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Nicolas Augier

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Contrôle adiabatique des systèmes quantiques

Thèse de doctorat de l'Université Paris-Saclay
préparée à l'École Polytechnique

Ecole doctorale n°574 Ecole doctorale de mathématiques Hadamard (EDMH)
Spécialité de doctorat : Mathématiques appliquées

Thèse présentée et soutenue à Palaiseau, le 27 septembre 2019, par

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Contrôle adiabatique des systèmes quantiques

Adiabatic control of quantum systems

Nicolas Augier

CMAP, Equipe INRIA CAGE (LJLL)

École Polytechnique

Thèse présentée pour l'obtention du grade de
Docteur en mathématiques de l'Université Paris-Saclay

Résumé

Le but principal de la thèse est d'étudier les liens entre les singularités du spectre d'un Hamiltonien quantique contrôlé et les questions de contrôlabilité de l'équation Schrödinger associée.

La question majeure qui se pose est de savoir comment contrôler une famille de systèmes quantiques dépendant des paramètres avec une entrée de commande commune. Ce problème de contrôlabilité d'ensemble est lié à la conception d'une stratégie de contrôle robuste lorsqu'un paramètre (une fréquence de résonance ou une inhomogénéité de champ de contrôle par exemple) est inconnu, et constitue un enjeu important pour les expérimentateurs. Grâce à l'étude des familles à un paramètre de Hamiltoniens et de leurs singularités génériques, nous donnons une stratégie de contrôle explicite pour le problème de contrôlabilité d'ensemble lorsque certaines conditions géométriques sur le spectre des Hamiltoniens sont satisfaites. Le résultat est basé sur la théorie de l'approximation adiabatique et sur la présence de courbes d'intersections coniques de valeurs propres du Hamiltonien contrôlé. La technique proposée fonctionne à la fois pour des systèmes évoluant dans des espaces de Hilbert de dimension finie et de dimension infinie. Nous étudions ensuite le problème de la contrôlabilité d'ensemble sous des hypothèses moins restrictives sur le spectre, à savoir la présence de singularités non-coniques. Sous des conditions génériques, de telles singularités n'apparaissent pas pour des systèmes uniques, mais apparaissent pour des familles de systèmes à un paramètre.

Pour l'étude d'un système unique, nous nous concentrons sur une classe de courbes dans l'espace des contrôles, appelées les courbes non-mixantes (définies dans [22]), qui peuvent optimiser la dynamique adiabatique près des intersections coniques et non coniques. Elles sont liées à la géométrie des espaces propres du Hamiltonien contrôlé et l'approximation adiabatique possède une meilleure précision le long de celles-ci.

Nous proposons d'étudier la compatibilité de l'approximation adiabatique avec la Rotating Wave Approximation. De telles approximations sont généralement combinées par les physiciens. On montre que cela ne se justifie pour les systèmes quantiques à dimensions finies que dans certaines conditions sur les échelles de temps. Nous étudions également les questions de contrôle d'ensemble dans ce cas.

Abstract

The main purpose of the thesis is to study the links between the singularities of the spectrum of a controlled quantum Hamiltonian and the controllability issues of the associated Schrödinger equation.

The principal issue that is developed is how to control a parameter-dependent family of quantum systems with a common control input. This problem of ensemble controllability is linked to the design of a robust control strategy when a parameter (a resonance frequency or a control field inhomogeneity for instance) is unknown, and is an important issue for experimentalists. Thanks to the study one-parametric families of Hamiltonians and their generic singularities, we give an explicit control strategy for the ensemble controllability problem when geometric conditions on the spectrum of the Hamiltonian are satisfied. The result is based on adiabatic approximation theory and on the presence of curves of conical eigenvalue intersections of the controlled Hamiltonian. The proposed technique works for systems evolving both in finite-dimensional and infinite-dimensional Hilbert spaces. Then we study the problem of ensemble controllability under less restrictive hypotheses on the spectrum, namely the presence of non-conical singularities. Under generic conditions such non-conical singularities are not present for single systems, but appear for one-parametric families of systems. , For the study of a single system, we focus on a class of curves in the space of controls, called the non-mixing curves (defined in [22]), that can optimize the adiabatic dynamics near conical and non-conical intersections. They are linked to the geometry of the eigenspaces of the controlled Hamiltonian and the adiabatic approximation holds with higher precision along them.

We propose to study the compatibility of the adiabatic approximation with the rotating wave approximation. Such approximations are usually done in cascade by physicists. It is shown in this work that this is justified for finite dimensional quantum systems only under certain conditions on the time scales. We also study ensemble control issues in this case.

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Chapitre **1**

Introduction

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1.1 Préliminaires de physique quantique, théorème adiabatique

Pour un système quantique fermé général sous l'action d'un contrôle u à valeurs dans un ouvert U de \mathbb{R}^m , nous sommes intéressés par l'équation contrôlée de la forme

$$i \frac{d\psi}{dt}(t) = H(u(t))\psi(t), \quad \psi(t) \in \mathcal{H}, \quad (1.1)$$

avec $H(u)$ essentiellement auto-adjoint sur l'espace de Hilbert complexe séparable \mathcal{H} pour chaque valeur de $u \in U$, avec un domaine dense commun pour tout $u \in U$. Pour \mathcal{H} de dimension finie, la contrôlabilité de l'équation (2.9) a été largement étudiée par des méthodes d'algèbre de Lie (voir [6, 9, 34]). Pour \mathcal{H} est de dimension infinie, l'équation (2.9) n'est en général pas contrôlable de façon exacte [11]. De nombreux résultats de contrôlabilité plus faibles ont été prouvés [17, 25, 22]. Cependant, dans les deux cas, il existe peu de résultats théoriques sur la robustesse des stratégies de contrôle par rapport aux variations des paramètres du système, sauf pour les systèmes à deux niveaux (voir [13, 63]). Le contrôle adiabatique est réputé pour être une bonne technique pour gérer les perturbations et les incertitudes. Dans sa forme la plus simple, le théorème adiabatique affirme que dans une condition de séparation sur les niveaux d'énergie du Hamiltonien contrôlé,

1.1. Préliminaires de physique quantique, théorème adiabatique

les probabilités d'occupation des niveaux d'énergie sont approximativement conservées lorsque les contrôles varient lentement. L'un de ses principaux avantages est qu'il fournit des lois de contrôle explicites et régulières. Il a donc été appliqué avec succès pour obtenir des stratégies de contrôle telles que les chirped pulses (voir par exemple [27, 74, 43]) pour les systèmes spin 1/2 à fréquence de Larmor dispersée. Une autre application classique du contrôle adiabatique à la contrôlabilité d'ensemble est ce qu'on appelle les impulsions contre-intuitives pour le processus STIRAP [38, 73, 83]. Une généralisation de cette approche a été proposée dans [62], et a soulevé de nombreuses questions intéressantes, en particulier sur la validité de l'approximation Rotating Wave dans ce cadre. Une théorie générale est alors nécessaire pour un contrôle robuste dans le cadre quantique. La principale contribution de la thèse est la compréhension de la robustesse des stratégies de contrôle adiabatique, en étudiant le problème du contrôle de familles paramétrées de systèmes quantiques avec une entrée de contrôle commune, c'est-à-dire le problème de la contrôlabilité d'ensemble. Nos principaux résultats à ce sujet sont présentés dans l'introduction de la section 2.2.1 avec deux contrôles réels et des Hamiltoniens réels, la plupart des arguments étant valables lorsque \mathcal{H} est de dimension finie ou infinie selon des hypothèses appropriées sur le Hamiltonien. Une extension de ceci avec une seule entrée de commande réelle utilisant l'approximation Rotating Wave (voir par exemple [53]) est exposée dans la section 2.2.3. Nous développerons ces questions dans les chapitres 3 et 6. Le point de départ de la thèse est le théorème adiabatique (voir par exemple [16, 55, 54, 47]), que nous énonçons dans sa forme générale, en adaptant les résultats exposés dans [78, Chapitre 2] à nos questions de théorie du contrôle.

Théorème adiabatique général Soit \mathcal{H} un espace de Hilbert séparable complexe et $k \in \mathbb{N}$. Designons l'ensemble des opérateurs linéaires essentiellement auto-adjoints sur \mathcal{H} par $\mathcal{L}_{sa}(\mathcal{H})$, et l'ensemble des fonctions C^j bornées entre deux espaces topologiques X et Y par $C_b^j(X, Y)$. Soit $H(\cdot) \in C_b(\mathbb{R}^k, \mathcal{L}_{sa}(\mathcal{H}))$. On dit que le spectre $\sigma(\cdot)$ de $H(\cdot)$ contient une partie séparée $\sigma_*(\cdot) \subset \sigma(\cdot)$ localement autour de $\bar{u} \in \mathbb{R}^k$ s'il existe deux fonctions continues et bornées $f, g \in C_b(\mathbb{R}^k, \mathbb{R})$ et un voisinage V de \bar{u} dans \mathbb{R}^k satisfaisant, pour chaque $u \in V$, $\sigma_*(u) \subset [f(u), g(u)]$ et $\inf_{u \in V} \text{dist}([f(u), g(u)], \sigma(u) \setminus \sigma_*(u)) > 0$. Pour $u \in V$, définissons $P_*(u)$ comme la projection spectrale de $H(u)$ sur l'espace propre de $H(u)$ associé à $\sigma_*(u)$. Soit $\gamma : [0, 1] \rightarrow V$ un chemin de contrôle régulier C^2 .

Nous sommes intéressés par les trajectoires $\psi^\epsilon(t) \in \mathcal{H}$ de l'Equation de Schrödinger Adiabatique :

$$i\dot{\psi}^\epsilon(t) = H(\gamma(\epsilon t))\psi^\epsilon(t), \quad \psi^\epsilon(0) = \psi_0,$$

où $\psi_0 \in \mathcal{H}$, $t \in [0, \frac{1}{\epsilon}]$, et $\epsilon > 0$. Dans la variable $\tau = \epsilon t \in [0, 1]$, la trajectoire reparamétrisée $\tilde{\psi}^\epsilon(\tau) = \psi^\epsilon(\tau\epsilon)$ satisfait

$$i\dot{\tilde{\psi}}^\epsilon(\tau) = \frac{1}{\epsilon}H(\gamma(\tau))\tilde{\psi}^\epsilon(\tau), \quad \tilde{\psi}^\epsilon(0) = \psi_0, \quad (1.2)$$

où $\tau \in [0, 1]$.

Définissons le *Hamiltonien adiabatique*, pour tout $\tau \in [0, 1]$, par

$$H_a^\epsilon(\tau) = H(\tau) - i\epsilon P_*(\gamma(\tau))\dot{P}_*(\gamma(\tau)) + i\epsilon(Id - P_*(\gamma(\tau)))\dot{P}_*(\gamma(\tau)),$$

où $\dot{P}_*(\gamma(\tau))$ est la dérivée de P_* le long du chemin de contrôle γ . Lorsqu'ils sont bien définis, définissons les deux propagateurs unitaires $U^\epsilon(\tau)$ et $U_a^\epsilon(\tau)$ sur \mathcal{H} de, respectivement, l'Equation (1.2) et $i\dot{\psi}^\epsilon(\tau) = \frac{1}{\epsilon}H_a^\epsilon(\gamma(\tau))\psi^\epsilon(\tau)$, pour $\tau \in [0, 1]$. Une propriété essentielle de U_a^ϵ est que pour tout $\tau \in [0, 1]$, $P_*(\gamma(\tau))U_a^\epsilon(\tau) = U_a^\epsilon(\tau)P_*(\gamma(0))$.

Theorem 1.1.1. [78, Theorems 2.1, 2.2] Soit V un ouvert de \mathbb{R}^k et $\gamma : [0, 1] \rightarrow V$ chemin de contrôle régulier C^2 . Soit $H(\cdot) \in C_b^2(V, \mathcal{L}_{sa}(\mathcal{H}))$ tel que les opérateurs $H(u)$ ont un domaine dense commun $D \subset \mathcal{H}$ pour tout $u \in V$, et sont minorés, uniformément par rapport à $u \in V$. Supposons que $\sigma_*(u) \subset \sigma(H(u))$ est une partie localement séparée de σ , pour $u \in V$. Alors $P_* \in C_b^2(V, \mathcal{L}_{sa}(\mathcal{H}))$, les propagateurs unitaires U_ϵ et U_a^ϵ sont bien définis, et il existe une constante $C < \infty$ telle que pour tout $\tau \in [0, 1]$,

$$\|U^\epsilon(\tau) - U_a^\epsilon(\tau)\| \leq C\epsilon.$$

Adiabatic decoupling Soit $j \in \mathbb{N}$. Supposons que les valeurs propres λ_j et λ_{j+1} de H sont séparées du reste du spectre pour u dans un voisinage V de $\bar{u} \in \mathbb{R}^k$. Remarquons qu'on ne suppose pas ici l'existence d'un gap entre λ_j et λ_{j+1} . En effet, le but de ce qui suit est d'avoir une approximation de la dynamique au voisinage d'un point \bar{u} tel que $\lambda_j(\bar{u}) = \lambda_{j+1}(\bar{u})$, c'est à dire une *intersection de valeurs propres*. Définissons pour $u \in V$, la projection spectrale $P_{j,j+1}(u)$ de $H(u)$ sur l'espace propre associé à $\sigma_*(u) = \{\lambda_j(u), \lambda_{j+1}(u)\}$. Considérons, pour $u \in V$, une base orthonormale $(\psi_j(u), \psi_{j+1}(u))$ de $\text{Im}P_{j,j+1}(u)$ qui est C^2 . Pour tout $u \in V$, considérons une application unitaire $I(u)$ de \mathbb{C}^2 à $\text{Im}P_{j,j+1}(u)$, qui est C^2 en $u \in V$, telle que $I(u)(e_1) = \psi_j(u)$ et $I(u)(e_2) = \psi_{j+1}(u)$, où (e_1, e_2) est la base canonique de \mathbb{C}^2 . Le long d'un chemin régulier de contrôle C^2 , noté $(\gamma(\tau))_{\tau \in [0,1]}$ dans V , nous définissons le *Hamiltonien effectif* pour tout $\tau \in [0, 1]$, par

$$H_{\text{eff}}(\gamma(\tau)) = h(\gamma(\tau)) - i\epsilon \begin{pmatrix} 0 & \langle \dot{\psi}_j(\gamma(\tau)), \psi_{j+1}(\gamma(\tau)) \rangle \\ \langle \dot{\psi}_{j+1}(\gamma(\tau)), \psi_j(\gamma(\tau)) \rangle & 0 \end{pmatrix}, \quad (1.3)$$

où, pour tout $u \in V$, $h(u) = I^{-1}(u)H(u)I(u)$ est une matrice hermitienne de dimension 2, C^2 en $u \in V$, et $\dot{\psi}_q(\gamma(\tau))$, $q \in \{j, j+1\}$ est la dérivée de ψ_q le long du chemin γ . En notant le propagateur associé à $H_{\text{eff}}(\gamma(\tau))$ par $U_{\text{eff}}^\epsilon(\tau)$, le théorème 1.1.1 prouve que :

$$\|(U^\epsilon(\tau) - I(\gamma(\tau))U_{\text{eff}}^\epsilon(\tau)I^{-1}(\gamma(0)))P_{j,j+1}(0)\| \leq C\epsilon, \quad (1.4)$$

pour tout $\tau \in [0, 1]$.

Une propriété importante obtenue en négligeant le second terme de H_{eff} par une procédure classique de moyennisation (voir le théorème 4.6.4 prouvé dans le chapitre 4 pour

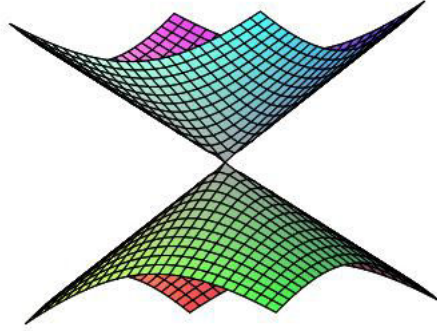


FIGURE 1.1 – Deux valeurs propres de $H(u)$ au voisinage d’une intersection conique, tracées en fonction de $u \in \mathbb{R}^k$ avec $k = 2$.

plus de précisions), est la suivante, qui est vérifiée sous des hypothèses convenables sur les valeurs propres de H , qui sont celles de h , et des vecteurs propres de H , qui sont ceux de h , modulo la transformation I unitaire. Pour un chemin de contrôle régulier $\gamma : [0, 1] \rightarrow V$ et $\tilde{\psi}_0 \in \mathbb{C}^2$, les solutions ψ et $\tilde{\psi}$ de, respectivement, $i \frac{d\psi}{dt} = H(\gamma(\epsilon t))\psi$, $\psi(0) = I(\gamma(0))\tilde{\psi}_0$, et $i \frac{d\tilde{\psi}}{dt} = h(\gamma(\epsilon t))\tilde{\psi}$, $\tilde{\psi}(0) = \tilde{\psi}_0$ sont telles que $\psi(1/\epsilon)$ est $O(\epsilon^\alpha)$ près de $I(\gamma(1))\tilde{\psi}(1/\epsilon)$. La valeur de $\alpha \in \mathbb{R}$ est positive et dépend de l’ordre du gap entre les valeurs propres λ_j et λ_{j+1} de H le long de γ , c’est à dire de la quantité $\lambda_{j+1} - \lambda_j$ et de ses dérivées (voir le théorème 4.6.4).

