligned}$$

This proves the desired inclusion. □

Proof of Lemma 6.7.12. One applies Lemma 6.7.13 to $\overline{\mathscr{H}_\alpha} = \bigoplus_{k\in\mathbb{Z}} \overline{A_\alpha(k)}$. □

6.7.7 Decomposition of the adjoint into singular terms

As alluded to at the end of Subsect. 6.6.2, let us show that the decomposition induced by (6.6.14) of a generic element in the domain of a uniformly fibred extension $\mathscr{H}_\alpha^{\mathrm{u.f.}}$, namely

$$(g_k)_{k\in\mathbb{Z}} \;=\; (\varphi_k)_{k\in\mathbb{Z}} + \big(g_{1,k}|x|^{1+\frac{\alpha}{2}}P\big)_{k\in\mathbb{Z}} + \big(g_{0,k}|x|^{-\frac{\alpha}{2}}P\big)_{k\in\mathbb{Z}}, \tag{6.7.40}$$

unavoidably displays a form of singularity, in the following sense.

Lemma 6.7.14. *Let $\alpha \in [0,1)$ and let $\mathscr{H}_\alpha^{\mathrm{u.f.}}$ be a uniformly fibred self-adjoint extension. There exists $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}_\alpha^{\mathrm{u.f.}})$ such that, with respect to the decomposition* (6.7.40)*,*

$$\begin{aligned}\big(g_{1,k}|x|^{1+\frac{\alpha}{2}}P\big)_{k\in\mathbb{Z}} &\notin \mathcal{D}(\mathscr{H}_\alpha^*),\\ \big(g_{0,k}|x|^{-\frac{\alpha}{2}}P\big)_{k\in\mathbb{Z}} &\notin \mathcal{D}(\mathscr{H}_\alpha^*),\end{aligned}$$

with the obvious exception of those terms above that are prescribed to be identically zero for all elements of the domain of the considered uniformly fibred extension.

Clearly, the fact that

$$(\varphi_k)_{k\in\mathbb{Z}} \in \ell^2(\mathbb{Z}, L^2(\mathbb{R}, \mathrm{d}x)) \tag{6.7.41}$$

follows at once by difference from (6.7.40), because owing to Corollary 6.6.3 both $(g_{1,k}|x|^{1+\frac{\alpha}{2}}P)_{k\in\mathbb{Z}}$ and $(g_{0,k}|x|^{-\frac{\alpha}{2}}P)_{k\in\mathbb{Z}}$ belong to $\ell^2(\mathbb{Z}, L^2(\mathbb{R}, \mathrm{d}x))$. However, whereas in (6.6.14)/(6.7.40) each φ_k belongs to $\mathcal{D}(\overline{A_\alpha(k)})$, their collection $(\varphi_k)_{k\in\mathbb{Z}}$ may fail to belong to $\mathcal{D}(\overline{\mathscr{H}_\alpha})$ because it may even fail to belong to $\mathcal{D}(\mathscr{H}_\alpha^*)$.

In preparation for the proof of Lemma 6.7.14, a simple computation shows that

$$\begin{aligned}A_\alpha^\pm(k)^*\big(|x|^{-\frac{\alpha}{2}}P\big) &= \alpha|x|^{-(1+\frac{\alpha}{2})}P' - |x|^{-\frac{\alpha}{2}}P'' + k^2|x|^{\frac{3\alpha}{2}}P\\ A_\alpha^\pm(k)^*\big(|x|^{1+\frac{\alpha}{2}}P\big) &= -(2+\alpha)|x|^{\frac{\alpha}{2}}P' - |x|^{1+\frac{\alpha}{2}}P'' + k^2|x|^{1+\frac{5\alpha}{2}}P\end{aligned}$$

for any $k \in \mathbb{Z}$ and $x \gtrless 0$ depending on the '+' or the '-' case. In particular, as the cut-off function P is constantly equal to one when $|x| < 1$,

$$\begin{aligned}\mathbf{1}_{I^\pm}(x)A_\alpha^\pm(k)^*\big(|x|^{-\frac{\alpha}{2}}P\big) &= \mathbf{1}_{I^\pm}(x)k^2|x|^{\frac{3\alpha}{2}}\\ \mathbf{1}_{I^\pm}(x)A_\alpha^\pm(k)^*\big(|x|^{1+\frac{\alpha}{2}}P\big) &= \mathbf{1}_{I^\pm}(x)k^2|x|^{1+\frac{5\alpha}{2}},\end{aligned} \tag{6.7.42}$$

where $I^- := (-1,0)$ and $I^+ := (0,1)$. We can see that this implies

$$\big\|(\mathscr{H}_\alpha^\pm)^*\big(g_{0,k}^\pm|x|^{-\frac{\alpha}{2}}P\big)_{k\in\mathbb{Z}}\big\|^2_{\mathcal{H}^\pm} \;\geqslant\; \sum_{k\in\mathbb{Z}} k^4|g_{0,k}^\pm|^2, \tag{6.7.43}$$

$$\big\|(\mathscr{H}_\alpha^\pm)^*\big(g_{1,k}^\pm|x|^{1+\frac{\alpha}{2}}P\big)_{k\in\mathbb{Z}}\big\|^2_{\mathcal{H}^\pm} \;\geqslant\; \sum_{k\in\mathbb{Z}} k^4|g_{1,k}^\pm|^2. \tag{6.7.44}$$

Indeed,

$$\begin{aligned}\big\|(\mathscr{H}_\alpha^+)^*\big(g_{1,k}^+x^{1+\frac{\alpha}{2}}P\big)_{k\in\mathbb{Z}}\big\|^2_{\mathcal{H}^+} &= \sum_{k\in\mathbb{Z}}\big\|A_\alpha^+(k)^*\big(g_{1,k}^+x^{1+\frac{\alpha}{2}}P\big)\big\|^2_{L^2(\mathbb{R}^+,\mathrm{d}x)}\\ &\geqslant \sum_{k\in\mathbb{Z}}\big\|g_{1,k}^+k^2x^{1+\frac{5\alpha}{2}}\big\|^2_{L^2((0,1),\mathrm{d}x)}\\ &= (3+5\alpha)^{-1}\sum_{k\in\mathbb{Z}}k^4|g_{1,k}^+|^2,\end{aligned}$$

where we used (6.7.8) in the first step and (6.7.42) in the second; all other cases for (6.7.43)-(6.7.44) are obtained in a completely analogous way.