Cette approximation est intéressante car elle préserve la structure adiabatique des Hamiltoniens, ceci étant important pour obtenir des estimations uniformes de la dynamique le long de tout chemin de contrôle suffisamment régulier dans V . En outre, la connaissance de h nous donne toute l’information requise à propos de la régularité locale des valeurs propres et vecteurs propres de H . Remarquons que h , appelé *Hamiltonien réduit* dépend du choix de la base de $\pi_{H(u)} = \text{Im}P_{j,j+1}(u)$, pour $u \in V$. Cependant, nous verrons en Section 4.6.3 que les propriétés géométriques et par conséquent les propriétés dynamiques de l’équation de Schrödinger qui nous intéressent sont invariantes par un tel changement de base. Nous avons prouvé en Section 4.6.2 que lorsque \mathcal{H} est de dimension finie, des propriétés génériques sur h et ses jets jusqu’à l’ordre 2 fournissent des propriétés génériques sur le Hamiltonien H et ses jets jusqu’à l’ordre 2.

Intersections coniques Une *intersection conique* (aussi appelée point diabolique) est une singularité de type cône du spectre de $H(u)$, vu comme une fonction du contrôle $u \in \mathbb{R}^k$. (voir la figure 1.1)

Les intersections coniques sont génériques au sens où elles sont les singularités les moins dégénérées du spectre d'un Hamiltonien. Elles ont été étudiées depuis les débuts de la théorie de la mécanique quantique [82]. Elles jouent un rôle important dans le contexte de l'analyse semi-classique [32, 33]. Les chemins adiabatiques passant à travers les intersections coniques peuvent être utilisés pour induire des superpositions d'états propres, comme montré dans [22, 46], ainsi que pour obtenir des tests pour la contrôlabilité exacte lorsque \mathcal{H} est de dimension finie et de contrôlabilité approchée lorsque \mathcal{H} est de dimension infinie [19]. Pour une large classe de systèmes, elles sont génériques et structurellement stables, au sens où elles ne peuvent pas être effacées par de petites perturbations du Hamiltonien.

Soit U un ouvert connexe de \mathbb{R}^2 . Par un léger abus de notations, pour $u \in \mathbb{R}^2$, désignons les composantes de u par (u, v) . Supposons que $H(u, v) = H_0 + uH_1 + vH_2$ où H_0, H_1, H_2 sont des opérateurs essentiellement auto-adjoints sur \mathcal{H} ayant un domaine dense commun \mathcal{D} telles que les conditions suivantes, que nous appellons (\mathcal{R}) sont satisfaites :

- H_0 a un spectre discret ;
- H_1, H_2 sont bornés ;
- Il existe une base orthonormal $(b_j)_j$ de l'espace de Hilbert \mathcal{H} tel que $\langle b_j, H_0 b_q \rangle, \langle b_j, H_1 b_q \rangle, \langle b_j, H_2 b_q \rangle$ sont réels pour tout j, q .

Sous ces hypothèses, on dit que $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ est une intersection conique entre les valeurs propres λ_j et λ_{j+1} si $\lambda_j(\bar{u}, \bar{v}) = \lambda_{j+1}(\bar{u}, \bar{v})$ a une multiplicité égale à 2 et il existe $C > 0$ tel que pour tout vecteur unitaire $\eta \in \mathbb{R}^2$ et $t > 0$ assez petit, $\lambda_{j+1}((\bar{u}, \bar{v}) + t\eta) - \lambda_j((\bar{u}, \bar{v}) + t\eta) > Ct$.

Soit $(\gamma(t))_{t \in [0,1]} = (u(t), v(t))_{t \in [0,1]}$ un chemin régulier de contrôle C^3 dans \mathbb{R}^2 . Considérons l'équation

$$i \frac{d\psi(t)}{dt} = H(\gamma(\epsilon t))\psi(t), \quad (1.5)$$

où $\psi(t) \in \mathcal{H}$. Supposons que H a une intersection conique en $(0, 0)$. Supposons $\gamma(t_0) = (0, 0)$ pour un $t_0 \in (0, 1)$, $\gamma(t) \neq 0$ pour tout $t \neq t_0$. Considérons une solution ψ_ϵ de l'équation (1.5) telle que $\psi_\epsilon(0) = \phi_j(\gamma(0))$. Alors

$$\left\| \psi_\epsilon\left(\frac{1}{\epsilon}\right) - e^{i\theta} \phi_{j+1}(\gamma(1)) \right\| = O(\epsilon^{1/2}), \quad (1.6)$$

où $\theta \in \mathbb{R}$ dépend possiblement de ϵ . Nous pouvons alors implémenter une stratégie pour effectuer des transitions d'états passant au travers des intersections coniques, comme exposé dans [22] (see Figure 1.2).

Nous nous intéressons à la notion suivante de contrôlabilité. On dit que l'équation (1.5) est *contrôlable de façon approchée* si pour tout $\epsilon > 0$ et $\psi_1 \in \mathcal{H}$, il existe un contrôle $\gamma(\cdot) = (u(\cdot), v(\cdot)) : [0, T] \rightarrow U$ tel que la solution de l'équation (1.5) avec condition initiale $\psi(0) = \psi_0$ satisfait $\|\psi(T) - \psi_1\| < \epsilon$. On dit que le spectre $\sigma(\cdot)$ de $H(\cdot)$ est *coniquement connexe* si toutes les intersections de valeurs propres sont coniques et si pour

1.2. Thèmes d'études

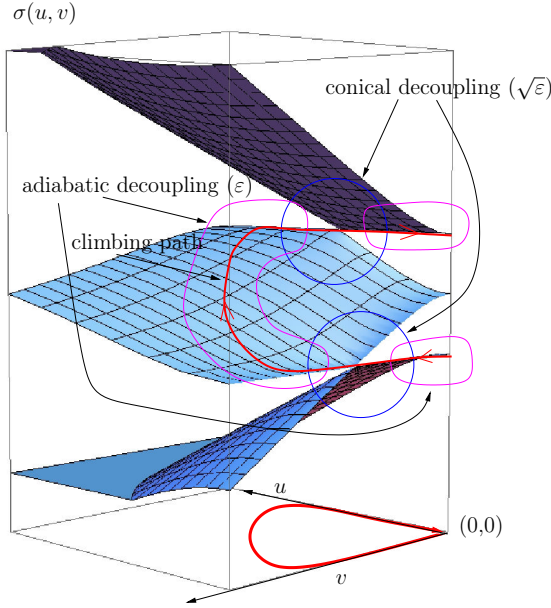


FIGURE 1.2 – Chemin de transition à la vitesse ϵ when $k = 2$.

tout j , il existe une intersection conique (\bar{u}_j, \bar{v}_j) entre les valeurs propres λ_j, λ_{j+1} , avec $\lambda_l(\bar{u}_j, \bar{v}_j)$ simple si $l \neq j, j + 1$. Nous avons les résultats généraux suivants.

Theorem 1.1.2 ([19]). *Supposons que le spectre de $H(\cdot)$ est coniquement connexe. Alors l'équation (1.5) est contrôlable de façon approchée.*

Theorem 1.1.3 ([19]). *Supposons que \mathcal{H} est de dimension finie. Supposons de plus que le spectre de $H(\cdot)$ est coniquement connexe. Alors l'équation (1.5) est contrôlable de façon exacte.*

Proposition 1.1.4 (Genericité). *Soit H_0 une matrice symétrique réelle de dimension n . Alors, génériquement par rapport à (H_1, H_2) dans l'espace des matrices symétriques réelles de dimension n , les intersections de valeurs propres de $H_0 + uH_1 + vH_2$ sont coniques.*

Certains résultats de généricité lorsque \mathcal{H} est de dimension infinie ont été prouvés dans [31, 22], dans le cas de potentiels réels contrôlés.

1.2 Thèmes d'études

Notre but est de continuer à explorer les liens entre les singularités du spectre des Hamiltoniens, la géométrie des espaces propres et les propriétés de contrôlabilité du système quantique associé. En particulier, comme annoncé précédemment, nous étudions le problème du contrôle des familles paramétrées de systèmes quantiques avec une entrée de contrôle commune. C'est une tâche importante pour de nombreuses applications en

contrôle quantique (voir [39] et ses références), notamment en résonance magnétique nucléaire [40]. Ce problème de contrôlabilité d'ensemble a été formulé mathématiquement par Li et Khaneja dans [63] et par Beauchard, Coron et Rouchon dans [13]. Les résultats pour le contrôle d'ensemble au-delà du cadre de contrôle quantique peuvent être trouvés dans [4, 50, 64, 72].

1.2.1 Contrôle d'ensemble avec deux contrôles réels

Pour un système quantique fermé général soumis à l'action d'un contrôle $u \in \mathbb{R}^m$ et dépendant d'un paramètre z , l'équation contrôlée associée est de la forme

$$i \frac{d\psi}{dt}(t) = H(u(t), z)\psi(t), \quad \psi(t) \in \mathcal{H}, \quad (1.7)$$

où $H(u, z)$ est essentiellement auto-adjoint sur l'espace de Hilbert \mathcal{H} pour toute valeur de u et z . Le paramètre z peut être utilisé soit pour décrire une famille de systèmes physiques sur lesquels agit un champ commun u ou bien un système physique pour lequel la valeur d'un des paramètres n'est pas connue précisément.

Les propriétés de contrôlabilité de systèmes de cette forme ont été étudiées à la fois pour des ensembles de paramètres discrets et continus. Le cas d'un ensemble fini de systèmes est caractérisé dans [14, 35]. Dans [29] la stabilisation asymptotique d'ensemble est étudiée pour des ensembles de paramètres dénombrables. Dans [63], [13] une preuve d'une forte notion de contrôlabilité d'ensemble a été obtenue pour un système à deux niveaux. Le contrôle d'ensemble numérique dans le cas d'un continuum de paramètres a fait l'objet d'études approfondies pour les systèmes à deux niveaux [79, 28, 75]. Notre but est de généraliser les théorèmes 2.1.2 et 2.1.3 à la question du contrôle d'ensemble.

Nous limitons notre étude au problème de la contrôlabilité d'ensemble approchée entre états propres. Sauf lorsque explicitement mentionné, nous étudierons les systèmes quantiques réels de dimension finie, c'est-à-dire les systèmes dont le Hamiltonien appartient à l'ensemble $S_n(\mathbb{R})$ des matrices réelles symétriques de dimension n . Cependant, les résultats principaux de contrôlabilité restent valides lorsque $H(u, v) = H_0 + uH_1 + vH_2$ où H_0, H_1, H_2 sont essentiellement auto-adjoints sur \mathcal{H} avec un domaine dense commun, et satisfont la condition (\mathcal{R}) , $(u, v) \in U$, où U est un ouvert connexe de \mathbb{R}^2 , et une adaptation de ces conditions au cas paramétrique (voir le chapitre 2.2.1).

Notations

- Soit $H \in C^k(U, S_n(\mathbb{R}))$. Pour $u \in U$, désignons le spectre de $H(u)$ by $(\lambda_j(u))_{j=1}^n$, où $j \mapsto \lambda_j(u)$ est la suite des valeurs propres de $H(u)$ dans l'ordre croissant, répétées selon leur multiplicités. Définissons $(\phi_1(u), \dots, \phi_n(u))$ une base orthonormale des vecteurs propres associés.

1.2. Thèmes d'études

- Soit $H \in C^k(U \times [z_0, z_1]), S_n(\mathbb{R})$. Pour $u \in U$, et $z \in [z_0, z_1]$, désignons le spectre de $H(u, z)$ par $(\lambda_j(u, z))_{j=1}^n$, où $j \mapsto \lambda_j(u, z)$ est la suite des valeurs propres de $H(u, z)$ dans l'ordre croissant, répétées selon leur multiplicités. Définissons $(\phi_1^z(u), \dots, \phi_n^z(u))$ une base orthonormale des vecteurs propres associés.

Definition 1.2.1. *Le système (1.7) est dit ensemble contrôlable de façon approchée entre les vecteurs propres si pour tout $\epsilon > 0$, $j, k \in \{1, \dots, n\}$, et $u_0, u_1 \in U$ tels que $\lambda_j(u_0, z)$ et $\lambda_k(u_0, z)$ sont simples pour tout $z \in [z_0, z_1]$, il existe un contrôle $u(\cdot) : [0, T] \rightarrow U$ tel que pour tout $z \in [z_0, z_1]$ la solution de (1.7) de condition initiale $\psi^z(0) = \phi_j^z(u_0)$ satisfait $\|\psi^z(T) - e^{i\theta} \phi_k^z(u_1)\| < \epsilon$, avec $\theta \in \mathbb{R}$ (possiblement dépendant de z et ϵ).*

En factorisant la dynamique par la trace, le Hamiltonien h défini en Section 1.1 peut être réduit à un Hamiltonien de trace nulle (à une phase globale près dans la dynamique). Dans le cas $k = 2$, on peut supposer sans perte de généralité que pour tout $(u, v) \in \mathbb{R}^2$ dans un voisinage de $(0, 0)$, $h(u, v) = H_f(u, v)$, où H_f est défini par

$$H_f(u, v) = \begin{pmatrix} f_1(u, v) & f_2(u, v) \\ f_2(u, v) & -f_1(u, v) \end{pmatrix},$$

avec $f = (f_1, f_1) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. Dans le cas paramétrique, pour tout $(u, v, z) \in \mathbb{R}^3$ au voisinage de $(0, 0, 0)$, on peut supposer $h(u, v, z) = H_f(u, v, z)$, où H_f est défini par

$$H_f(u, v, z) = \begin{pmatrix} f_1(u, v, z) & f_2(u, v, z) \\ f_2(u, v, z) & -f_1(u, v, z) \end{pmatrix},$$

avec $f = (f_1, f_1) \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. Des intersections de valeurs propres transverses dans toutes les directions de \mathbb{R}^2 et tangentes dans une direction spécifique, appelée la *direction non conique*, apparaissent génériquement. Celles-ci sont appelées *intersections semi-coniques* (see Figure 2.3), et sont définies rigoureusement en Section 4.2.1. Nous allons étudier des formes normales pour ce cas générique.

Formes normales

Transformations admissibles de systèmes à deux niveaux Nous définissons les transformations admissibles qui nous permettent d'obtenir des formes normales pour les Hamiltoniens H_f . Considérons l'équation de Schrödinger, définie pour $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ par

$$i \frac{d\psi(t)}{dt} = H_f(u(t), v(t))\psi(t), \tag{1.8}$$

où $\psi(t) \in \mathbb{C}^2$, et l'équation de Schrödinger d'ensemble, définie pour $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ par

$$i \frac{d\psi(t)}{dt} = H_f(u(t), v(t), z)\psi(t), \tag{1.9}$$

où $\psi(t) \in \mathbb{C}^2$. Les fonctions de contrôle u, v sont dans $L^\infty(\mathbb{R}, \mathbb{R})$ et le paramètre z appartient à $[z_0, z_1]$ où $z_0, z_1 \in \mathbb{R}$.

Les trois transformations correspondent aux représentations équivalentes des systèmes dynamiques (1.8) et (1.9) respectivement, par la reparamétrisation temporelle, par difféomorphisme de l'espace des états, et des transformations difféomorphes indépendantes de l'espace des contrôles et de l'espace du paramètre z .

Definition 1.2.2. On dit que f et \tilde{f} dans $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ sont équivalentes en 0 s'il existe $(\phi, \theta, \xi) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2) \times [-\pi, \pi] \times C^\infty(\mathbb{R}^2, \mathbb{R} \setminus \{0\})$ où ϕ est un difféomorphisme satisfaisant $\phi(0) = 0$, et $\zeta = \pm 1$, tel que pour tout (u, v) dans un voisinage de 0,

$$\begin{cases} \tilde{f}_1(u, v) = \xi(u, v)(\cos(2\theta)f_1 \circ \phi(u, v) - \zeta \sin(2\theta)f_2 \circ \phi(u, v)), \\ \tilde{f}_2(u, v) = \xi(u, v)(\sin(2\theta)f_1 \circ \phi(u, v) + \zeta \cos(2\theta)f_2 \circ \phi(u, v)). \end{cases}$$

Definition 1.2.3. On dit que f et \tilde{f} dans $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ sont équivalentes en 0 s'il existe $(\phi, \theta, \xi) \in C^\infty(\mathbb{R}^3, \mathbb{R}^3) \times [-\pi, \pi] \times C^\infty(\mathbb{R}^2, \mathbb{R} \setminus \{0\})$ où ϕ est un difféomorphisme de la forme $\phi : (u, v, z) \mapsto (\phi_1(u, v), \phi_2(u, v), \phi_3(z))$, où $\phi_1, \phi_2 \in C^\infty(\mathbb{R}^2, \mathbb{R})$ et $\phi_3 \in C^\infty(\mathbb{R}, \mathbb{R})$, satisfait $\phi(0) = 0$, et $\zeta = \pm 1$, tel que pour tout (u, v, z) dans un voisinage de 0,

$$\begin{cases} \tilde{f}_1(u, v, z) = \xi(u, v)(\cos(2\theta)f_1 \circ \phi(u, v, z) - \zeta \sin(2\theta)f_2 \circ \phi(u, v, z)), \\ \tilde{f}_2(u, v, z) = \xi(u, v)(\sin(2\theta)f_1 \circ \phi(u, v, z) + \zeta \cos(2\theta)f_2 \circ \phi(u, v, z)). \end{cases}$$

Ceci permet de classifier les comportements génériques des systèmes quantiques par rapport à (u, v) .

Cas non-paramétrique Considérons $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. Alors H_f a une intersection conique en $(0, 0)$ si et seulement si f est équivalent à $(u, v) \mapsto \begin{pmatrix} u & v \\ v & -u \end{pmatrix}$. Un Hamiltonien générique n'admet que des singularités coniques.

On dit que H_f a une *intersection semi-conique* (voir Figure 2.3) en $(0, 0)$ si et seulement si f est équivalent à $(u, v) \mapsto \begin{pmatrix} h(u)u \\ u + v^2 \end{pmatrix}$ où $h : \mathbb{R} \rightarrow \mathbb{R}$ est une fonction lisse satisfaisant $h(0) = 1$. Les intersections semi-coniques ne sont pas génériques pour $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, cependant, nous allons voir qu'elles peuvent apparaître en des points isolés lorsque l'on considère le cas paramétrique. Le Hamiltonien correspondant $\begin{pmatrix} h(u)u & u + v^2 \\ u + v^2 & -h(u)u \end{pmatrix}$ est tel que ses valeurs propres sont tangentes le long d'un chemin de contrôle tangent à $e_2 = (0, 1)$, c'est à dire à la direction non-conique en $(0, 0)$, alors qu'elles sont transverses dans toutes les autres directions.

Nous classifions maintenant les comportements génériques des systèmes quantiques par rapport à (u, v, z) .

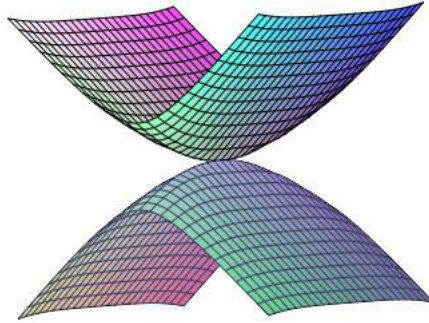


FIGURE 1.3 – Les deux valeurs propres de $H_f(u, v)$ au voisinage d'une intersection semi-conique, tracées en fonction of (u, v) .

Cas paramétrique Nous définissons les intersections F-coniques et F-semi-coniques, qui sont les deux cas génériques pour les Hamiltoniens paramétriques. Ils correspondent, pour $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$, au cas où $H_f(\cdot, 0)$ a une intersection conique ou semi-conique, combiné à des hypothèses additionnelles de régularité en le paramètre z .

Soit $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$.

- On dit que 0 est *F-conical* pour f si et seulement si il existe $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R})$ satisfaisant $h_1(0) = h_2(0) = 1$, tels que f est équivalente à

$$(u, v, z) \mapsto \begin{pmatrix} h_1(u, v, z)(z - u) \\ h_2(u, v, z)(z - v) \end{pmatrix};$$

- On dit que 0 est *F-semi-conique* pour $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ si et seulement si il existe $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ satisfaisant $h_1(0) = h_2(0) = 1$ et $m \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfaisant $m(0) \notin \{-1, 0\}$ tel que f est équivalent à

$$(u, v, z) \mapsto \begin{pmatrix} h_1(u, v, z)(z - m(u)u) \\ h_2(u, v, z)(z + u + v^2) \end{pmatrix}.$$

Systèmes à n -niveaux Soit $H \in C^\infty(\mathbb{R}^2, S_n(\mathbb{R}))$. On prouve que H a une intersection conique en $(0, 0)$ entre les niveaux λ_j et λ_{j+1} si et seulement si il existe un Hamiltonien réduit h de H localement en $(0, 0)$ ayant une intersection conique en $(0, 0)$. Par conséquent, il est cohérent de donner la définition suivante d'intersection semi-conique pour H .

Definition 1.2.4. On dit que H a une intersection semi-conique en $(0, 0)$ entre les niveaux λ_j et λ_{j+1} s'il existe un Hamiltonien réduit h de H ayant une intersection semi-conique en $(0, 0)$.

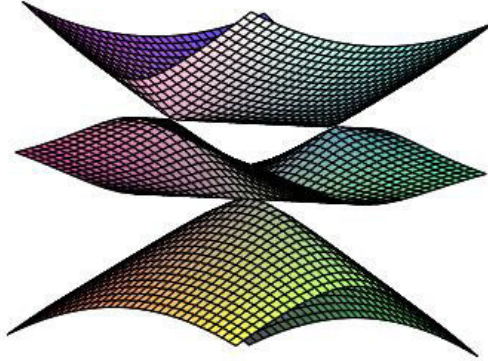


FIGURE 1.4 – Intersection semi-conique pour un processus STIRAP dégénéré

Nous prouvons en Section 4.6.3 que ces propriétés ne dépendent pas de l'application unitaire $I(u, v)$, pour (u, v) dans un voisinage de $(0, 0)$, utilisé pour le découplage adiabatique comme en Section 2.1 de l'introduction.

Dans le cas paramétrique, on dit que H a une intersection F-conique (respectivement, F-semi-conique) en $(0, 0, 0)$ s'il existe un Hamiltonien réduit h of H ayant une intersection F-conique (respectivement, F-semi-conique) en $(0, 0, 0)$. En Section 4.6.3, on montre que, generiquement par rapport à $H \in C^\infty(\mathbb{R}^3, S_n(\mathbb{R}))$, une intersection de valeur propre $(u, v, z) \in \mathbb{R}^3$ de H est soit F-conique soit F-semi-conique.

Les intersections semi-coniques apparaissent notamment lorsque, pour $(u, v) \in \mathbb{R}^2$,

$$H(u, v) = \begin{pmatrix} E & u & 0 \\ u & E & v \\ 0 & v & E' \end{pmatrix}, \text{ avec } E < E', \text{ cas que nous appelons } \textit{STIRAP dégénéré}.$$

Sur la Figure 2.4, nous avons tracé le spectre de $H(u, v)$ en fonction de (u, v) pour un Hamiltonien de ce type. Nous remarquons la présence d'une intersection semi-conique entre les deux niveaux les plus bas et deux intersections coniques entre les deux niveaux les plus hauts.

Propriétés dynamiques aux intersections semi-coniques Grâce aux formes normales, nous pouvons estimer l'approximation adiabatique pour des systèmes à n -niveaux. Soit $H \in C^\infty(\mathbb{R}^2, S_n(\mathbb{R}))$, ayant une intersection semi-conique en $(0, 0)$. Désignons par η la direction non-conique.. Soit $(\gamma(t))_{t \in [0,1]} = (u(t), v(t))_{t \in [0,1]}$ un chemin de contrôle régulier lisse de \mathbb{R}^2 tel que $\gamma(t_0) = (0, 0)$ pour $t_0 \in (0, 1)$, $\gamma(t) \neq 0$ pour tout $t \neq t_0$, et γ est tangent à η en $t = t_0$. Considérons une solution ψ_ϵ de l'équation

$$i \frac{d\psi(t)}{dt} = H(u(\epsilon t), v(\epsilon t))\psi(t), \quad (1.10)$$

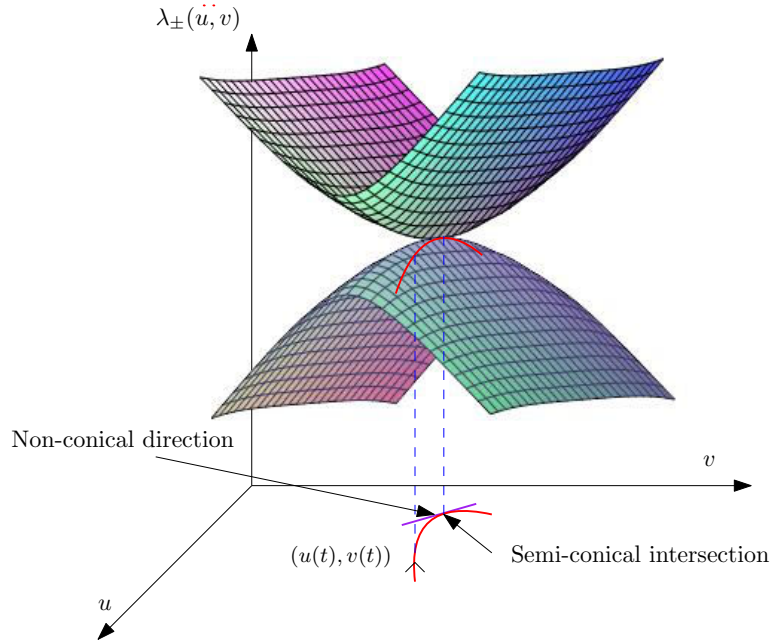


FIGURE 1.5 – Chemin de contrôle passant à travers la singularité dans la direction non-conique.

où $\psi(t) \in \mathbb{C}^n$, tel que $\psi_\epsilon(0) = \phi_j(\gamma(0))$. Alors $\|\psi_\epsilon(\frac{1}{\epsilon}) - e^{i\theta}\phi_j(\gamma(1))\| = O(\epsilon^{1/3})$, où $\theta \in \mathbb{R}$ est possiblement dépendant de ϵ (voir Figure 1.5 pour une représentation graphique du chemin de contrôle passant à travers la singularité dans la direction non-conique).

Lorsque la conicité est préservée quand le paramètre z varie

Dans le chapitre 3 nous proposons un cadre pour le contrôle adiabatique d'ensemble d'un continuum de systèmes à n -niveaux avec un Hamiltonien réel, pilotés par deux contrôles et ayant des intersections coniques entre les valeurs propres. L'idée principale est que, si un système correspondant à un paramètre fixe a des intersections coniques entre deux valeurs propres, alors une petite perturbation du paramètre donne une courbe d'intersections coniques, chaque point de la courbe correspondant exactement à une valeur du paramètre. On peut alors suivre adiabatement de telles courbes dans l'espace de contrôle et obtenir un transfert de population entre les deux niveaux pour l'ensemble des systèmes. Ce résultat a été écrit sans recourir aux formes normales en raison de l'estimation déjà bien connue de la dynamique adiabatique aux intersections coniques dans la littérature. Cependant, le même résultat peut aussi être déduit de l'étude locale des formes normales.

Soit U un ouvert connexe de \mathbb{R}^2 . Pour $j \in \{1 \dots n\}$, désignons par γ_j l'ensemble $\{(u, v, z) \in U \times [z_0, z_1] \mid \lambda_j(u, v, z) = \lambda_{j+1}(u, v, z)\}$, où par convention $\gamma_0 = \gamma_n = \emptyset$.

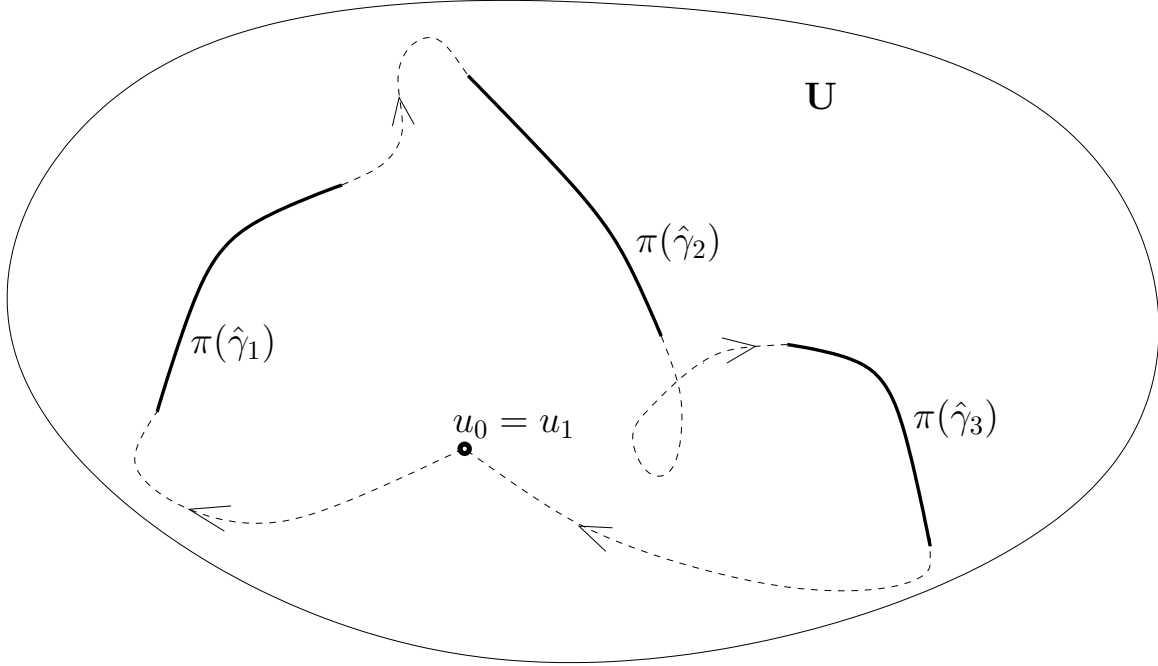


FIGURE 1.6 – Un contrôle réalisant une transition d'ensemble entre $\phi_1^z(u_0, v_0)$ et $\phi_4^z(u_0, v_0)$.

Notons la projection de $(u, v, z) \in \mathbb{R}^3$ sur la composante (u, v) par π .

ASSUMPTION A_j . Il existe une composante connexe $\hat{\gamma}_j$ de γ_j et une application $\beta_j : [z_0, z_1] \rightarrow U$ telle que β_j est un plongement C^3 et

- $\pi(\hat{\gamma}_j)$ est inclus dans $U \times [z_0, z_1] \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_{j+1}))$;
- $\pi(\hat{\gamma}_j) = \beta_j([z_0, z_1])$;
- Pour tout $z \in [z_0, z_1]$, $\lambda_j(\cdot, z)$ et $\lambda_{j+1}(\cdot, z)$ ont une unique intersection dans $\pi(\hat{\gamma}_j)$, qui est conique et a lieu en $\beta_j(z)$.

En outre, l'ensemble $U \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_j) \cup \pi(\gamma_{j+1}))$ est connexe par arcs.

Remarquons que les secondes et troisièmes conditions sont équivalentes à dire que les courbes $\hat{\gamma}_j$ formées que d'intersections F-coniques et que $\pi(\hat{\gamma}_j)$ est une courbe plongée dans \mathbb{R}^2 sans auto-intersection. Le résultat qui suit est le résultat principal de l'article [10] et du chapitre 3.

Theorem 1.2.5. *Considérons une application C^3 , $U \times [z_0, z_1] \ni (u, v, z) \mapsto H(u, v, z) \in S_n(\mathbb{R})$. Supposons que Assumption A_j est satisfaite pour tout $j \in \{1 \dots n\}$. Alors l'équation $i \frac{d\psi}{dt} = H(u, v, z)\psi$ est ensemble contrôlable entre états propres de façon approchée.*

Méthode de contrôle Notre méthode de contrôle est présentée sur la figure 1.6, avec un chemin $(u(t), v(t))_{t \in [0,1]}$, parcouru à la vitesse ϵ . L'erreur dans le régime adiabatique est d'ordre $\sqrt{\epsilon}$.

Lorsque qu'une intersection semi-conique apparait quand le paramètre z varie

L'argument esquissé ci-dessus repose sur l'hypothèse que pour toutes les valeurs du paramètre, les intersections de valeurs propres restent coniques et décrivent une courbe lisse. Ces hypothèses sont satisfaites pour de petites perturbations génériques du paramètre. Pour de grandes perturbations génériques, il peut arriver que la conicité des intersections de valeurs propres soit perdue en des points isolés de la courbe. L'objectif est d'étendre l'analyse à ce cas.

Dans le cas où des intersections F-semi-coniques sont présentes sur γ_j , la question que l'on pose est celle de la validité de l'approximation adiabatique lorsque le chemin de contrôle passe par de tels points. En utilisant les formes normales, nous remarquons que $\pi(\hat{\gamma}_j)$ est tangent à la direction non-conique en une intersection F-semi-conique. Par conséquent, lorsqu'un chemin de contrôle suit $\pi(\hat{\gamma}_j)$, il passe dans l'intersection semi-conique pour $H(\cdot, z)$ dans la direction non-conique, et il n'y a alors pas de transition d'état pour le système de paramètre z . Cependant, nous montrons que sous l'hypothèse appelée Assumption \tilde{A}_j qui suit, l'approximation adiabatique est uniforme par rapport au paramètre $z \in [z_0, z_1]$ et le système est alors ensemble contrôlable entre les états propres de façon approchée. Dans ce cas, nous ne pouvons considérer un plongement de $[z_0, z_1]$ dans $\pi(\hat{\gamma}_j)$ puisque la même valeur du paramètre z correspond à différentes intersections de valeurs propres de $H(\cdot, z)$. C'est pourquoi nous faisons les hypothèses suivantes.

ASSUMPTION \tilde{A}_j . Il existe une composante connexe $\hat{\gamma}_j$ de γ_j telle que

- $\hat{\gamma}_j$ est une sous-variété de dimension 1 de \mathbb{R}^3 composée uniquement d'intersections F-coniques et F-semi-coniques.
- Il existe $(u_0, v_0) \in U$ et $(u_1, v_1) \in U$ tel que $(u_0, v_0, z_0), (u_1, v_1, z_1) \in \hat{\gamma}_j$ sont des intersections F-coniques pour H ;
- $\pi(\hat{\gamma}_j)$ est une courbe C^∞ plongée dans \mathbb{R}^2 sans auto-intersection, contenue dans $U \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_{j+1}))$.

En outre, l'ensemble $U \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_j) \cup \pi(\gamma_{j+1}))$ est connexe par arcs.