Proof of Lemma 6.7.14. Let us discuss case by case all possible types of uniformly fibred extensions. For arbitrary $\varepsilon > 0$ let

$$a_k(\varepsilon) := \begin{cases}|k|^{\frac{1}{1+\alpha}-\frac{1}{2}(1+\varepsilon)} & \text{if } k \in \mathbb{Z}\setminus\{0\}\\ 0 & \text{if } k = 0\end{cases}$$

$$b_k(\varepsilon) := \begin{cases}|k|^{-\frac{1}{1+\alpha}-\frac{1}{2}(1+\varepsilon)} & \text{if } k \in \mathbb{Z}\setminus\{0\}\\ 0 & \text{if } k = 0.\end{cases}$$

(i) Friedrichs extension $\mathscr{H}_{\alpha,F} = \bigoplus_{k\in\mathbb{Z}} A_{\alpha,F}(k)$. For this case we choose $(g_k)_{k\in\mathbb{Z}}$ with

$$g_k \;:=\; \begin{pmatrix} a_k(\varepsilon)\,\widetilde{\Psi}_{\alpha,k} \\ a_k(\varepsilon)\,\widetilde{\Psi}_{\alpha,k} \end{pmatrix}.$$

With respect to the representation (6.5.10), $c^{\pm}_{0,k} = 0$ and $c^{\pm}_{1,k} = a_k(\varepsilon)$. Therefore,

$$\sum_{k\in\mathbb{Z}} |k|^{-\frac{2}{1+\alpha}} |c^{\pm}_{1,k}|^2 \;=\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-1-\varepsilon} \;<\; +\infty$$

and, owing to Lemma 6.5.2, $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}^*_\alpha)$. Moreover, by construction g_k satisfies the conditions of self-adjointness characterising $\mathcal{D}(A_{\alpha,F}(k))$ stated in Theorem 6.4.2; thus, $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}_{\alpha,F})$. Expressing now $(g_k)_{k\in\mathbb{Z}}$ in the representation (6.7.40), formulas (6.6.25)-(6.6.26) yield

$$g^{\pm}_{0,k} \;=\; 0, \qquad g^{\pm}_{1,k} \;\sim\; |k|^{-\frac{1}{2}(\frac{2}{1+\alpha}+\varepsilon)} \quad (k\neq 0),$$

whence

$$\sum_{k\in\mathbb{Z}\setminus\{0\}} k^4 |g^{\pm}_{1,k}|^2 \;\sim\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{2+4\alpha}{1+\alpha}-\varepsilon} \;=\; +\infty \quad \Leftrightarrow \quad \varepsilon\in(0,\tfrac{3+5\alpha}{1+\alpha}]\,.$$

Thus, for $\varepsilon\in(0,\frac{3+5\alpha}{1+\alpha}]$, we deduce from (6.7.44) that $(g_{1,k}|x|^{1+\frac{\alpha}{2}}P)_{k\in\mathbb{Z}} \notin \mathcal{D}(\mathscr{H}^*_\alpha)$.

(ii) Extensions of type I_R: for $\gamma\in\mathbb{R}$ let us consider $\mathscr{H}^{[\gamma]}_{\alpha,R} = \bigoplus_{k\in\mathbb{Z}} A^{[\gamma]}_{\alpha,R}(k)$. For this case we choose $(g_k)_{k\in\mathbb{Z}}$ with

$$g_k \;:=\; \begin{pmatrix} a_k(\varepsilon)\widetilde{\Psi}_{\alpha,k} \\ \beta_k b_k(\varepsilon)\widetilde{\Psi}_{\alpha,k} + b_k(\varepsilon)\widetilde{\Phi}_{\alpha,k} \end{pmatrix}$$

and β_k given by

$$\gamma \;=\; \tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)}}{\pi(1+\alpha)}\,\beta_k - 1\Big)\,.$$

From (6.3.16), $\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)} \sim |k|^{-\frac{2}{1+\alpha}}$ (for some multiplicative α-dependent constant), whence $\beta_k \sim |k|^{\frac{2}{1+\alpha}}$ at the leading order in $k\in\mathbb{Z}\setminus\{0\}$. With respect to the representation (6.5.10),

$$\begin{aligned} c^-_{0,k} \;&=\; 0, & c^-_{1,k} \;&=\; a_k(\varepsilon) \;=\; |k|^{\frac{1}{1+\alpha}-\frac{1}{2}(1+\varepsilon)}, \\ c^+_{0,k} \;&=\; b_k(\varepsilon) \;=\; |k|^{-\frac{1}{1+\alpha}-\frac{1}{2}(1+\varepsilon)}, & c^+_{1,k} \;&=\; \beta_k b_k(\varepsilon) \;\sim\; |k|^{\frac{1}{1+\alpha}-\frac{1}{2}(1+\varepsilon)}, \end{aligned}$$

at the leading order in $k\in\mathbb{Z}\setminus\{0\}$, whereas all the above coefficients vanish for $k=0$. Therefore,