Theorem 1.2.6. *Considérons une application C^4 , $U \times [z_0, z_1] \ni (u, v, z) \mapsto H(u, v, z) \in S_n(\mathbb{R})$. Supposons que Assumption \tilde{A}_j est satisfaite pour tout $j \in \{1 \dots n\}$. Alors l'équation $i \frac{d\psi}{dt} = H(u, v, z)\psi$ est ensemble contrôlable entre les états propres de façon approchée.*

Méthode de contrôle Sur la figure 1.7, nous proposons un chemin de contrôle lisse (u, v) (voir Theorem 4.1.3 pour plus de précisions) réalisant des transitions entre les niveaux j et $j + 1$ uniformément par rapport au paramètre $z \in [z_0, z_1]$. Le chemin de contrôle (u, v) entre dans $\pi(\gamma)$ en un point (u_0, v_0) tel que (u_0, v_0, z_0) est une intersection de valeurs propres F-conique de $H(u, v, z_0)$ entre les niveaux j et $j + 1$, et quittant $\pi(\gamma)$ en un point (u_1, v_1) tel que (u_1, v_1, z_1) est une intersection F-conique de valeurs propres de $H(u, v, z_1)$ entre les niveaux j et $j+1$. De façon à garantir que les transitions sont effectuées

pour tout $z \in [z_0, z_1]$, le chemin de contrôle doit passer un nombre impair de fois à travers des intersections F-coniques de $H(u, v, z)$ entre les niveaux j et $j+1$, pour tout $z \in [z_0, z_1]$. En outre, l'uniformité de l'approximation adiabatique par rapport au paramètre z est assurée lorsque le chemin de contrôle est choisi de façon à avoir $z \in [z_0, z_1]$ pour tous z et t tels que $(u(t), v(t), z) \in \gamma$. L'erreur commise dans l'approximation adiabatique pour un tel chemin de contrôle parcouru à la vitesse ϵ est d'ordre $\epsilon^{\frac{1}{3}}$.

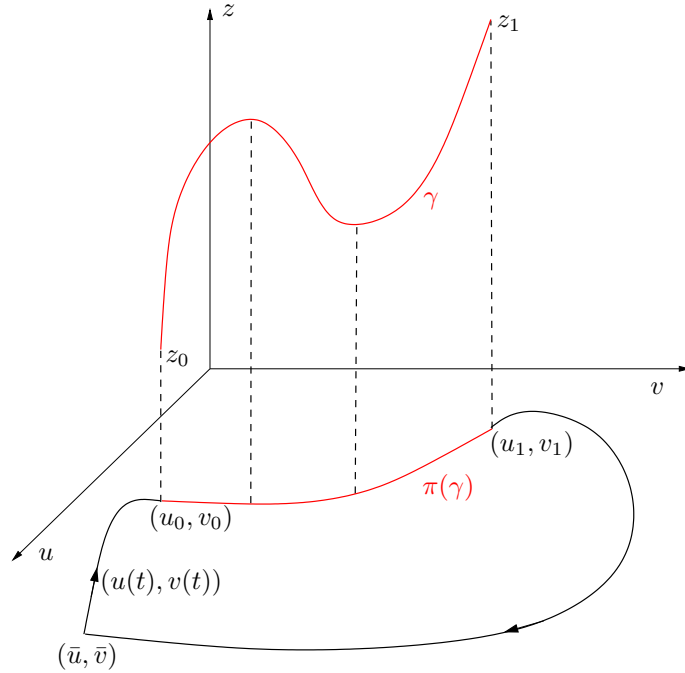


FIGURE 1.7 – Une courbe de contrôles (u, v) réalisant des transitions uniformes en $z \in [z_0, z_1]$ entre deux niveaux comportant des intersections F-semi-coniques

1.2.2 Classification des singularités du champ non-mixant

Pour un Hamiltonien H dépendant de deux contrôles, les courbes non-mixantes entre λ_{j-1} et λ_j pour $j \geq 2$ ont été définies dans [22] comme les courbes $\gamma = (\gamma(t))_{t \in [0,1]}$ de \mathbb{R}^2 le long desquelles $\dot{\phi}_{j-1}(\gamma(t))$ est orthogonal à $\phi_j(\gamma(t))$, pour tout $t \in [0, 1]$. Alors, par le théorème 1.1.1, la précision de l'approximation adiabatique suivant une telle courbe est améliorée. En particulier, l'erreur d'ordre $\sqrt{\epsilon}$ obtenue pour la dynamique de l'équation (??) pour un chemin de contrôle passant à travers une intersection conique devient d'ordre ϵ en suivant une courbe non-mixante. Cette propriété a été utilisée dans [22] pour un contrôle précis de l'équation de Schrödinger pour un Hamiltonien réel soumis à deux contrôles réels et une généralisation a été publiée dans [31] pour un Hamiltonien complexe soumis à trois contrôles réels.

1.2. Thèmes d'études

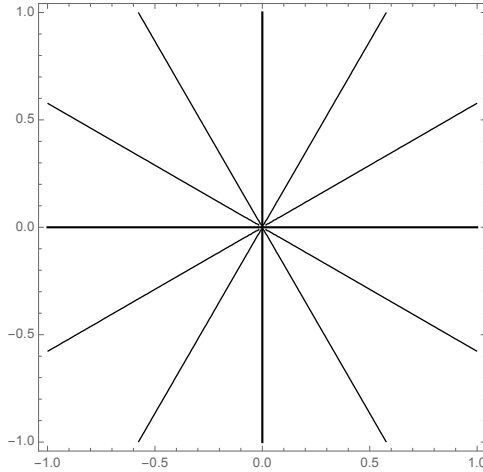


FIGURE 1.8 – Un noeud critique

Dans cette section, nous proposons d'étudier les singularités des courbes non-mixantes d'abord pour des systèmes à deux niveaux, puis pour des systèmes quantiques plus généraux.

Le champ non-mixant pour les systèmes à deux niveaux et ses singularités dans ce cas

Pour f dans $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, étudions la dynamique de

$$i \frac{d\psi_\epsilon(t)}{dt} = H_f(u(\epsilon t), v(\epsilon t))\psi_\epsilon(t), \quad \psi_\epsilon(0) = \tilde{\psi}_0 \in \mathbb{C}^2, \quad (1.11)$$

où $t \in [0, \frac{1}{\epsilon}]$ et $\tilde{\psi}_0$ est indépendant de ϵ .

Le long de γ , l'erreur commise dans le théorème adiabatique est nulle, c'est à dire que les courbes non-mixantes peuvent être suivies à une vitesse arbitraire, la dynamique suit de façon exacte l'évolution des vecteurs propres (à phase près) le long de γ , quelle que soit la vitesse de parcours. Nous montrons dans un premier temps que de telles courbes sont courbes intégrales d'un champ de vecteur lisse $\chi(f)$, qu'on appelle *champ non-mixant*.

Theorem 1.2.7. *Génériquement par rapport à $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, $\chi(f)$ a des singularités de trois types, à un changement de coordonnées C^∞ -difféomorphe de \mathbb{R}^2 dans \mathbb{R}^2 près :*

- *Des noeuds critiques (voir Figure 1.8) aux points d'intersections de valeurs propres de H_f (c'est à dire des zéros de f),*
- *Des selles et des centres aux points qui ne sont pas des intersections de valeurs propres de H_f .*

Une famille générique à un paramètre de Hamiltoniens peut être mise, au voisinage d'une intersection de valeurs propres, sous une des formes normales suivantes par une

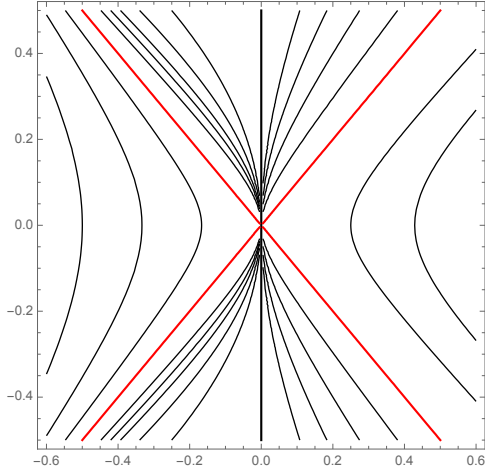


FIGURE 1.9 – Un exemple de singularité semi-conique hyperbolique. L'indice est 0. La direction non-conique est $(0, 1)$. Deux droites (en rouge) traversent la singularité dans la direction non-mixante

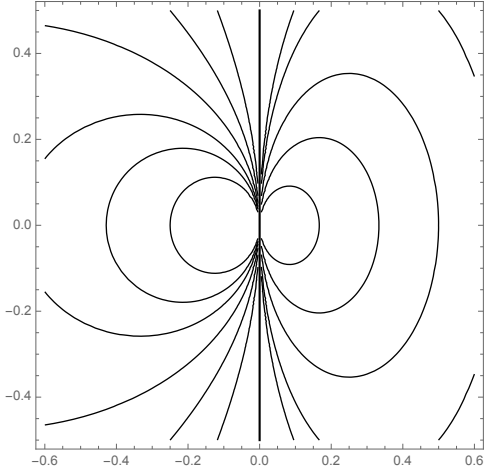


FIGURE 1.10 – Un exemple de singularité semi-conique elliptique. L'indice est 2. La direction non-conique est $(0, 1)$. Toute courbe non-mixante passe à la singularité dans la direction non-conique.

transformation admissible :

$$H(u, v, z) = \begin{pmatrix} h_1(u, v, z)(z - u) & h_2(u, v, z)(z - v) \\ h_2(u, v, z)(z - v) & -h_1(u, v, z)(z - u) \end{pmatrix},$$

ou

$$H(u, v, z) = \begin{pmatrix} h_1(u, v, z)(z - m(u)u) & h_2(u, v, z)(z + u + v^2) \\ h_2(u, v, z)(z + u + v^2) & -h_1(u, v, z)(z - m(u)u) \end{pmatrix},$$

où $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R})$ satisfont $h_1(0) = h_2(0) = 1$, et $m \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfait $m(0) \notin \{-1, 0\}$.

Cette propriété nous permet d'étudier les bifurcations des singularités du champ non-mixant données dans le théorème 1.2.7 lorsqu'un paramètre z varie. Pour tout $z \in \mathbb{R}$, soit $\chi_z(f)$ le champ non-mixant associé à $f(\cdot, \cdot, z) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$.

Theorem 1.2.8. *Génériquement par rapport à $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$, pour tout $z \in \mathbb{R}$, $\chi_z(f)$ possède les singularités suivantes à un changement de coordonnées C^∞ -diffeomorphe de \mathbb{R}^2 dans \mathbb{R}^2 près :*

- Des noeuds critiques aux points d'intersections de valeurs propres de H_f ,
- Des singularités semi-coniques elliptiques ou hyperboliques aux intersections semi-coniques de valeurs propres de H_f (voir le chapitre 5 Section 5.2.2 pour une définition précise, et les figures 5.3 et 5.2),
- Des selles, des centres ou des cusps aux points qui ne sont pas des intersections de valeurs propres de H_f .

Le champ non-mixant pour des systèmes plus généraux

Pour des systèmes de plus grande dimension, les courbes non-mixantes ont été étudiées dans [22]. Dans ce qui suit, nous considérons $H_0, H_1, H_2 \in S_n(\mathbb{R})$, et nous définissons $H(u, v) = H_0 + uH_1 + vH_2$. Dans ce cas, il a été montré dans [22] que les courbes non-mixantes sont les courbes intégrales d'un champ de direction sur \mathbb{R}^2 , défini par $\chi_{j-1,j}(u, v) = \begin{pmatrix} -\langle H_2\phi_{j-1}(u, v), \phi_j(u, v) \rangle \\ \langle H_1\phi_{j-1}(u, v), \phi_j(u, v) \rangle \end{pmatrix}$ où \langle, \rangle est le produit scalaire Euclidien sur \mathbb{R}^n .

Remarquons que $\chi_{j-1,j}$ est défini au signe près aux points $(u, v) \in \mathbb{R}^2$ tels que $\lambda_{j-1}(u, v) \neq \lambda_j(u, v)$. Le long de ces courbes, l'approximation adiabatique a une plus grande précision, c'est-à-dire que l'erreur est de l'ordre de ϵ le long d'un chemin de contrôle de vitesse ϵ , même quand la courbe passe par des intersections de valeurs propres. Contrairement à ce que l'on pourrait penser, les courbes non-mixantes d'un Hamiltonien de niveau n avec $n \geq 3$ ne correspondent pas localement à celles d'un Hamiltonien réduit de deux niveaux tel que défini dans Section 2.1. Il s'agit d'une structure plus complexe qui présente des propriétés topologiques intéressantes. En effet, nous allons voir que le champ non-mixant peut avoir à la fois des singularités d'indice entier qui sont génériques pour un champ de vecteurs de \mathbb{R}^2 et des singularités d'indice demi-entier qui sont génériques pour un champ de directions de \mathbb{R}^2 , alors que l'espace des champs de vecteurs et des champs de directions sont munis de topologies différentes, telles que les combinaisons de ces deux types de singularités semble à première vue être impossible génériquement. Ce type de structures a déjà été observé dans des cristaux liquides (voir [26] pour une revue générale de la théorie des cristaux liquides et la Figure 1.11 pour une illustration de telles singularités). D'autres recherches sur ce type de structures seront menées dans le cadre de travaux futurs. Notre but est de classifier les singularités du champ de direction $\chi_{j-1,j}$, nous avons d'abord besoin de rappeler quelques outils topologiques.

Propriétés des champs de directions Soit (M, g) une variété Riemannienne de dimension 2, et K un sous-ensemble fermé de M . Un champ de direction L sur M est une section de $PT(M \setminus K)$. L'ensemble K est l'ensemble singulier de L . Comme prouvé dans [21], tout champ de direction peut être obtenu par bisection angulaire (définie pour la métrique g) de deux champs de vecteurs X et Y sur M . Lorsqu'un champ de directions L est bisection de deux champs de vecteurs X et Y , on dit que L est défini comme un *proto champ de direction*. Les zéros de X et Y correspondent aux singularités de L . Avec cette définition, la topologie de Whitney sur les paires de champs de vecteurs sur M définissent une topologie sur les champs de directions sur M . Il a été prouvé dans [21] que génériquement, un proto champ de direction n'a que des singularités *Darbouxiennes*, c'est à dire que ses courbes intégrales sont localement homéomorphes à celles des proto

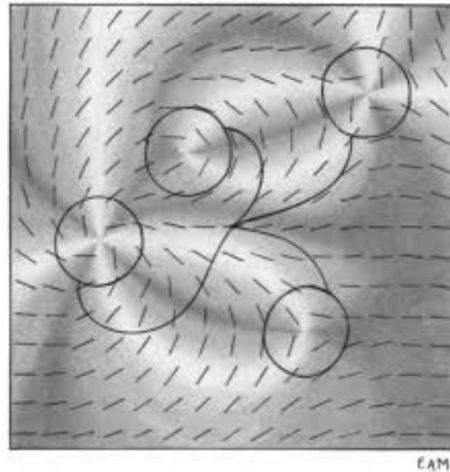


FIGURE 1.11 – Combinaison de singularités d’indice demi-entier et entier dans les cristaux liquides, image issue de [8]

champs de directions définis par (X_L, Y_L) , (X_M, Y_M) and (X_S, Y_S) comme suit :

- Le *Lemon proto champ de direction* (voit la figure 5.15) est la paire de champs de vecteurs sur $(\mathbb{R}^2, Eucl)$ définis par

$$X_L(x, y) = \begin{pmatrix} x + y \\ y - x \end{pmatrix}, \quad Y_L(x, y) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

- Le *Monstar proto champ de direction* (voir la figure 5.16) est la paire de champs de vecteurs sur $(\mathbb{R}^2, Eucl)$ définis par

$$X_M(x, y) = \begin{pmatrix} x \\ 3y \end{pmatrix}, \quad Y_M(x, y) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

- Le *Star proto champ de direction* (voir la figure 5.17) est la paire de champs de vecteurs sur $(\mathbb{R}^2, Eucl)$ définis par

$$X_S(x, y) = \begin{pmatrix} x \\ -y \end{pmatrix}, \quad Y_S(x, y) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

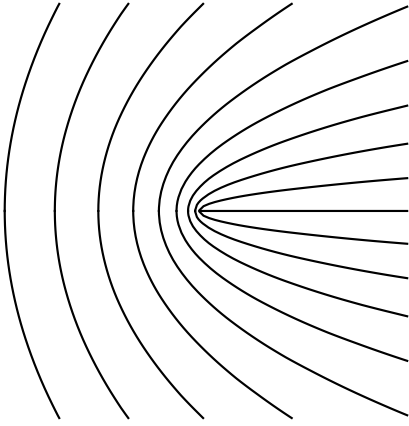


FIGURE 1.12 – La singularité Lemon, d'indice $\frac{1}{2}$.

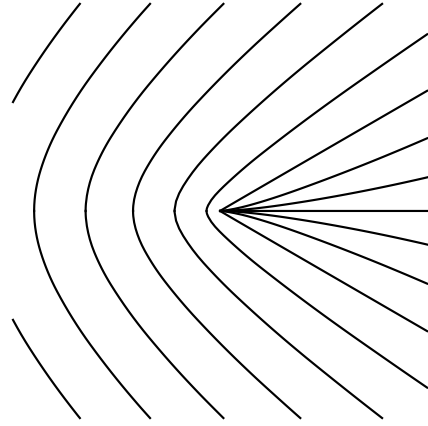


FIGURE 1.13 – La singularité Monster, d'indice $\frac{1}{2}$.

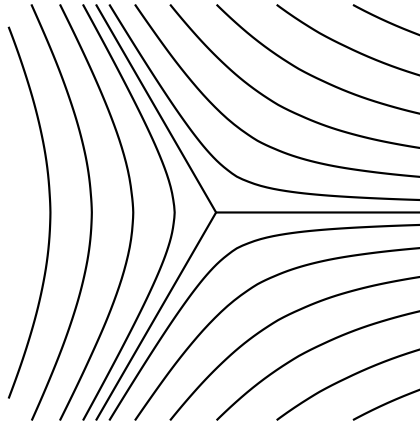


FIGURE 1.14 – La singularité Star, d'indice $-\frac{1}{2}$.

Courbes non-mixantes pour systèmes à n -niveaux aux intersections entre les niveaux $j-1$ et j Au voisinage d'une intersection conique $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ entre les niveaux $j-1$ et j ,

- Il existe un choix lisse du signe des vecteurs propres $\phi_{j-1}(u, v)$ et $\phi_j(u, v)$ tel que $\chi_{j-1,j}$ définit un champ de vecteur C^∞ dans un voisinage épointé de (\bar{u}, \bar{v}) ,
- Les courbes intégrales de $\chi_{j-1,j}$ sont C^∞ et les vecteurs propres ϕ_{j-1} et ϕ_j sont C^∞ le long de ces courbes,
- Pour toute direction η de \mathbb{R}^2 , il existe une courbe intégrale $\gamma : [0, 1] \rightarrow \mathbb{R}^2$ de $\chi_{j-1,j}$ telle que $\gamma(1) = (\bar{u}, \bar{v})$, $\lim_{t \rightarrow 1^-} \frac{\dot{\gamma}(t)}{\|\dot{\gamma}(t)\|} = \eta$.

Dans ce cas, on dit que $\chi_{j,j-1}$ a une singularité de type **(N)**.

Courbes non-mixantes pour systèmes à n -niveaux aux intersections entre les niveaux j et $j+1$ (respectivement $j-2$ et $j-1$) Pour compléter la classification

des singularités du champ non-mixant aux intersections de valeurs propres, nous nous concentrons maintenant sur les singularités de $\chi_{j-1,j}$ aux intersections coniques entre les niveaux j et $j + 1$.

Soit $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ une intersection conique entre λ_j et λ_{j+1} . On introduit la condition suivante :

Condition (C) : Les vecteurs $P_{j,j+1}H_1\phi_{j-1}(u, v)$ et $P_{j,j+1}H_2\phi_{j-1}(u, v)$ ne sont pas colinéaires.

Nous prouvons le théorème suivant.

Theorem 1.2.9. *Soit $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ tel que $\lambda_j(\bar{u}, \bar{v}) = \lambda_{j+1}(\bar{u}, \bar{v})$ est une intersection conique. Supposons que Condition (C) est satisfaite en (\bar{u}, \bar{v}) . Alors $\chi_{j-1,j}$ a une singularité Darbouxienne en (\bar{u}, \bar{v}) .*

Corollary 1.2.10. *Soit $E_1, E_2, E_3 \in \mathbb{R}$ tels que $E_1 < E_2 < E_3$ et $H(u, v) = \begin{pmatrix} E_1 & u & 0 \\ u & E_2 & v \\ 0 & v & E_3 \end{pmatrix}$.*

Alors $\chi_{1,2}$ (respectivement $\chi_{2,3}$) possède des singularités Darbouxiennes aux points $(u, v) \in \mathbb{R}^2$ tels que $\lambda_2(u, v) = \lambda_3(u, v)$ (respectivement, $\lambda_1(u, v) = \lambda_2(u, v)$) qui sont

$$(u, v) = (\pm\sqrt{(E_1 - E_3)(E_2 - E_3)}, 0) \text{ (respectivement } (\pm\sqrt{(E_1 - E_3)(E_1 - E_2)}, 0)).$$

Le tracé des courbes intégrales de $\chi_{1,2}$ est effectué en Figure 1.15. Nous remarquons qu'il y a une singularité de Type (N) aux intersections coniques entre λ_1 et λ_2 , alors qu'il y a des singularités Star aux intersections coniques entre λ_2 and λ_3 .

1.2.3 Vers le contrôle d'ensemble avec un seul contrôle

Un enjeu important du contrôle quantique est de concevoir des lois de contrôle explicites pour le problème de l'équation de Schrödinger bilinéaire avec un seul contrôle, à savoir

$$i \frac{d\psi}{dt} = (H_0 + uH_1) \psi \tag{1.12}$$

où ψ appartient à la sphère unité d'un espace de Hilbert \mathcal{H} , H_0 est un opérateur auto-adjoint représentant un terme de dérive appelé *Hamiltonien libre*, H_1 est un opérateur auto-adjoint représentant le couplage de contrôle et $u : [0, T] \rightarrow \mathbb{R}$, $T > 0$. D'importants résultats théoriques de contrôlabilité ont été prouvés avec différentes techniques (voir [7, 12, 17] et les références qui y figurent). mais les contrôles explicites sont souvent difficiles à calculer. Pour le problème avec deux entrées ou plus, les méthodes adiabatiques sont considérées aujourd'hui comme façon classique d'obtenir une expression explicite des contrôles et peuvent être utilisées sous des conditions géométriques sur le spectre du Hamiltonien contrôlé (voir les articles [10, 22, 62] et leurs références), et nos résultats sur ces méthodes sont présentés dans la section 2.2.1 de l'Introduction et sont développés

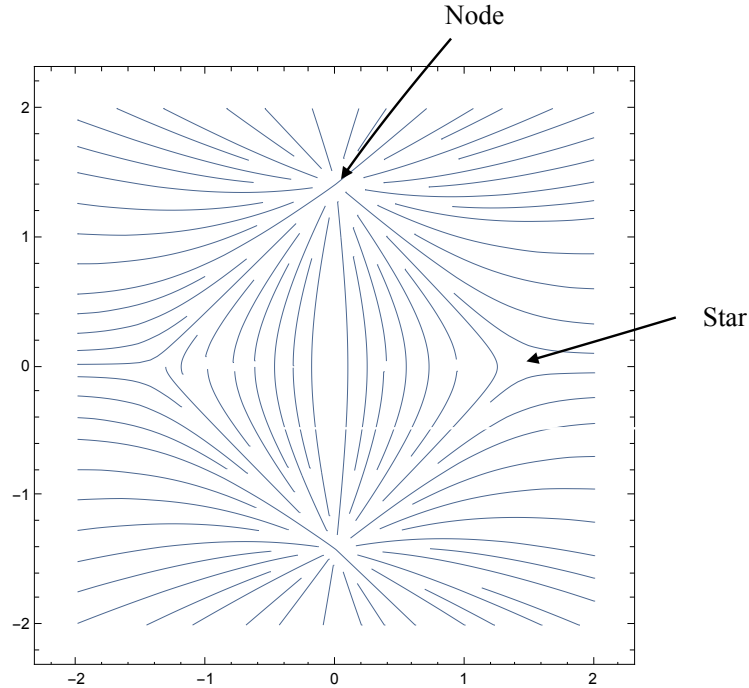


FIGURE 1.15 – Champ non-mixant entre λ_1 et λ_2 pour le STIRAP du Corollaire 1.2.10.

dans le Chapitre 3. Cependant, ces méthodes sont efficaces pour des systèmes ayant au moins eux contrôles et ne peuvent pas être appliquées au cas de l'équation (2.12). Notre objectif est alors d'étendre une équation de Schrödinger bilinéaire avec un seul contrôle en une équation de Schrödinger bilinéaire avec deux contrôles dans le même esprit que les extensions de Lie introduites par Sussmann et Liu dans [66] et [77], puis d'appliquer au système étendu les techniques adiabatiques connues. La première étape de cette procédure est l'approximation Rotating Wave (RWA, en abrégé), et est bien connue des physiciens. C'est une approximation de découplage qui permet de se débarrasser des termes très oscillants lorsque le système est commandé par un contrôle réel. Cette approximation est basée sur une procédure de moyennisation du premier ordre (voir [71, 77, 66, 23] pour plus d'informations sur la moyennisation des systèmes dynamiques). Cette approximation est connue pour bien fonctionner pour un faible désaccord par rapport à fréquence de résonance du système et une petite amplitude. Pour un récapitulatif de la RWA et de ses limites, voir [37] et [44, 45, 51]. Dans [24], un cadre mathématique a été établi pour les systèmes quantiques de dimension infinie, formalisant ce que les physiciens appellent *oscillations de Rabi généralisées* et montrant que la RWA est valide pour une large classe de systèmes quantiques. L'approximation adiabatique et la RWA impliquent des échelles de temps différentes, et il est naturel de se demander si elles peuvent ou non être utilisées en cascade. Le but du chapitre 2.2.3 est de montrer la validité d'une telle approximation

sous une certaine condition sur les échelles de temps impliquées dans la dynamique, en utilisant une procédure de calcul de moyennisation. Ensuite, les résultats bien connus de la théorie adiabatique (voir [22, 18, 78]) peuvent être appliqués afin d’obtenir des transitions entre les états propres du Hamiltonien libre H_0 . Cela nous amène à concevoir des lois de contrôle permettant l’inversion d’une particule Spin- $\frac{1}{2}$ et des transferts de population dans le processus STIRAP qui sont robustes par rapport aux inhomogénéités de l’amplitude de l’entrée de contrôle (voir [81, 10] et le chapitre 3). Comme conséquence de l’utilisation d’un contrôle oscillant avec un petit désaccord de fréquence, la méthode proposée n’est pas robuste par rapport aux inhomogénéités des fréquences de résonance, c’est-à-dire les inhomogénéités du terme de drift H_0 .

Pour de tels systèmes, lorsque \mathcal{H} est de dimension finie, nous proposons d’utiliser des contrôles sous la forme

$$u_\epsilon(t) = 2\epsilon^\alpha \sum_{(j,k) \in \{1 \dots N\}^2} v_{jk}(\epsilon^{\alpha+1}t) \cos(\beta_{jk}t + \frac{1}{\epsilon} \phi_{jk}(\epsilon^{\alpha+1}t)),$$

où, pour tous $j, k \in \{1 \dots N\}$, $v_{jk}, \phi_{jk} \in C^\infty([0, 1], \mathbb{R})$ tels que $\phi_{jk}(0) = 0$ et $\beta_{jk} \in \mathbb{R}$, $N \in \mathbb{N} \setminus \{0\}$, puis nous étudions le comportement asymptotique du système quantique associé (1.12) lorsque $\epsilon \rightarrow 0$ sur l’intervalle de temps $t \in [0, \frac{1}{\epsilon^{\alpha+1}}]$. En supposant $\alpha > 1$, par un bon choix de (v_{kj}, ϕ_{kj}) , et β_{kj} pour tous k, j , nous montrons un théorème général d’approximation (voir les théorèmes 6.1.3 et 6.2.11) qui permet de concevoir des lois de contrôle explicites qui sont robustes par rapport aux inhomogénéités de l’amplitude du contrôle. Ce résultat nous a permis de prouver les résultats suivants.

Soit U un intervalle ouvert de \mathbb{R} contenant 0.

Theorem 1.2.11. *Soit $E \in \mathbb{R} \setminus \{0\}$. L’équation*

$$i \frac{d\psi}{dt} = \begin{pmatrix} E & \delta u \\ \delta u & -E \end{pmatrix} \psi \tag{1.13}$$

est ensemble contrôlable de façon approchée entre les états propres de $H_0 = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$

uniformément par rapport à $\delta \in [a, b] \subset (0, +\infty)$ et $u \in U$.

Theorem 1.2.12. *Soient $E_1, E_2, E_3 \in \mathbb{R}$ tels que $|E_k - E_q| \neq |E_j - E_l|$, pour tous $k, q, j, l \in \{1 \dots 3\}$ tels que $(k, q) \notin \{(j, l), (l, j)\}$. L’équation*

$$i \frac{d\psi}{dt} = \begin{pmatrix} E_1 & \delta_1 u & 0 \\ \delta_1 u & E_2 & \delta_2 u \\ 0 & \delta_2 u & E_3 \end{pmatrix} \psi \tag{1.14}$$

est ensemble contrôlable de façon approchée entre les états propres de $H_0 = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix} \psi$

uniformément par rapport à $\delta_1 \in [a_1, b_1] \subset (0, +\infty)$, $\delta_2 \in [a_2, b_2] \subset (0, +\infty)$ et $u \in U$.

1.2. Thèmes d'études

Une question ouverte est celle de la contrôlabilité d'ensemble par rapport à $\delta \in [a, b] \subset (0, +\infty)$ de l'équation

$$i \frac{d\psi}{dt} = (H_0 + \delta u H_1) \psi,$$

où $H_0, H_1 \in S_n(\mathbb{R})$, en supposant que H_0, H_1 sont tels que l'équation (2.12) est contrôlable. Des questions similaires en dimension infinie seraient aussi très intéressantes à étudier. Un autre projet d'étude est de comprendre comment contrôler de façon robuste une équation où le terme de drift est incertain.

Chapitre
2

Introduction

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2.1 Quantum physics preliminaries, adiabatic theorem

For a general closed quantum system under the action of a control u having values in an open set U of \mathbb{R}^m , we are interested in the controlled equation of the form

$$i \frac{d\psi}{dt}(t) = H(u(t))\psi(t), \quad \psi(t) \in \mathcal{H}, \tag{2.1}$$

with $H(u)$ essentially self-adjoint on the complex separable Hilbert space \mathcal{H} for every value of u , with a common dense domain for every $u \in U$. If \mathcal{H} is finite dimensional, the controllability of Equation (2.9) has been extensively studied by Lie-algebraic methods (see [6, 9, 34]). If \mathcal{H} is infinite dimensional, then Equation (2.9) is in general not exactly controllable [11]. Many results concerning weaker notions of controllability have been proved [17, 25, 22]. However, in both cases, there exist few theoretical results about the robustness of the control strategies with respect to variations of the parameters of the system, except for two level systems (see [13, 63]). Adiabatic control is known as a powerful technique which can be used to handle perturbations and uncertainties. The adiabatic theorem states, in its simplest form, that under a separation condition on the energy levels of the controlled Hamiltonian, the occupation probabilities of the energy levels are approximately conserved when the controls are slowly varying. One of its main advantages

2.1. Quantum physics preliminaries, adiabatic theorem

is that it provides explicit and regular control laws. It has hence been successfully applied to obtain control strategies such as the chirp pulses (see, for instance [27, 74, 43]) for spin 1/2 systems with dispersed Larmor frequency. Another nowadays classical application of adiabatic control to ensemble controllability are the so-called counterintuitive pulses for the STIRAP process [38, 73, 83]. A generalization of this approach has been proposed in [62], and has raised many interesting questions, in particular about the validity of the Rotating Wave Approximation in this framework. Hence, a general theory is needed for the robust control in the quantum framework. The main contribution of the thesis is the understanding of the robustness of adiabatic control strategies, by studying the problem of controlling parametrized families of quantum systems with a common control input, that is the *Ensemble controllability* problem. Our main results about this topic are presented in the introduction in Section 2.2.1 with two real control inputs and real Hamiltonians, most of the arguments are valid both when \mathcal{H} is finite dimensional or infinite dimensional under suitable assumptions on the Hamiltonian. An extension of this with a single real control input using the Rotating Wave Approximation (see, for instance [53]) is exposed in Section 2.2.3. We will develop these issues in the chapters 3 and 6.

The starting point of the thesis is the adiabatic theorem (see, for instance [16, 55, 54, 47]), that we state in its general form, adapting the results exposed in [78, Chapter 2] to our issues of control theory.

General adiabatic theorem Let \mathcal{H} be a complex separable Hilbert space and $k \in \mathbb{N}$. Denote the set of essentially self-adjoint linear operators on \mathcal{H} by $\mathcal{L}_{sa}(\mathcal{H})$, and the set of C^j and bounded functions between two topological spaces X and Y by $C_b^j(X, Y)$. Let $H(\cdot) \in C_b(\mathbb{R}^k, \mathcal{L}_{sa}(\mathcal{H}))$. We say that the spectrum $\sigma(\cdot)$ of $H(\cdot)$ contains a separated part $\sigma_*(\cdot) \subset \sigma(\cdot)$ locally around $\bar{u} \in \mathbb{R}^k$ if there exists two bounded and continuous functions $f, g \in C_b(\mathbb{R}^k, \mathbb{R})$ and a neighborhood V of \bar{u} in \mathbb{R}^k satisfying, for every $u \in V$, $\sigma_*(u) \subset [f(u), g(u)]$ and $\inf_{u \in V} \text{dist}([f(u), g(u)], \sigma(u) \setminus \sigma_*(u)) > 0$. For $u \in V$, define $P_*(u)$ as the spectral projection of $H(u)$ on the eigenspace of $H(u)$ associated with $\sigma_*(u)$. Let $\gamma : [0, 1] \rightarrow V$ be a regular C^2 control path. We are interested in the trajectories $\psi^\epsilon(t) \in \mathcal{H}$ of the *Adiabatic Schrödinger Equation*:

$$i\dot{\psi}^\epsilon(t) = H(\gamma(\epsilon t))\psi^\epsilon(t), \quad \psi^\epsilon(0) = \psi_0,$$

where $\psi_0 \in \mathcal{H}$, $t \in [0, \frac{1}{\epsilon}]$, and $\epsilon > 0$. In the variable $\tau = \epsilon t \in [0, 1]$, the reparameterized trajectory $\tilde{\psi}^\epsilon(\tau) = \psi^\epsilon(\tau/\epsilon)$ satisfies

$$i\dot{\tilde{\psi}}^\epsilon(\tau) = \frac{1}{\epsilon}H(\gamma(\tau))\tilde{\psi}^\epsilon(\tau), \quad \tilde{\psi}^\epsilon(0) = \psi_0, \quad (2.2)$$

where $\tau \in [0, 1]$.