$$\begin{aligned} \sum_{k\in\mathbb{Z}} |k|^{-\frac{2}{1+\alpha}} |c^+_{0,k}|^2 \;&=\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{4}{1+\alpha}-1-\varepsilon} \;<\; +\infty, \\ \sum_{k\in\mathbb{Z}} |k|^{-\frac{2}{1+\alpha}} |c^{\pm}_{1,k}|^2 \;&=\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-1-\varepsilon} \;<\; +\infty, \end{aligned}$$

which implies, owing to Lemma 6.5.2, that $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}^*_\alpha)$. Moreover, by construction g_k satisfies the conditions of self-adjointness characterising $\mathcal{D}(A^{[\gamma]}_{\alpha,R}(k))$ stated in Theorem 6.4.2; thus, $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}^{[\gamma]}_{\alpha,R})$. Expressing now $(g_k)_{k\in\mathbb{Z}}$ in the representation (6.7.40), formulas (6.6.25)-(6.6.26) yield

$$\begin{aligned} g^-_{0,k} \;&=\; 0, & g^-_{1,k} \;&\sim\; |k|^{-\frac{1}{2}(\frac{2}{1+\alpha}+\varepsilon)}, \\ g^+_{0,k} \;&\sim\; |k|^{-\frac{1}{2}(\frac{4+2\alpha}{1+\alpha}+\varepsilon)}, & g^+_{1,k} \;&\sim\; |k|^{-\frac{1}{2}(\frac{4+2\alpha}{1+\alpha}+\varepsilon)}, \end{aligned}$$

for $k\in\mathbb{Z}\setminus\{0\}$, up to multiplicative pre-factors depending on α and γ only, all the above coefficients vanishing for $k=0$. From this one obtains

$$\begin{aligned} \sum_{k\in\mathbb{Z}} k^4 |g^+_{0,k}|^2 \;&\sim\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{2\alpha}{1+\alpha}-\varepsilon} \;=\; +\infty \quad \Leftrightarrow \quad \varepsilon\in(0,\tfrac{1+3\alpha}{1+\alpha}], \\ \sum_{k\in\mathbb{Z}} k^4 |g^+_{1,k}|^2 \;&\sim\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{2\alpha}{1+\alpha}-\varepsilon} \;=\; +\infty \quad \Leftrightarrow \quad \varepsilon\in(0,\tfrac{1+3\alpha}{1+\alpha}], \\ \sum_{k\in\mathbb{Z}} k^4 |g^-_{1,k}|^2 \;&\sim\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{2+4\alpha}{1+\alpha}-\varepsilon} \;=\; +\infty \quad \Leftrightarrow \quad \varepsilon\in(0,\tfrac{3+5\alpha}{1+\alpha}]\,. \end{aligned}$$

Thus, for $\varepsilon \in (0, \frac{1+3\alpha}{1+\alpha}]$, we deduce from (6.7.43)-(6.7.44) that $(g_{0,k}|x|^{-\frac{\alpha}{2}}P)_{k\in\mathbb{Z}} \notin \mathcal{D}(\mathscr{H}^*_\alpha)$ and $(g_{1,k}|x|^{1+\frac{\alpha}{2}}P)_{k\in\mathbb{Z}} \notin \mathcal{D}(\mathscr{H}^*_\alpha)$.

(iii) Extensions of type I_L: for $\gamma \in \mathbb{R}$ let us consider $\mathscr{H}^{[\gamma]}_{\alpha,L} = \bigoplus_{k\in\mathbb{Z}} A^{[\gamma]}_{\alpha,L}(k)$. For this case we choose $(g_k)_{k\in\mathbb{Z}}$ with

$$g_k \;:=\; \begin{pmatrix} \beta_k b_k(\varepsilon)\widetilde{\Psi}_{\alpha,k} + b_k(\varepsilon)\widetilde{\Phi}_{\alpha,k} \\ a_k(\varepsilon)\widetilde{\Psi}_{\alpha,k} \end{pmatrix},$$

with the same β_k as in case (ii). With the obvious inversion between '-' and '+' components, the reasoning is the same as in case (ii).

(iv) Extensions of type II_a for given $a \in \mathbb{C}\setminus\{0\}$: for $\gamma \in \mathbb{R}$ let us consider $\mathscr{H}^{[\gamma]}_{\alpha,a} = \bigoplus_{k\in\mathbb{Z}} A^{[\gamma]}_{\alpha,a}(k)$. For this case we choose $(g_k)_{k\in\mathbb{Z}}$ with

$$g_k \;:=\; \begin{pmatrix} \big(\tau_k b_k(\varepsilon) + a_k(\varepsilon)\big)\widetilde{\Psi}_{\alpha,k} + b_k(\varepsilon)\widetilde{\Phi}_{\alpha,k} \\ \big(\tau_k a b_k(\varepsilon) - \overline{a}^{-1} a_k(\varepsilon)\big)\widetilde{\Psi}_{\alpha,k} + a b_k(\varepsilon)\widetilde{\Phi}_{\alpha,k} \end{pmatrix}$$

and τ_k given by

$$\gamma \;:=\; (1+|a|^2)\tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)}}{\pi(1+\alpha)}\,\tau_k - 1\Big).$$