Define the *adiabatic Hamiltonian*, for every $\tau \in [0, 1]$, by

$$H_a^\epsilon(\tau) = H(\tau) - i\epsilon P_*(\gamma(\tau))\dot{P}_*(\gamma(\tau)) + i\epsilon(Id - P_*(\gamma(\tau)))\dot{P}_*(\gamma(\tau)),$$

where $\dot{P}_*(\gamma(\tau))$ is the derivative of P_* along the control path γ . When they are well defined, define the two unitary propagators $U^\epsilon(\tau)$ and $U_a^\epsilon(\tau)$ on \mathcal{H} of, respectively, Equation (2.2) and $i\dot{\psi}^\epsilon(\tau) = \frac{1}{\epsilon}H_a^\epsilon(\gamma(\tau))\psi^\epsilon(\tau)$, for $\tau \in [0, 1]$. An essential property of U_a^ϵ is that for every $\tau \in [0, 1]$, $P_*(\gamma(\tau))U_a^\epsilon(\tau) = U_a^\epsilon(\tau)P_*(\gamma(0))$.

Theorem 2.1.1. [78, Theorems 2.1, 2.2] *Let V be an open set of \mathbb{R}^k and $\gamma : [0, 1] \rightarrow V$ be a regular C^2 control path. Let $H(\cdot) \in C_b^2(V, \mathcal{L}_{sa}(\mathcal{H}))$ such that the operators $H(u)$ have a common dense domain $D \subset \mathcal{H}$ for every $u \in V$, and are bounded from below, uniformly with respect to $u \in V$. Assume that $\sigma_*(u) \subset \sigma(H(u))$ is a locally separated part of σ , for $u \in V$.*

Then $P_ \in C_b^2(V, \mathcal{L}_{sa}(\mathcal{H}))$, the unitary propagators U_ϵ and U_a^ϵ are well defined, and there is a constant $C < \infty$ such that for all $\tau \in [0, 1]$,*

$$\|U^\epsilon(\tau) - U_a^\epsilon(\tau)\| \leq C\epsilon.$$

Adiabatic decoupling Let $j \in \mathbb{N}$. Assume that the eigenvalues λ_j and λ_{j+1} of H are separated from the rest of the spectrum for u in a neighborhood V of $\bar{u} \in \mathbb{R}^k$. Notice that we do not assume here the existence of a gap between λ_j and λ_{j+1} . Indeed, the aim of what follows is to get an appropriate approximation of the dynamics in a neighborhood of a point \bar{u} such that $\lambda_j(\bar{u}) = \lambda_{j+1}(\bar{u})$, that is, an *intersection of eigenvalues*. Set for every $u \in V$, the spectral projection $P_{j,j+1}(u)$ of $H(u)$ on the eigenspace associated with $\sigma_*(u) = \{\lambda_j(u), \lambda_{j+1}(u)\}$. Consider, for every $u \in V$, a C^2 orthonormal basis $(\psi_j(u), \psi_{j+1}(u))$ of $\text{Im}P_{j,j+1}(u)$. For every $u \in V$, consider a unitary mapping $I(u)$ from \mathbb{C}^2 to $\text{Im}P_{j,j+1}(u)$, which is C^2 with respect to $u \in V$, such that $I(u)(e_1) = \psi_j(u)$ and $I(u)(e_2) = \psi_{j+1}(u)$, where (e_1, e_2) is the canonical basis of \mathbb{C}^2 . Along every regular C^2 control path $(\gamma(\tau))_{\tau \in [0,1]}$ in V we define the *effective Hamiltonian* for every $\tau \in [0, 1]$, by

$$H_{\text{eff}}(\gamma(\tau)) = h(\gamma(\tau)) - i\epsilon \begin{pmatrix} 0 & \langle \dot{\psi}_j(\gamma(\tau)), \psi_{j+1}(\gamma(\tau)) \rangle \\ \langle \dot{\psi}_{j+1}(\gamma(\tau)), \psi_j(\gamma(\tau)) \rangle & 0 \end{pmatrix}, \quad (2.3)$$

where, for every $u \in V$, $h(u) = I^{-1}(u)H(u)I(u)$ is a two-dimensional hermitian matrix, C^2 in $u \in V$, and $\dot{\psi}_q(\gamma(\tau))$, $q \in \{j, j+1\}$ is the derivative of ψ_q along the path γ . Denoting the propagator associated with $H_{\text{eff}}(\gamma(\tau))$ by $U_{\text{eff}}^\epsilon(\tau)$, Theorem 2.1.1 yields

$$\|(U^\epsilon(\tau) - I(\gamma(\tau))U_{\text{eff}}^\epsilon(\tau)I^{-1}(\gamma(0)))P_{j,j+1}(0)\| \leq C\epsilon, \quad (2.4)$$

for every $\tau \in [0, 1]$.

An important property, obtained by deleting the second term of H_{eff} by a standard averaging procedure (see Theorem 4.6.4 proved in Chapter 4 for a precise statement), is the following, which is valid under suitable assumptions on the eigenvalues of H , which are those of h , and the eigenvectors of H , which are those of h up to the transformation

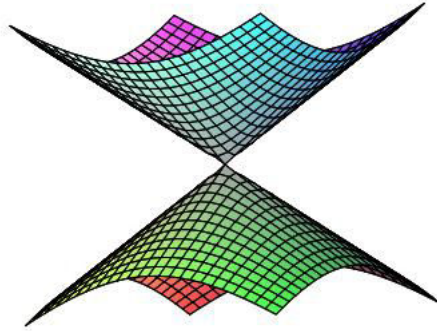


Figure 2.1 – Two eigenvalues of $H(u)$ in a neighborhood of a conical intersection when $k = 2$, as a function of $u \in \mathbb{R}^2$.

I. Given a sufficiently regular path $\gamma : [0, 1] \rightarrow V$ and $\tilde{\psi}_0 \in \mathbb{C}^2$, the solutions ψ and $\tilde{\psi}$ of, respectively, $i \frac{d\psi}{dt} = H(\gamma(\epsilon t))\psi$, $\psi(0) = I(\gamma(0))\tilde{\psi}_0$, and $i \frac{d\tilde{\psi}}{dt} = h(\gamma(\epsilon t))\tilde{\psi}$, $\tilde{\psi}(0) = \tilde{\psi}_0$ are such that $\psi(1/\epsilon)$ is ϵ^α -close, up to phases, to $I(\gamma(1))\tilde{\psi}(1/\epsilon)$. The value of $\alpha \in \mathbb{R}$ is positive and depends on the order of the gap between the eigenvalues λ_j and λ_{j+1} of H along the path γ , that is on the quantity $\lambda_{j+1} - \lambda_j$ and its derivatives (see Theorem 4.6.4).

This approximation is interesting because it preserves the adiabatic structure of the Hamiltonians, it is important to get uniform estimations of the dynamics holding along every sufficiently regular control path of \mathbb{R}^k . Moreover, the knowledge of h provides all the information needed about the local regularity of the eigenpairs of H . Notice that h , called *reduced Hamiltonian* depends on the choice of a basis of $\pi_{H(u)} = \text{Im}P_{j,j+1}(u)$, for $u \in V$. However, we will see in Section 4.6.3 that the geometric properties and hence the dynamical properties of the Schrödinger equation that we are interested in are invariant by such a change of basis. We have proved (see Section 4.6.2) that, when \mathcal{H} is finite dimensional, generic properties on h and its jet until order 2 provide generic properties on the Hamiltonian H and its jet until order 2.

Conical intersections A conical intersection (also called diabolic point) is a cone-like singularity of the spectrum of $H(u)$, seen as a function of the control $u \in \mathbb{R}^k$ (see Figure 2.1)

In the case where $H(u)$ is real and $k = 2$, they are generic in the sense that they are the least degenerate singularities of the spectrum of a Hamiltonian and have been studied since the beginning of quantum mechanics [82]. They play an important role in the context of semiclassical analysis [32, 33]. Adiabatic paths through conical intersections can be used

to induce superpositions of eigenstates, as shown in [22, 46] and to obtain tests for exact controllability when \mathcal{H} is finite-dimensional and approximate controllability when \mathcal{H} is infinite-dimensional [19]. For a large class of systems, they are generic and structurally stable, in the sense that they are not removed by small perturbations of the Hamiltonian.

Let U be a connected open set of \mathbb{R}^2 . By a slight abuse of notations, for $u \in \mathbb{R}^2$, denote the components of u by (u, v) . Assume that $H(u, v) = H_0 + uH_1 + vH_2$ where H_0, H_1, H_2 are self-adjoint operators on \mathcal{H} having a common domain \mathcal{D} such that the following conditions, that we refer as (\mathcal{R}) are satisfied:

- H_0 has a discrete spectrum;
- H_1, H_2 are bounded;
- There exists an orthonormal basis $(b_j)_j$ of the Hilbert space \mathcal{H} such that $\langle b_j, H_0 b_q \rangle, \langle b_j, H_1 b_q \rangle, \langle b_j, H_2 b_q \rangle$ are real for every j, q .

We say that $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ is a conical intersection between two eigenvalues λ_j and λ_{j+1} if $\lambda_j(\bar{u}, \bar{v}) = \lambda_{j+1}(\bar{u}, \bar{v})$ has multiplicity two and there exists $C > 0$ such that for every unit vector $\eta \in \mathbb{R}^2$ and $t > 0$ small enough, $\lambda_{j+1}((\bar{u}, \bar{v}) + t\eta) - \lambda_j((\bar{u}, \bar{v}) + t\eta) > Ct$.

Let $(\gamma(t))_{t \in [0,1]} = (u(t), v(t))_{t \in [0,1]}$ be a C^3 regular path of \mathbb{R}^2 . Consider the equation

$$i \frac{d\psi(t)}{dt} = H(\gamma(zt))\psi(t), \quad (2.5)$$

where $\psi(t) \in \mathcal{H}$. Assume that H has a conical intersection at $(0, 0)$. Assume that $\gamma(t_0) = (0, 0)$ for $t_0 \in (0, 1)$, $\gamma(t) \neq 0$ for every $t \neq t_0$. Consider a solution ψ_ϵ of Equation (2.5) such that $\psi_\epsilon(0) = \phi_j(\gamma(0))$. Then

$$\left\| \psi_\epsilon\left(\frac{1}{\epsilon}\right) - e^{i\theta} \phi_{j+1}(\gamma(1)) \right\| = O(\epsilon^{1/2}), \quad (2.6)$$

where $\theta \in \mathbb{R}$ is possibly depending on ϵ . We can then implement a strategy in order to make transitions of states passing through conical intersections, as it has been exposed in [22] (see Figure 2.2).

We are interested in the following notion of controllability. We say that Equation (2.5) is *approximately controllable* if for every $\epsilon > 0$ and $\psi_1 \in \mathcal{H}$, there exists a control $\gamma(\cdot) = (u(\cdot), v(\cdot)) : [0, T] \rightarrow U$ such that the solution of Equation (2.5) with initial condition $\psi(0) = \psi_0$ satisfies $\|\psi(T) - \psi_1\| < \epsilon$. We say that the spectrum $\sigma(\cdot)$ of $H(\cdot)$ is *conically connected* if all eigenvalue intersections are conical and for every j , there exists a conical intersection (\bar{u}_j, \bar{v}_j) between the eigenvalues λ_j, λ_{j+1} , with $\lambda_l(\bar{u}_j, \bar{v}_j)$ simple if $l \neq j, j+1$. We have the following general results.

Theorem 2.1.2 ([19]). *Assume that the spectrum of $H(\cdot)$ is conically connected. Then Equation (2.5) is approximately controllable.*

Theorem 2.1.3 ([19]). *Assume that \mathcal{H} is finite dimensional. Assume that the spectrum of $H(\cdot)$ is conically connected. Then Equation (2.5) is exactly controllable.*

2.2. Topics of investigation

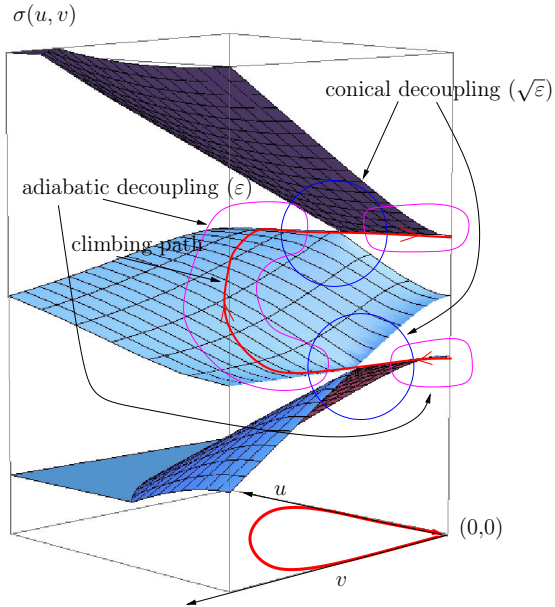


Figure 2.2 – Climbing path at speed ϵ when $k = 2$.

Proposition 2.1.4 (Genericity). *Let H_0 be a n -dimensional real symmetric matrix. Then, generically with respect to (H_1, H_2) in the space of n -dimensional real symmetric matrices, all intersections of eigenvalues of $H_0 + uH_1 + vH_2$ are conical.*

Some results of genericity of conical intersections when \mathcal{H} is infinite dimensional have been proved in [31, 22], in the cases of real controlled potentials.

2.2 Topics of investigation

Our aim is to continue exploring the links between singularities of the spectrum of Hamiltonians, the geometry of the eigenspaces, and controllability properties of the associated quantum system. In particular, as announced previously, we study the problem of controlling parametrized families of quantum systems with a common control input. It is a critical task for many applications in quantum control (see [39] and references therein), notably in Nuclear Magnetic Resonance [40]. This issue of ensemble controllability has been formulated mathematically by Li and Khaneja in [63] and by Beauchard, Coron and Rouchon in [13]. Results for ensemble control beyond the quantum control setting can be found in [4, 50, 64, 72].

2.2.1 Ensemble control with two real controls

For a general closed quantum system under the action of a control $u \in \mathbb{R}^m$ and depending on a parameter z , the corresponding controlled equation is of the form

$$i \frac{d\psi}{dt}(t) = H(u(t), z)\psi(t), \quad \psi(t) \in \mathcal{H}, \quad (2.7)$$

with $H(u, z)$ essentially self-adjoint on the separable complex Hilbert space \mathcal{H} for every value of u and z . The parameter z can be used either to describe a family of physical systems on which acts a common field driven by u or a physical systems for which the value of one parameter is not known precisely.

The controllability properties of systems of this form has been studied both for discrete and continuous sets of parameters. The case of a finite set of systems is characterized in [14, 35]. In [29] the asymptotic ensemble stabilization is studied for countable sets of parameters. In [63], [13] a proof of a strong notion of ensemble controllability has been obtained for a two-level system. Numerical ensemble control in the case of a continuum of parameters has been throughly studied for two-level systems [79, 28, 75]. Our aim is to generalize the theorems 2.1.2 and 2.1.3 to the issue of Ensemble control.

We restrict our study to the problem of *ensemble approximate controllability between eigenstates*. Excepted when it is explicitly mentioned, we will study finite dimensional real quantum systems, that is systems whose Hamiltonian belong to the set $S_n(\mathbb{R})$ of real symmetric n -dimensional matrices. However the main results of controllability remain valid when $H(u, v) = H_0 + uH_1 + vH_2$ where H_0, H_1, H_2 are essentially self-ajoint operators on \mathcal{H} with a common dense domain, and satisfying Condition (\mathcal{R}) , $(u, v) \in U$, where U is a connected open set of \mathbb{R}^2 , and an adaptation of this condition to the parametric case (see Chapter 2.2.1).

Notations

- Let $H \in C^k(U, S_n(\mathbb{R}))$. For $u \in U$, denote the spectrum of $H(u)$ by $(\lambda_j(u))_{j=1}^n$, where $j \mapsto \lambda_j(u)$ is the nondecreasing sequence of eigenvalues of $H(u)$ repeated according to their multiplicities. We write $(\phi_1(u), \dots, \phi_n(u))$ to denote an orthonormal basis of associated eigenvectors.
- Let $H \in C^k(U \times [z_0, z_1], S_n(\mathbb{R}))$. For $u \in U$, and $z \in [z_0, z_1]$, denote the spectrum of $H(u, z)$ by $(\lambda_j(u, z))_{j=1}^n$, where $j \mapsto \lambda_j(u, z)$ is the nondecreasing sequence of eigenvalues of $H(u, z)$ repeated according to their multiplicities. We write $(\phi_1^z(u), \dots, \phi_n^z(u))$ to denote an orthonormal basis of associated eigenvectors.