In particular, $\tau_k \sim |k|^{\frac{2}{1+\alpha}}$ at the leading order in $k \in \mathbb{Z}\setminus\{0\}$. With respect to the representation (6.5.10),

$$c^{\pm}_{0,k} \;\sim\; |k|^{-\frac{1}{1+\alpha}-\frac{1}{2}(1+\varepsilon)}, \qquad c^{\pm}_{1,k} \;\sim\; |k|^{\frac{1}{1+\alpha}-\frac{1}{2}(1+\varepsilon)}$$

at the leading order in $k \in \mathbb{Z}\setminus\{0\}$, whereas all the above coefficients vanish for $k = 0$. Therefore,

$$\sum_{k\in\mathbb{Z}} |k|^{-\frac{2}{1+\alpha}}|c^{\pm}_{0,k}|^2 \;=\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-\frac{4}{1+\alpha}-1-\varepsilon} \;<\; +\infty,$$
$$\sum_{k\in\mathbb{Z}} |k|^{-\frac{2}{1+\alpha}}|c^{\pm}_{1,k}|^2 \;=\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{-1-\varepsilon} \;<\; +\infty,$$

which implies, owing to Lemma 6.5.2, that $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}^*_\alpha)$. Moreover, by construction g_k satisfies the conditions of self-adjointness characterising $\mathcal{D}(A^{[\gamma]}_{\alpha,a}(k))$ stated in Theorem 6.4.2; thus, $(g_k)_{k\in\mathbb{Z}} \in \mathcal{D}(\mathscr{H}^{[\gamma]}_{\alpha,a})$. Expressing now $(g_k)_{k\in\mathbb{Z}}$ in the representation (6.7.40), formulas (6.6.25)-(6.6.26) yield

$$g^{\pm}_{0,k} \;\sim\; |k|^{-\frac{1}{2}(\frac{4+2\alpha}{1+\alpha}-\varepsilon)}, \qquad g^{\pm}_{1,k} \;\sim\; |k|^{-\frac{1}{2}(\frac{2}{1+\alpha}+\varepsilon)}$$

at the leading order in $k \in \mathbb{Z}\setminus\{0\}$, all the above coefficients vanishing for $k = 0$. From this one obtains

$$\sum_{k\in\mathbb{Z}} k^4|g^{\pm}_{0,k}|^2 \;\sim\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{2\alpha}{1+\alpha}-\varepsilon} \;=\; +\infty \quad\Leftrightarrow\quad \varepsilon \in (0, \tfrac{1+3\alpha}{1+\alpha}],$$
$$\sum_{k\in\mathbb{Z}} k^4|g^{\pm}_{1,k}|^2 \;\sim\; \sum_{k\in\mathbb{Z}\setminus\{0\}} |k|^{\frac{2+4\alpha}{1+\alpha}-\varepsilon} \;=\; +\infty \quad\Leftrightarrow\quad \varepsilon \in (0, \tfrac{3+5\alpha}{1+\alpha}].$$

Thus, for $\varepsilon \in (0, \frac{1+3\alpha}{1+\alpha}]$, we deduce from (6.7.43)-(6.7.44) that $(g_{0,k}|x|^{-\frac{\alpha}{2}}P)_{k\in\mathbb{Z}} \notin \mathcal{D}(\mathscr{H}^*_\alpha)$ and $(g_{1,k}|x|^{1+\frac{\alpha}{2}}P)_{k\in\mathbb{Z}} \notin \mathcal{D}(\mathscr{H}^*_\alpha)$.

(v) Extensions of type III: for $\Gamma \in \mathbb{R}^4$ let us consider $\mathscr{H}^{[\Gamma]}_\alpha = \bigoplus_{k\in\mathbb{Z}} A^{[\Gamma]}_\alpha(k)$. For this case we choose $(g_k)_{k\in\mathbb{Z}}$ with

$$g_k \;:=\; \begin{pmatrix} \big(\tau_{1,k} + \tau_{2,k} + \mathrm{i}\tau_{3,k}\big)b_k(\varepsilon)\widetilde{\Psi}_{\alpha,k} + b_k(\varepsilon)\widetilde{\Phi}_{\alpha,k} \\ \big(\tau_{2,k} - \mathrm{i}\tau_{3,k} + \tau_{4,k}\big)b_k(\varepsilon)\widetilde{\Psi}_{\alpha,k} + b_k(\varepsilon)\widetilde{\Phi}_{\alpha,k} \end{pmatrix}$$

and $(\tau_{1,k}, \tau_{2,k}, \tau_{3,k}, \tau_{4,k})$ given by

$$\gamma_1 \;=\; \tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)}}{\pi(1+\alpha)}\,\tau_{1,k} - 1\Big)$$
$$\gamma_2 + \mathrm{i}\gamma_3 \;=\; (\tau_{2,k} + \mathrm{i}\tau_{3,k})\tfrac{2|k|}{\pi(1+\alpha)^2}\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)}$$
$$\gamma_4 \;=\; \tfrac{|k|}{1+\alpha}\Big(\tfrac{2\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)}}{\pi(1+\alpha)}\,\tau_{4,k} - 1\Big).$$

In particular,

$$\tau_{1,k} \;\sim\; |k|^{\frac{2}{1+\alpha}}, \qquad \tau_{2,k} \pm \mathrm{i}\tau_{3,k} \;\sim\; |k|^{\frac{1-\alpha}{1+\alpha}}, \qquad \tau_{4,k} \;\sim\; |k|^{\frac{2}{1+\alpha}},$$

at the leading order in $k \in \mathbb{Z}\setminus\{0\}$. With respect to the representation (6.5.10),

$$c^{\pm}_{0,k} \;\sim\; |k|^{-\frac{1}{1+\alpha}-\frac{1}{2}(1+\varepsilon)}, \qquad c^{\pm}_{1,k} \;\sim\; |k|^{\frac{1}{1+\alpha}-\frac{1}{2}(1+\varepsilon)}$$

at the leading order in $k \in \mathbb{Z}\setminus\{0\}$, whereas all the above coefficients vanish for $k = 0$. From this point one repeats verbatim the reasoning of part (iv). □