Definition 2.2.1. *We say that system (2.7) is ensemble approximately controllable between eigenstates if for every $\epsilon > 0$, $j, k \in \{1, \dots, n\}$, and $u_0, u_1 \in U$ such that $\lambda_j(u_0, z)$ and $\lambda_k(u_0, z)$ are simple for every $z \in [z_0, z_1]$, there exists a control $u(\cdot) : [0, T] \rightarrow U$*

2.2. Topics of investigation

such that for every $z \in [z_0, z_1]$ the solution of (2.7) with initial condition $\psi^z(0) = \phi_z^z(u_0)$ satisfies $\|\psi^z(T) - e^{i\theta} \phi_k^z(u_1)\| < \epsilon$ for some $\theta \in \mathbb{R}$ (possibly depending on z and ϵ).

By a factorization of the dynamics by the trace, the reduced Hamiltonian h defined in Section 2.1 can be reduced to a zero trace Hamiltonian. In the case $k = 2$, we can assume, without loss of generality that for every $(u, v) \in \mathbb{R}^2$ in a neighborhood of $(0, 0)$, $h(u, v) = H_f(u, v)$, where H_f is defined by

$$H_f(u, v) = \begin{pmatrix} f_1(u, v) & f_2(u, v) \\ f_2(u, v) & -f_1(u, v) \end{pmatrix},$$

with $f = (f_1, f_2) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. In the parametric case, for every $(u, v, z) \in \mathbb{R}^3$ in a neighborhood of $(0, 0, 0)$, we can assume $h(u, v, z) = H_f(u, v, z)$, where H_f is defined by

$$H_f(u, v, z) = \begin{pmatrix} f_1(u, v, z) & f_2(u, v, z) \\ f_2(u, v, z) & -f_1(u, v, z) \end{pmatrix},$$

with $f = (f_1, f_2) \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. In this case, intersections of eigenvalues which are transverse in every direction and tangent in a specific direction, called the *non-conical direction*, appear generically. They are called *semi-conical* intersections (see Figure 2.3), and are defined rigorously in Section 4.2.1. We are going to study normal forms for this generic case.

Normal forms

Admissible transformations of two-level systems We define admissible transformations in order to get normal forms for the Hamiltonians H_f . Consider the *Schrödinger Equation*, defined for $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ by

$$i \frac{d\psi(t)}{dt} = H_f(u(t), v(t))\psi(t), \quad (2.8)$$

where $\psi(t) \in \mathbb{C}^2$, and the *Ensemble Schrödinger Equation*, defined for $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ by

$$i \frac{d\psi(t)}{dt} = H_f(u(t), v(t), z)\psi(t), \quad (2.9)$$

where $\psi(t) \in \mathbb{C}^2$. The control functions u, v are in $L^\infty(\mathbb{R}, \mathbb{R})$ and the parameter z belongs to $[z_0, z_1]$ where $z_0, z_1 \in \mathbb{R}$.

The three transformations correspond to equivalent representations of the dynamical systems (2.8) and (2.9) achieved, respectively, by time-reparameterization, state-space diffeomorphism, and independent diffeomorphic transformations of both the space of controls and the space of the parameter z .

Definition 2.2.2. We say that two elements f and \tilde{f} of $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ are equivalent at 0 if there exists $(\phi, \theta, \xi) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2) \times [-\pi, \pi] \times C^\infty(\mathbb{R}^2, \mathbb{R} \setminus \{0\})$ where ϕ is a diffeomorphism satisfying $\phi(0) = 0$, and $\zeta = \pm 1$, such that for every (u, v) in a neighborhood of 0,

$$\begin{cases} \tilde{f}_1(u, v) = \xi(u, v)(\cos(2\theta)f_1 \circ \phi(u, v) - \zeta \sin(2\theta)f_2 \circ \phi(u, v)), \\ \tilde{f}_2(u, v) = \xi(u, v)(\sin(2\theta)f_1 \circ \phi(u, v) + \zeta \cos(2\theta)f_2 \circ \phi(u, v)). \end{cases}$$

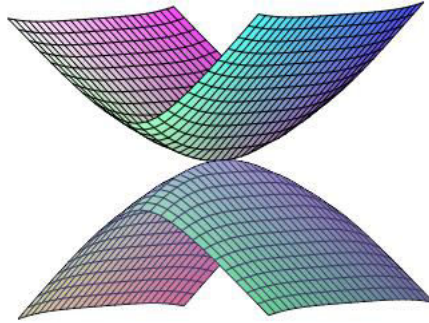


Figure 2.3 – The two eigenvalues of $H_f(u, v)$ in a neighborhood of a semi-conical intersection, as a function of (u, v) .

Definition 2.2.3. We say that two elements f and \tilde{f} of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ are equivalent at 0 if there exists $(\phi, \theta, \xi) \in C^\infty(\mathbb{R}^3, \mathbb{R}^3) \times [-\pi, \pi] \times C^\infty(\mathbb{R}^2, \mathbb{R} \setminus \{0\})$ where ϕ is a diffeomorphism of the form $\phi : (u, v, z) \mapsto (\phi_1(u, v), \phi_2(u, v), \phi_3(z))$, where $\phi_1, \phi_2 \in C^\infty(\mathbb{R}^2, \mathbb{R})$ and $\phi_3 \in C^\infty(\mathbb{R}, \mathbb{R})$, satisfying $\phi(0) = 0$, and $\zeta = \pm 1$, such that for every (u, v, z) in a neighborhood of 0,

$$\begin{cases} \tilde{f}_1(u, v, z) = \xi(u, v)(\cos(2\theta)f_1 \circ \phi(u, v, z) - \zeta \sin(2\theta)f_2 \circ \phi(u, v, z)), \\ \tilde{f}_2(u, v, z) = \xi(u, v)(\sin(2\theta)f_1 \circ \phi(u, v, z) + \zeta \cos(2\theta)f_2 \circ \phi(u, v, z)). \end{cases}$$

This allows to classify the generic local behaviours of quantum systems with respect to (u, v) .

Non-parametric case Consider $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. Then H_f has a conical intersection at $(0, 0)$ if and only if f is equivalent to $(u, v) \mapsto \begin{pmatrix} u & v \\ v & -u \end{pmatrix}$. A generic Hamiltonian has only conical singularities.

We say that H_f has a *semi-conical intersection* (see Figure 2.3) at $(0, 0)$ if and only if f is equivalent to $(u, v) \mapsto \begin{pmatrix} h(u)u & \\ u + v^2 & \end{pmatrix}$ where $h : \mathbb{R} \rightarrow \mathbb{R}$ is a smooth function satisfying $h(0) = 1$. Semi-conical intersections are not generic for $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, however, we are going to see that they may appear at isolated points when considering the parametric case. The corresponding Hamiltonian $\begin{pmatrix} h(u)u & u + v^2 \\ u + v^2 & -h(u)u \end{pmatrix}$ is such that its eigenvalues are tangent along a control path tangent to $e_2 = (0, 1)$, that is, the non-conical direction at $(0, 0)$, while they are transverse in every other directions.

2.2. Topics of investigation

Then we classify the different generic local behaviours of quantum systems with respect to (u, v, z) .

Parametric case Now we can define F-conical and F-semi-conical intersections, which are the two generic cases for parametric Hamiltonians. They correspond, for $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$, to the case where $H_f(\cdot, 0)$ has conical or semi-conical intersections, combined with additional regularity hypothesis with respect to the parameter z .

Let $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$.

- We say that 0 is *F-conical* for f if and only if there exist $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R})$ satisfying $h_1(0) = h_2(0) = 1$, such that f is equivalent to

$$(u, v, z) \mapsto \begin{pmatrix} h_1(u, v, z)(z - u) \\ h_2(u, v, z)(z - v) \end{pmatrix};$$

- We say that 0 is *F-semi-conical* for $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ if and only if there exist $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ satisfying $h_1(0) = h_2(0) = 1$ and $m \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfying $m(0) \notin \{-1, 0\}$ such that f is equivalent to

$$(u, v, z) \mapsto \begin{pmatrix} h_1(u, v, z)(z - m(u)u) \\ h_2(u, v, z)(z + u + v^2) \end{pmatrix}.$$

n -level systems Let $H \in C^\infty(\mathbb{R}^2, S_n(\mathbb{R}))$. We prove that H has a conical intersection at $(0, 0)$ between the levels λ_j and λ_{j+1} if and only if there exists a reduced Hamiltonian h of H locally around $(0, 0)$ having a conical intersection at $(0, 0)$. As a consequence, it is coherent to give the following definition of semi-conical intersections for H .

Definition 2.2.4. *We say that H has a semi-conical intersection at $(0, 0)$ between the levels λ_j and λ_{j+1} if there exists a reduced Hamiltonian h of H having a semi-conical intersection at $(0, 0)$.*

We prove in Section 4.6.3 that these properties do not depend on the mapping $I(u, v)$, for (u, v) in a neighborhood of $(0, 0)$, used for the adiabatic decoupling as in Section 2.1 of the introduction.

In the parametric case, we say that H has a F-conical intersection (respectively, F-semi-conical intersection) at $(0, 0, 0)$ if there exists a reduced Hamiltonian h of H having a F-conical intersection (respectively, F-semi-conical intersection) at $(0, 0, 0)$. In Section 4.6.3, we show that, generically with respect to $H \in C^\infty(\mathbb{R}^3, S_n(\mathbb{R}))$, an eigenvalue intersection $(u, v, z) \in \mathbb{R}^3$ of H is either F-conical or F-semi-conical.

Actually, semi-conical intersections are not so rare. For instance, they can appear when,

for $(u, v) \in \mathbb{R}^2$, $H(u, v) = \begin{pmatrix} E & u & 0 \\ u & E & v \\ 0 & v & E' \end{pmatrix}$, where $E < E'$, we call this case the *degenerate*

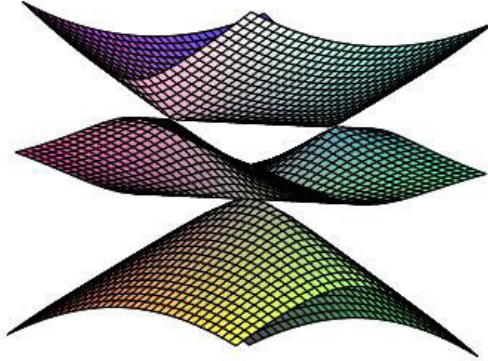


Figure 2.4 – Semi-conical intersection for a degenerate STIRAP process

STIRAP. On Figure 2.4, we have plotted the spectrum of $H(u, v)$ as a function of (u, v) for such a Hamiltonian. We can notice that there is a semi-conical intersection between the first and second levels, and two conical intersections between the second and third levels.

Dynamical properties at semi-conical intersections Thanks to the normal forms, we can estimate the adiabatic approximation for general n -level Hamiltonians. Let $H \in C^\infty(\mathbb{R}^2, \mathcal{S}_n(\mathbb{R}))$, having a semi-conical intersection at $(0, 0)$. Denote by η the non-conical direction. Let $(\gamma(t))_{t \in [0, 1]} = (u(t), v(t))_{t \in [0, 1]}$ be a smooth regular path of \mathbb{R}^2 such that $\gamma(t_0) = (0, 0)$ for $t_0 \in (0, 1)$, $\gamma(t) \neq 0$ for every $t \neq t_0$, and γ is tangent to η at $t = t_0$. Consider a solution ψ_ϵ of the equation

$$i \frac{d\psi(t)}{dt} = H(u(\epsilon t), v(\epsilon t))\psi(t), \quad (2.10)$$

where $\psi(t) \in \mathbb{C}^n$, such that $\psi_\epsilon(0) = \phi_j(\gamma(0))$. Then $\|\psi_\epsilon(\frac{1}{\epsilon}) - e^{i\theta} \phi_j(\gamma(1))\| = O(\epsilon^{1/3})$, where $\theta \in \mathbb{R}$ is possibly depending on ϵ (see Figure 2.5 for a graphic representation of the control path passing through the singularity in the non-conical direction).

When conicity is preserved when the parameter z varies

In Chapter 3 we propose a framework for the adiabatic ensemble control of a continuum of n -level systems with real Hamiltonian, driven by two controls and having conical intersections between the eigenvalues. The main idea is that, if a system corresponding to a fixed parameter has conical intersections between two eigenvalues, then a small perturbation of the parameter yields a curve of conical intersections, each point of the curve

2.2. Topics of investigation

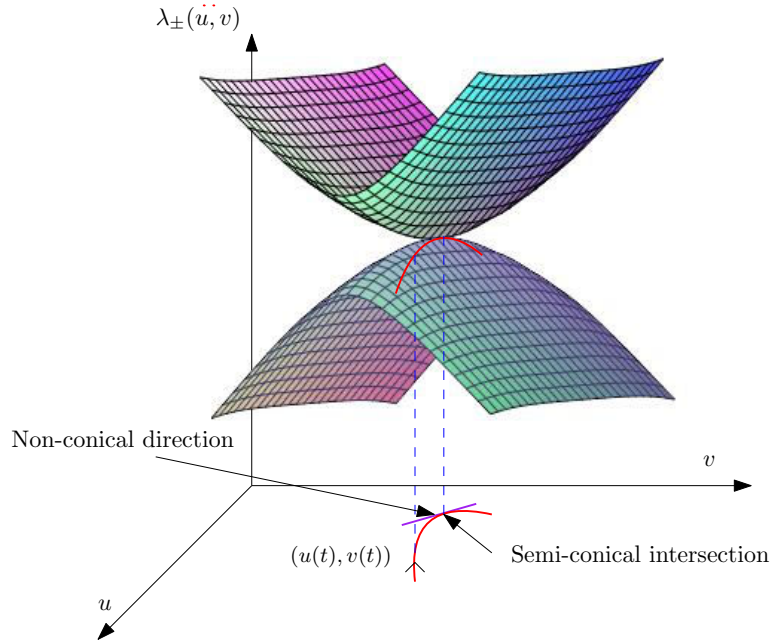


Figure 2.5 – Control path passing in the non-conical direction.

corresponding to exactly one value of the parameter. One can then follow adiabatically such curves in the space of controls and obtain a population transfer between the two levels for the whole ensemble of systems. This result has been written without resorting to the normal forms because of the already well-known estimation of the adiabatic dynamics at conical intersections in the literature. However, the same result can be deduced also from the local study of normal forms.

Let U be an open set of \mathbb{R}^2 . For $j \in \{1 \dots n\}$, let us denote by γ_j the set $\{(u, v, z) \in U \times [z_0, z_1] \mid \lambda_j(u, v, z) = \lambda_{j+1}(u, v, z)\}$, where by convention $\gamma_0 = \gamma_n = \emptyset$. Denote the projection of $(u, v, z) \in \mathbb{R}^3$ onto the (u, v) -component by π .

ASSUMPTION A_j . There exist a connected component $\hat{\gamma}_j$ of γ_j and a map such that $\beta_j : [z_0, z_1] \rightarrow U$ such that β_j is a C^3 embedding and

- $\pi(\hat{\gamma}_j)$ is contained in $U \times [z_0, z_1] \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_{j+1}))$;
- $\pi(\hat{\gamma}_j) = \beta_j([z_0, z_1])$;
- for every $z \in [z_0, z_1]$, $\lambda_j(\cdot, z)$ and $\lambda_{j+1}(\cdot, z)$ have a unique intersection on $\pi(\hat{\gamma}_j)$, which is conical and occurs at $\beta_j(z)$.

Moreover the set $U \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_j) \cup \pi(\gamma_{j+1}))$ is pathwise connected.

Notice that the second and third conditions are equivalent to say that $\hat{\gamma}_j$ has F-conical intersections only and $\pi(\hat{\gamma}_j)$ is an embedded curve of \mathbb{R}^2 without self-intersections. The following result is the main result of the article [10] and of the chapter 3.

Theorem 2.2.5. Consider a C^3 map $U \times [z_0, z_1] \ni (u, v, z) \mapsto H(u, v, z) \in S_n(\mathbb{R})$. Let

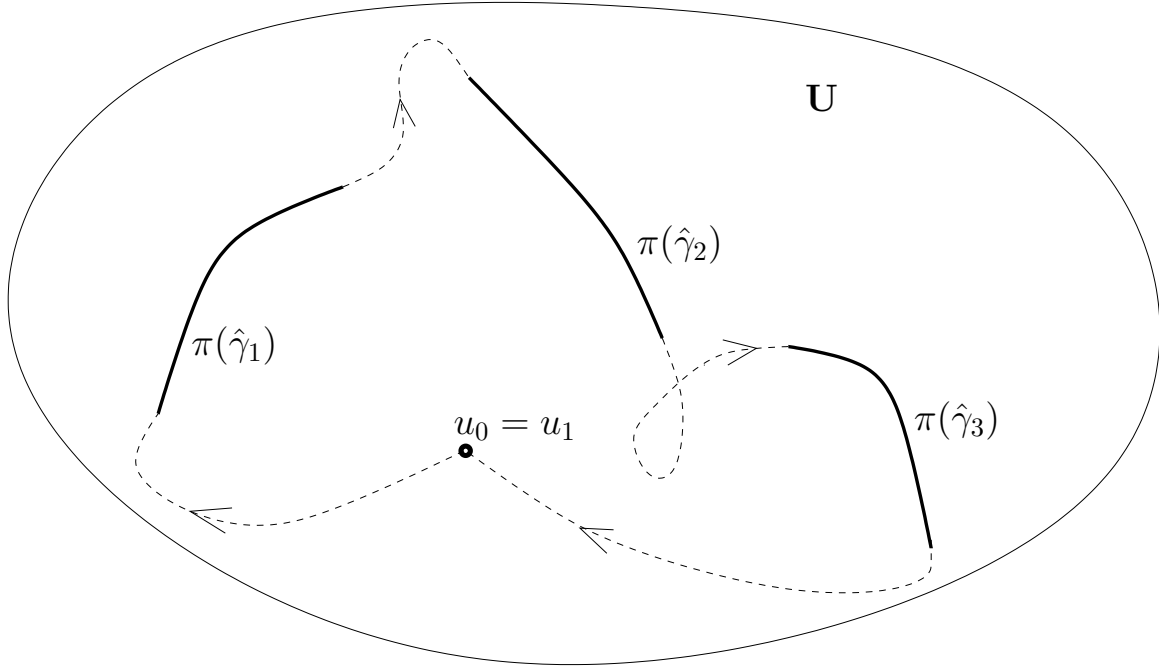


Figure 2.6 – A control realizing an ensemble transition between $\phi_1^z(u_0, v_0)$ and $\phi_4^z(u_0, v_0)$.

assumption A_j be satisfied for every $j \in \{1 \dots n\}$. Then the equation $i \frac{d\psi}{dt} = H(u, v, z)\psi$ is ensemble approximately controllable between eigenstates.