6.7.8 Proof of Proposition 6.6.13

In preparation for the proof of Proposition 6.6.13, in terms of the functions

$$\begin{aligned} h_{0,k} &:= \sqrt{\tfrac{2}{\pi(1+\alpha)}}\,|k|^{\frac{1}{2(1+\alpha)}}\Big(\Phi_{\alpha,k} - \sqrt{\tfrac{\pi(1+\alpha)}{2|k|}}\,x^{-\frac{\alpha}{2}} + \sqrt{\tfrac{\pi|k|}{2(1+\alpha)}}\,x^{1+\frac{\alpha}{2}}\Big) \\ h_{1,k} &:= \sqrt{\tfrac{2}{\pi(1+\alpha)}}\,|k|^{\frac{5}{2(1+\alpha)}}\Big(\Psi_{\alpha,k} - \sqrt{\tfrac{2|k|}{\pi(1+\alpha)^3}}\,\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)}\,|x|^{1+\frac{\alpha}{2}}\Big) \end{aligned} \tag{6.7.45}$$

defined on $\mathbb{R}^+$ for each $k \in \mathbb{Z}\setminus\{0\}$, one sees from (6.6.31)-(6.6.32) that

$$\begin{aligned} \vartheta^{\pm}_{0,k}(x) &= c^{\pm}_{0,k}\sqrt{\tfrac{\pi(1+\alpha)}{2}}\,|k|^{-\frac{1}{2(1+\alpha)}}\,h_{0,k}(|x|) \qquad 0 < \pm x < 1\,, \\ \vartheta^{\pm}_{1,k}(x) &= c^{\pm}_{1,k}\sqrt{\tfrac{\pi(1+\alpha)}{2}}\,|k|^{-\frac{5}{2(1+\alpha)}}\,h_{1,k}(|x|) \qquad 0 < \pm x < 1\,. \end{aligned} \tag{6.7.46}$$

Clearly the above identities are not valid when $|x| > 1$.

Lemma 6.7.15. *Let $\alpha \in [0,1)$ and $k \in \mathbb{Z}\setminus\{0\}$. For $x \in \mathbb{R}^+$ one has*

$$h_{0,k}(x) := w_0\big(|k|x^{1+\alpha}\big), \qquad h_{1,k}(x) := w_1\big(|k|x^{1+\alpha}\big) \tag{6.7.47}$$

with

$$w_0(x) := x^{-\frac{\alpha}{2(1+\alpha)}}\big(e^{-\frac{x}{1+\alpha}} - 1 + \tfrac{x}{1+\alpha}\big) \tag{6.7.48}$$

and

$$\begin{aligned} w_1(x) := {} & x^{-\frac{\alpha}{2(1+\alpha)}}\,e^{-\frac{x}{1+\alpha}}\int_0^{x^{\frac{1}{1+\alpha}}} \mathrm{d}\rho\,\rho^{-\alpha}\sinh\big(\tfrac{\rho^{1+\alpha}}{1+\alpha}\big)\,e^{-\frac{\rho^{1+\alpha}}{1+\alpha}} \\ & + x^{-\frac{\alpha}{2(1+\alpha)}}\,\sinh\big(\tfrac{x}{1+\alpha}\big)\int_{x^{\frac{1}{1+\alpha}}}^{+\infty}\mathrm{d}\rho\,\rho^{-\alpha}\,e^{-\frac{2\rho^{1+\alpha}}{1+\alpha}} \\ & - 2^{-\frac{1-\alpha}{1+\alpha}}\,(1+\alpha)^{-\frac{1+3\alpha}{1+\alpha}}\,\Gamma\big(\tfrac{1-\alpha}{1+\alpha}\big)\,x^{\frac{2+\alpha}{2(1+\alpha)}}\,. \end{aligned} \tag{6.7.49}$$

Proof. Plugging the explicit expression (6.3.13) for $\Phi_{\alpha,k}$ into the first formula in (6.7.45) one finds

$$h_{0,k}(x) = \big(|k|^{\frac{1}{1+\alpha}}x\big)^{-\frac{\alpha}{2}}\Big(e^{-\frac{|k|}{1+\alpha}x^{1+\alpha}} - 1 + \tfrac{|k|x^{1+\alpha}}{1+\alpha}\Big) = w_0\big(|k|x^{1+\alpha}\big)$$

with w_0 defined by (6.7.48). Analogously, inserting the expression (6.3.31) for $\Psi_{\alpha,k}$ and the expression (6.3.16) for $\|\Phi_{\alpha,k}\|^2_{L^2(\mathbb{R}^+)}$ into the second formula in (6.7.45), one obtains

$$\begin{aligned} h^{\pm}_{1,k}(x) &= \big(|k|^{\frac{1}{1+\alpha}}x\big)^{-\frac{\alpha}{2}}\,e^{-\frac{|k|x^{1+\alpha}}{1+\alpha}}\int_0^{x|k|^{\frac{1}{1+\alpha}}}\mathrm{d}\rho\,\rho^{-\alpha}\sinh\big(\tfrac{\rho^{1+\alpha}}{1+\alpha}\big)\,e^{-\frac{\rho^{1+\alpha}}{1+\alpha}} \\ &\quad + \big(|k|^{\frac{1}{1+\alpha}}x\big)^{-\frac{\alpha}{2}}\,\sinh\big(\tfrac{|k|x^{1+\alpha}}{1+\alpha}\big)\int_{x|k|^{\frac{1}{1+\alpha}}}^{+\infty}\mathrm{d}\rho\,\rho^{-\alpha}\,e^{-\frac{2\rho^{1+\alpha}}{1+\alpha}} \\ &\quad - 2^{-\frac{1-\alpha}{1+\alpha}}\,(1+\alpha)^{-\frac{1+3\alpha}{1+\alpha}}\,\Gamma\big(\tfrac{1-\alpha}{1+\alpha}\big)\,\big(|k|^{\frac{1}{1+\alpha}}x\big)^{1+\frac{\alpha}{2}} \\ &= w_1\big(|k|x^{1+\alpha}\big) \end{aligned}$$

with w_1 defined by (6.7.49). □

Lemma 6.7.16. *Let $\alpha \in [0,1)$ and $k \in \mathbb{Z}\setminus\{0\}$. The functions $h_{0,k}$ and $h_{1,k}$ defined in* (6.7.45) *satisfy*

$$\big\|x^{-2}h_{j,k}\big\|^2_{L^2((0,1))} \leqslant |k|^{\frac{3}{1+\alpha}}\,\big\|x^{-2}h_{j,1}\big\|^2_{L^2(\mathbb{R}^+)} \tag{6.7.50}$$

$$\big\|h''_{j,k}\big\|^2_{L^2((0,1))} \leqslant |k|^{\frac{3}{1+\alpha}}\,\big\|h''_{j,1}\big\|^2_{L^2(\mathbb{R}^+)} \tag{6.7.51}$$

for $j \in \{0,1\}$.

Proof. By means of the homogeneity properties (6.7.47) one finds

$$\begin{aligned}\big\|x^{-2}h_{j,k}\big\|^2_{L^2((0,1))} &= \int_0^1 \big|x^{-2}w_j\big(|k|x^{1+\alpha}\big)\big|^2\,\mathrm{d}x\\ &= |k|^{\frac{3}{1+\alpha}}\int_0^{|k|^{\frac{1}{1+\alpha}}} |x^{-2}w_j(x^{1+\alpha})|^2\,\mathrm{d}x\\ &\leqslant |k|^{\frac{3}{1+\alpha}}\int_0^{+\infty} |x^{-2}h_{j,1}(x)|^2\,\mathrm{d}x\end{aligned}$$

and

$$\begin{aligned}\big\|h''_{j,k}\big\|^2_{L^2((0,1))} &= \int_0^1 \Big|\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,w_j\big(|k|x^{1+\alpha}\big)\Big|^2\,\mathrm{d}x\\ &= \int_0^1 \big|(1+\alpha)^2|k|^2x^{2\alpha}w''_j\big(|k|x^{1+\alpha}\big)+\alpha(1+\alpha)|k|x^{-(1-\alpha)}w'_j\big(|k|x^{1+\alpha}\big)\big|^2\,\mathrm{d}x\\ &= |k|^{\frac{3}{1+\alpha}}\int_0^{|k|^{\frac{1}{1+\alpha}}} \big|(1+\alpha)^2x^{2\alpha}w''_j\big(x^{1+\alpha}\big)+\alpha(1+\alpha)x^{-(1-\alpha)}w'_j\big(x^{1+\alpha}\big)\big|^2\,\mathrm{d}x\\ &= |k|^{\frac{3}{1+\alpha}}\int_0^{|k|^{\frac{1}{1+\alpha}}} \Big|\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,w_j\big(x^{1+\alpha}\big)\Big|^2\,\mathrm{d}x \;\leqslant\; |k|^{\frac{3}{1+\alpha}}\int_0^{+\infty} |h''_{j,1}(x)|^2\,\mathrm{d}x\,,\end{aligned}$$

which proves, respectively, (6.7.50) and (6.7.51). □

Lemma 6.7.17. *Let $\alpha\in[0,1)$. The functions $h_{0,1}$ and $h_{1,1}$ defined in* (6.7.45) *satisfy*

$$\big\|x^{-2}h_{j,1}\big\|^2_{L^2(\mathbb{R}^+)} < +\infty \tag{6.7.52}$$

$$\big\|h''_{j,1}\big\|^2_{L^2(\mathbb{R}^+)} < +\infty \tag{6.7.53}$$

for $j\in\{0,1\}$.

Proof. As $h_{0,1}$ (resp., $h_{1,1}$) only agrees with $\vartheta^+_{0,1}$ (resp., $\vartheta^+_{1,1}$) over the interval $(0,1)$, apart from a α-dependent pre-factor, one cannot deduce (6.7.52)-(6.7.53) from (6.6.33), because the considered norms are over the whole $\mathbb{R}^+$. However, the reasoning made in the proof of Theorem 6.4.3, which led to (6.6.33), can be essentially repeated here. Clearly, both $h_{0,1}$ and $h_{1,1}$ are $C^\infty(\mathbb{R}^+)$-functions; therefore, the finiteness of the norms in (6.7.52)-(6.7.53) is only to be checked as $x\downarrow 0$ and $x\to+\infty$. In fact, for

$$h_{0,1} = x^{-\frac{\alpha}{2}}\big(e^{-\frac{x^{1+\alpha}}{1+\alpha}}-1+\tfrac{x^{1+\alpha}}{1+\alpha}\big)$$

one can perform a straightforward computation and find

$$\begin{aligned}h_{0,1}(x) &\overset{x\downarrow 0}{=} x^{2+\frac{3}{2}\alpha}(1+O(x^{1+\alpha}))\,,\\ h_{0,1}(x) &\overset{x\to+\infty}{=} \tfrac{1}{1+\alpha}x^{1-\frac{\alpha}{2}}(1+O(x^{-1}))\,,\end{aligned}$$

and

$$\begin{aligned}h''_{0,1}(x)(x) &\overset{x\downarrow 0}{=} x^{\frac{3}{2}\alpha}\big(\tfrac{9}{8}-\tfrac{1}{8(1+\alpha)^2}\big)(1+O(x^{1+\alpha}))\,,\\ h''_{0,1}(x) &\overset{x\to+\infty}{=} \tfrac{\alpha(2+\alpha)}{4(1+\alpha)}x^{-(1+\frac{\alpha}{2})}(1+o(1))\,.\end{aligned}$$

Such asymptotics imply (6.7.52)-(6.7.53) when $j=0$, as $\alpha\in(0,1)$. Concerning

$$h_{1,1} = \sqrt{\tfrac{2}{\pi(1+\alpha)}}\,\Psi_{\alpha,1}-\tfrac{2}{\pi(1+\alpha)^2}\,\|\Phi_{\alpha,1}\|^2_{L^2(\mathbb{R}^+)}\,x^{1+\frac{\alpha}{2}}\,,$$

the square-integrability of $x^{-2}h_{1,1}$ is controlled analogously to the proof of Theorem 6.4.3: the short-distance asymptotics (6.3.29) for $\Psi_{\alpha,1}$ gives a convenient compensation in $h_{1,1}$ as $x\downarrow 0$, whereas at infinity the control can be simply made term by term, as $\Psi_{\alpha,1}\in L^2(\mathbb{R}^+)$. Thus, (6.7.52) is also proved for $j=1$. Next, we consider

$$h''_{1,1} = \sqrt{\tfrac{2}{\pi(1+\alpha)}}\,\Psi''_{\alpha,1}-\tfrac{2}{\pi(1+\alpha)^2}\,\|\Phi_{\alpha,1}\|^2_{L^2(\mathbb{R}^+)}\,\tfrac{\alpha(2+\alpha)}{2}\,x^{-(1-\frac{\alpha}{2})}\,.$$

As $\Psi_{\alpha,1} = R_{G_{\alpha,1}}\Phi_{\alpha,1}$ and $R_{G_{\alpha,1}} = (A^+_{\alpha,F}(1))^{-1}$ (see (6.3.28) and Prop. 6.3.15 above), then

$$\begin{aligned}\Psi''_{\alpha,1} &= -\big(-\tfrac{\mathrm{d}^2}{\mathrm{d}x^2} + x^{2\alpha} + \tfrac{\alpha(2+\alpha)}{2}x^{-2}\big)R_{G_{\alpha,1}}\Phi_{\alpha,1} + \big(x^{2\alpha} + \tfrac{\alpha(2+\alpha)}{2}x^{-2}\big)\Psi_{\alpha,1} \\ &= -\Phi_{\alpha,1} + \big(x^{2\alpha} + \tfrac{\alpha(2+\alpha)}{2}x^{-2}\big)\Psi_{\alpha,1}\,,\end{aligned}$$

whence

$$\begin{aligned}h''_{1,1} &= -\sqrt{\tfrac{2}{\pi(1+\alpha)}}\,\Phi_{1,\alpha} + \sqrt{\tfrac{2}{\pi(1+\alpha)}}\big(x^{2\alpha} + \tfrac{\alpha(2+\alpha)}{2}x^{-2}\big)\Psi_{\alpha,1} \\ &\qquad - \tfrac{2}{\pi(1+\alpha)^2}\,\|\Phi_{\alpha,1}\|^2_{L^2(\mathbb{R}^+)}\,\tfrac{\alpha(2+\alpha)}{2}\,x^{-(1-\frac{\alpha}{2})} \\ &= -\sqrt{\tfrac{2}{\pi(1+\alpha)}}\,\Phi_{1,\alpha} + \sqrt{\tfrac{2}{\pi(1+\alpha)}}\,x^{2\alpha}\,\Psi_{\alpha,1} + \tfrac{\alpha(2+\alpha)}{2}\,x^{-2}\,h_{1,1}\,.\end{aligned}$$

Each of the three summands in the r.h.s. above belongs to $L^2(\mathbb{R}^+)$: in particular, the second does so because $\Psi_{\alpha,1} \in \operatorname{ran} R_{G_{\alpha,k}} \subset L^2(\mathbb{R}^+, \langle x\rangle^{4\alpha}\mathrm{d}x)$ (Corollary 6.3.5). This proves (6.7.53) for $j = 1$. □

From (6.7.46), and from Lemmas 6.7.16 and 6.7.17, one immediately deduces:

Corollary 6.7.18. *Let $\alpha \in [0,1)$ and $k \in \mathbb{Z}\setminus\{0\}$. Then*

$$\begin{aligned}\big\|x^{-2}\vartheta^\pm_{0,k}\big\|^2_{L^2(I^\pm)} &\lesssim |c^\pm_{0,k}|^2\,|k|^{\frac{2}{1+\alpha}} \\ \big\|(\vartheta^\pm_{0,k})''\big\|^2_{L^2(I^\pm)} &\lesssim |c^\pm_{0,k}|^2\,|k|^{\frac{2}{1+\alpha}}\end{aligned} \tag{6.7.54}$$

and

$$\begin{aligned}\big\|x^{-2}\vartheta^\pm_{1,k}\big\|^2_{L^2(I^\pm)} &\lesssim |c^\pm_{1,k}|^2\,|k|^{-\frac{2}{1+\alpha}} \\ \big\|(\vartheta^\pm_{1,k})''\big\|^2_{L^2(I^\pm)} &\lesssim |c^\pm_{1,k}|^2\,|k|^{-\frac{2}{1+\alpha}}\end{aligned} \tag{6.7.55}$$

with $I^+ = (0,1)$ and $I^- = (-1,0)$, where the constants in the above inequalities only depend on α.

In fact, (6.7.54)-(6.7.55) are trivially true also for $k = 0$: recall indeed (see (6.6.29) above) that $\vartheta_0 \equiv 0$.

Proof of Proposition 6.6.13. It clearly suffices to discuss the proof for the '+' component $\vartheta^+ = \mathcal{F}_2^{-1}(\vartheta^+_k)_{k\in\mathbb{Z}}$. Recall also that $\vartheta^+_0 \equiv 0$.

Now, owing to Corollary 6.7.18,

$$\begin{aligned}\big\|x^{-2}(\vartheta^+_{0,k})_{k\in\mathbb{Z}}\big\|^2_{\ell^2(\mathbb{Z},L^2((0,1),\mathrm{d}x))} &\lesssim \sum_{k\in\mathbb{Z}\setminus\{0\}} |c^\pm_{0,k}|^2\,|k|^{\frac{2}{1+\alpha}} \\ \big\|((\vartheta^\pm_{0,k})'')_{k\in\mathbb{Z}}\big\|^2_{\ell^2(\mathbb{Z},L^2((0,1),\mathrm{d}x))} &\lesssim \sum_{k\in\mathbb{Z}\setminus\{0\}} |c^\pm_{0,k}|^2\,|k|^{\frac{2}{1+\alpha}}\,.\end{aligned}$$

The series in the r.h.s. above are *finite*, because of the enhanced summability of the $c_{0,k}$'s due to the fact that the initially considered $(g_k)_{k\in\mathbb{Z}}$ belongs to the domain of a uniformly fibred extension (as observed already in Remark 6.6.5).

As a first consequence, $(\vartheta^+_{0,k})_{k\in\mathbb{Z}}$ belongs to $\ell^2(\mathbb{Z}, L^2((0,1),\mathrm{d}x))$, and so too does $(\vartheta^+_{1,k})_{k\in\mathbb{Z}}$ by difference from $(\vartheta^+_k)_{k\in\mathbb{Z}}$: therefore, the inverse Fourier transform can be separately applied to

$$\vartheta^+ \;=\; \mathcal{F}_2^{-1}(\vartheta^+_k)_{k\in\mathbb{Z}} \;=\; \mathcal{F}_2^{-1}(\vartheta^+_{0,k})_{k\in\mathbb{Z}} + \mathcal{F}_2^{-1}(\vartheta^+_{1,k})_{k\in\mathbb{Z}}\,.$$

As a further consequence, the above estimates imply, by means of Plancherel's formula,

$$\begin{aligned}\big\|x^{-2}\mathcal{F}_2^{-1}(\vartheta^+_{0,k})_{k\in\mathbb{Z}}\big\|^2_{L^2((0,1)\times S^1,\mathrm{d}x\mathrm{d}y)} &= \big\|x^{-2}(\vartheta^+_{0,k})_{k\in\mathbb{Z}}\big\|^2_{\ell^2(\mathbb{Z},L^2((0,1),\mathrm{d}x))} < +\infty, \\ \big\|\partial_x^2\mathcal{F}_2^{-1}(\vartheta^+_{0,k})_{k\in\mathbb{Z}}\big\|^2_{L^2((0,1)\times S^1,\mathrm{d}x\mathrm{d}y)} &= \big\|(\partial_x^2\vartheta^+_{0,k})_{k\in\mathbb{Z}}\big\|^2_{\ell^2(\mathbb{Z},L^2((0,1),\mathrm{d}x))} < +\infty\,.\end{aligned}$$

Analogously, Corollary 6.7.18 also implies

$$\begin{aligned}\big\|x^{-2}(\vartheta^+_{1,k})_{k\in\mathbb{Z}}\big\|^2_{\ell^2(\mathbb{Z},L^2((0,1),\mathrm{d}x))} &\lesssim \sum_{k\in\mathbb{Z}\setminus\{0\}} |c^\pm_{1,k}|^2\,|k|^{-\frac{2}{1+\alpha}}\,, \\ \big\|((\vartheta^\pm_{1,k})'')_{k\in\mathbb{Z}}\big\|^2_{\ell^2(\mathbb{Z},L^2((0,1),\mathrm{d}x))} &\lesssim \sum_{k\in\mathbb{Z}\setminus\{0\}} |c^\pm_{1,k}|^2\,|k|^{-\frac{2}{1+\alpha}}\,,\end{aligned}$$

and the series in the r.h.s. above are *finite* because of the general summability for elements in $\mathcal{D}(\mathscr{H}_\alpha^*)$ established in Lemma 6.5.2, formula (6.5.13). Thus, for almost every $y \in S^1$,

$$\begin{aligned} \left\| x^{-2}\mathcal{F}_2^{-1}(\vartheta^+_{1,k})_{k\in\mathbb{Z}} \right\|^2_{L^2((0,1)\times S^1,\mathrm{d}x\mathrm{d}y)} &< +\infty \\ \left\| \partial_x^2\mathcal{F}_2^{-1}(\vartheta^+_{1,k})_{k\in\mathbb{Z}} \right\|^2_{L^2((0,1)\times S^1,\mathrm{d}x\mathrm{d}y)} &< +\infty\,. \end{aligned}$$

Summarising,

$$\|x^{-2}\vartheta^+\|_{L^2((0,1)\times S^1,\mathrm{d}x\mathrm{d}y)} + \|\partial_x^2\vartheta^+\|_{L^2((0,1)\times S^1,\mathrm{d}x\mathrm{d}y)} < +\infty\,.$$

Therefore, ϑ^+ satisfies the assumptions (a) and (b) of Lemma 6.6.6 (for obviously $|x^{-(\frac{3}{2}+\frac{\alpha}{2})}\vartheta^+(x,y)| \leqslant |x^{-2}\vartheta^+(x,y)|$ when $x \in (0,1)$, since $\alpha \in (0,1)$). The thesis then follows by applying Lemma 6.6.6. □

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