Method of control The method of control is presented on Figure 2.6, with a path $(u(t), v(t))_{t \in [0,1]}$, followed at a speed ϵ . The error in the adiabatic regime has order $\sqrt{\epsilon}$ on an interval of time of length $\frac{1}{\epsilon}$.

When a semi-conical intersection appears when the parameter z varies

The argument sketched above works under the assumption that for all values of the parameter eigenvalue intersections remain conical and describe a smooth curve. These assumptions are satisfied for generic small parametric perturbations. For generic large perturbations it may happen that conicity of eigenvalue intersections is lost at isolated points of the curve. The goal is to extend the analysis to this case.

Controllability properties In the case where there are F-semi-conical intersections of eigenvalues on γ_j , the question is whether or not the adiabatic approximation remains valid when the control path passes through such points. Using the normal forms, we notice that $\pi(\hat{\gamma}_j)$ is tangent to the non-conical direction at a F-semi-conical intersection. Hence, when a control path follows $\pi(\hat{\gamma}_j)$, it passes into the semi-conical intersection for $H(\cdot, z)$ in the non-conical direction, and hence there is no transition between eigenstates for the system with parameter z .

2.2. Topics of investigation

However, we show that under the assumption \tilde{A}_j that follows, the adiabatic approximation is uniform with respect to the parameter $z \in [z_0, z_1]$ and the system is ensemble approximately controllable between eigenstates. In this case, we cannot consider an embedding from $[z_0, z_1]$ to $\pi(\hat{\gamma}_j)$ because the same value of the parameter z corresponds to different intersections of eigenvalues of $H(\cdot, z)$. This is why we consider the following assumptions.

Controllability properties ASSUMPTION \tilde{A}_j . There exist a connected component $\hat{\gamma}_j$ of γ_j such that

- $\hat{\gamma}_j$ is a one-dimensional submanifold of \mathbb{R}^3 made of F-conical intersections and F-semi-conical intersections only;
- There exist $(u_0, v_0) \in U$ and $(u_1, v_1) \in U$ such that $(u_0, v_0, z_0), (u_1, v_1, z_1) \in \hat{\gamma}_j$ are F-conical intersections for H ;
- $\pi(\hat{\gamma}_j)$ is a C^∞ embedded curve of \mathbb{R}^2 without self-intersections, which is contained in $U \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_{j+1}))$.

Moreover the set $U \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_j) \cup \pi(\gamma_{j+1}))$ is pathwise connected.

Theorem 2.2.6. *Consider a C^4 map $U \times [z_0, z_1] \ni (u, v, z) \mapsto H(u, v, z) \in S_n(\mathbb{R})$. Let assumption \tilde{A}_j be satisfied for every $j \in \{1 \dots n\}$. Then the equation $i \frac{d\psi}{dt} = H(u, v, z)\psi$ is ensemble approximately controllable between eigenstates.*

Method of control On figure 2.7, we give a smooth control path (u, v) (see Theorem 4.1.3 for more precisions) achieving transitions between two levels j and $j + 1$ which are uniform with respect to the parameter $z \in [z_0, z_1]$. The control path (u, v) enters in $\pi(\gamma)$ at a point (u_0, v_0) such that (u_0, v_0, z_0) is a F-conical intersection of eigenvalues of $H(u, v, z_0)$ between the levels j and $j + 1$, and exiting at a point (u_1, v_1) such that (u_1, v_1, z_1) is a F-conical intersection of eigenvalues of $H(u, v, z_1)$ between the levels j and $j + 1$. In order to guarantee that transitions are achieved for every $z \in [z_0, z_1]$, the control path has to pass an odd number of times through F-conical intersections of $H(u, v, z)$, for every $z \in [z_0, z_1]$. Moreover the uniformity of the adiabatic approximation with respect to the parameter z is ensured when the control path is chosen such that we have $z \in [z_0, z_1]$ for every z and t such that $(u(t), v(t), z) \in \gamma$. The error made in the adiabatic approximation for such a path of speed ϵ has order $\epsilon^{\frac{1}{3}}$.

2.2.2 Classification of the singularities of the non-mixing field

For a general Hamiltonian H depending on two real controls, the non-mixing curves between λ_{j-1} and λ_j for $j \geq 2$ have been defined in [22] as the curves $\gamma = (\gamma(t))_{t \in [0,1]}$ of \mathbb{R}^2 along which $\dot{\phi}_{j-1}(\gamma(t))$ is orthogonal to $\phi_j(\gamma(t))$, for every $t \in [0, 1]$. Then, by Theorem 2.1.1, the precision of the adiabatic approximation along such a curve is improved. In

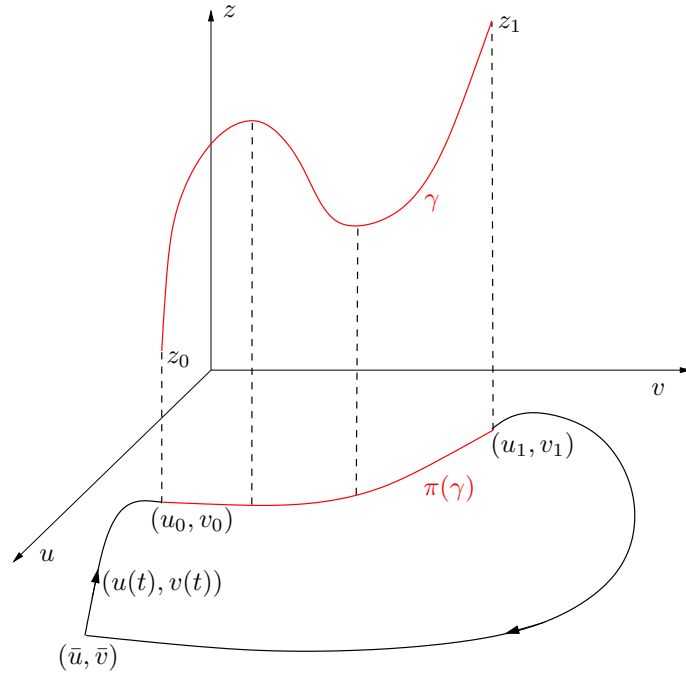


Figure 2.7 – A curve of controls (u, v) achieving uniform transitions w.r.t. $z \in [z_0, z_1]$ between two levels having F-semi-conical intersections

particular, the error of order $\sqrt{\epsilon}$ in Equation (2.6) for a control path at a conical intersection is transformed into ϵ along a non-mixing curve. This property has been used in [22] for a precise control of the Schrödinger Equation with real Hamiltonians and an extension has been presented in [31] for complex Hamiltonians with three real controls.

In this section, we study the singularities of the non-mixing curves for two level systems, then for more general quantum system.

Non-mixing field for two-level systems and singularities in this case

For f in $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, let us study the dynamics of

$$i \frac{d\psi_\epsilon(t)}{dt} = H_f(u(\epsilon t), v(\epsilon t))\psi_\epsilon(t), \quad \psi_\epsilon(0) = \tilde{\psi}_0 \in \mathbb{C}^2, \quad (2.11)$$

where $t \in [0, \frac{1}{\epsilon}]$ and $\tilde{\psi}_0$ is independent of ϵ .

Along a non-mixing curve γ , the error occurring in the adiabatic theorem is equal to 0, that is, the non-mixing curves can be followed at an arbitrary speed. We show that they are integral curves of a smooth vector field $\chi(f)$, namely the *non-mixing field*.

Theorem 2.2.7. *Generically with respect to $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, $\chi(f)$ has three types of singularities, up to a C^∞ diffeomorphic coordinate change from \mathbb{R}^2 to \mathbb{R}^2 :*

- *Critical nodes (see Figure 2.8) at intersections of eigenvalues,*

2.2. Topics of investigation

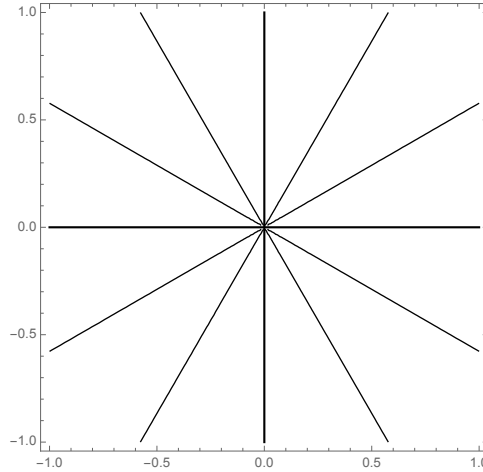


Figure 2.8 – A critical node

— *Saddles and centers at points that are not intersections of eigenvalues.*

By admissible transformations, generic one-parameter perturbation of a Hamiltonian can be transformed locally around eigenvalue intersections into:

$$H(u, v, z) = \begin{pmatrix} h_1(u, v, z)(z - u) & h_2(u, v, z)(z - v) \\ h_2(u, v, z)(z - v) & -h_1(u, v, z)(z - u) \end{pmatrix},$$

or

$$H(u, v, z) = \begin{pmatrix} h_1(u, v, z)(z - m(u)u) & h_2(u, v, z)(z + u + v^2) \\ h_2(u, v, z)(z + u + v^2) & -h_1(u, v, z)(z - m(u)u) \end{pmatrix},$$

where $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R})$ satisfy $h_1(0) = h_2(0) = 1$, and $m \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfies $m(0) \notin \{-1, 0\}$.

This property allows to study the bifurcations of singularities occurring in Theorem 2.2.7 when a parameter z varies. For every z in \mathbb{R} , let $\chi_z(f)$ be the non-mixing field associated with $f(\cdot, \cdot, z) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$.

Theorem 2.2.8. *Generically with respect to $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$, for every $z \in \mathbb{R}$, $\chi_z(f)$ has the following singularities, up to a C^∞ -diffeomorphic coordinate change from \mathbb{R}^2 to \mathbb{R}^2 :*

- *Critical nodes at conical intersections of eigenvalues,*
- *Hyperbolic or elliptic semi-conical singularities at semi-conical intersections of eigenvalues (see Chapter 5 Section 5.2.2 for a precise definition, and the figures 5.3 and 5.2),*
- *Saddles, centers or cusps at points that are not intersections of eigenvalues.*

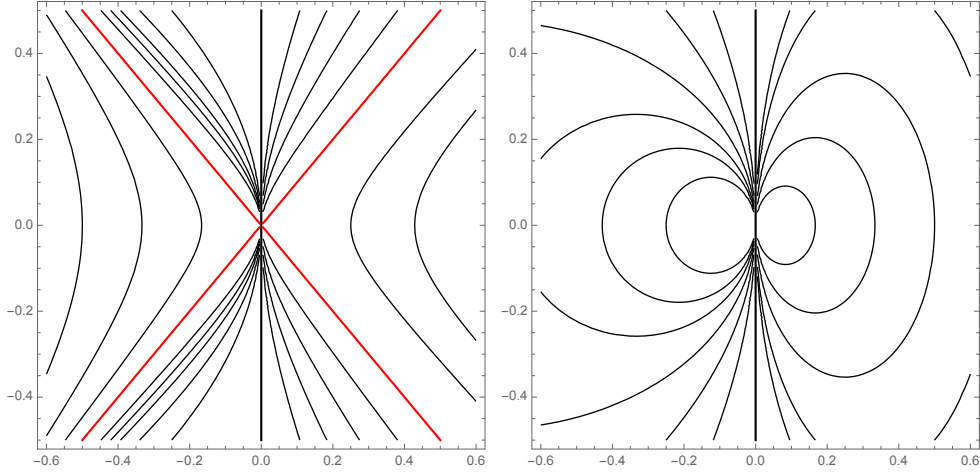


Figure 2.9 – A *hyperbolic semi-conical singularity*. The non-conical direction is $(0, 1)$. The red curves are the only non-mixing curves passing through the singularity in the non-conical direction. The index is 0. Figure 2.10 – An *elliptic semi-conical singularity*. The non-conical direction is $(0, 1)$. Every non-mixing curve passes through the singularity in the non-conical direction. The index is 2.

Non-mixing field for higher dimensional systems

For higher dimensional systems, the non-mixing curves have been studied in [22]. In the following, we consider $H_0, H_1, H_2 \in S_n(\mathbb{R})$, and we define

$$H(u, v) = H_0 + uH_1 + vH_2.$$

In this case, it has been shown in [22] that the non-mixing curves are the integral curves of a line field on \mathbb{R}^2 , defined up to a sign, for $(u, v) \in \mathbb{R}^2$, by

$$\chi_{j-1,j}(u, v) = \begin{pmatrix} -\langle H_2 \phi_{j-1}(u, v), \phi_j(u, v) \rangle \\ \langle H_1 \phi_{j-1}(u, v), \phi_j(u, v) \rangle \end{pmatrix},$$

where $\langle \cdot, \cdot \rangle$ is the natural Euclidean scalar product on \mathbb{R}^n . Notice that $\chi_{j-1,j}$ is defined up to a sign at the points $(u, v) \in \mathbb{R}^2$ such that $\lambda_{j-1}(u, v) \neq \lambda_j(u, v)$. Along these curves the adiabatic approximation has a higher precision, that is the error has an order ϵ along a control path of speed ϵ , even when it passes through crossings of eigenvalues. Contrarily to what one could think, the non-mixing curves for a n -level Hamiltonian with $n \geq 3$ do not correspond locally to those of a reduced two level Hamiltonian as defined in Section 2.1. They involve a more complex structure that has interesting topological properties. Indeed, we are going to see that the non-mixing field may have both singularities of integer index which are generic for a vector field of \mathbb{R}^2 and singularities of half-integer index which are generic for a line field of \mathbb{R}^2 , while the space of vector fields and of line fields are used to be

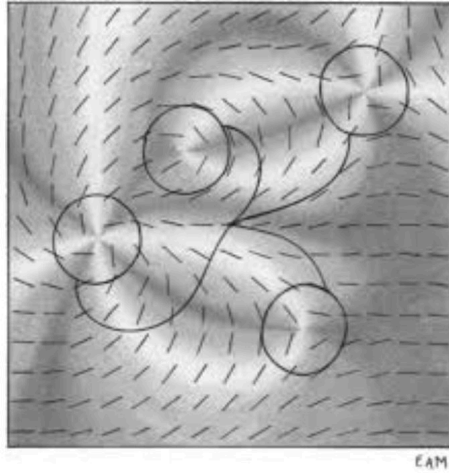


Figure 2.11 – Combination of integer and half-integer index singularities in nematic crystals, picture taken from [8]

endowed with different topologies so that at first view such a combination of singularities seems to be impossible generically. These kind of structures have already been observed in nematic liquid crystals (see [26] for a general review on nematic crystals and Figure 2.11 for an illustration of such a behaviour). Further investigations on this type of structures will be made in future works.

We aim at classifying the singularities of the line field $\chi_{j-1,j}$, and we first need to recap some topological tools.

Basic facts about line-fields Let (M, g) be a 2-dimensional Riemannian manifold, and K be a closed subset of M . A line field L on M is a section of $PT(M \setminus K)$. The set K is the set of singularities of L . As it has been proved in [21], any line field with singularities can be realized as the bisection for the angle defined for the Riemannian metric g of two vector fields X and Y on M . When a line field L is a bisection of the vector fields X and Y , we say that L is defined as a *proto-line-field*. The zeros of X and Y become singularities of the associated proto-line-field. With this definition, the Whitney topology on pairs of vector fields on M defines a topology on line fields on M . It has been proved in [21] that generically, a proto-line-field has only Darbouxian singularities, that is, its integral manifolds are homeomorphic to those of the proto-line-fields defined by (X_L, Y_L) , (X_M, Y_M) and (X_S, Y_S) as follows:

- The *Lemon proto-line-field* (see Figure 5.15) is the pair of vector fields on $(\mathbb{R}^2, Eucl)$ defined by

$$X_L(x, y) = \begin{pmatrix} x + y \\ y - x \end{pmatrix}, \quad Y_L(x, y) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

- The *Monstar proto-line-field* (see Figure 5.16) is the pair of vector fields on $(\mathbb{R}^2, Eucl)$

defined by

$$X_M(x, y) = \begin{pmatrix} x \\ 3y \end{pmatrix}, \quad Y_M(x, y) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

- The *Star proto-line-field* (see Figure 5.17) is the pair of vector fields on $(\mathbb{R}^2, Eucl)$ defined by

$$X_S(x, y) = \begin{pmatrix} x \\ -y \end{pmatrix}, \quad Y_S(x, y) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

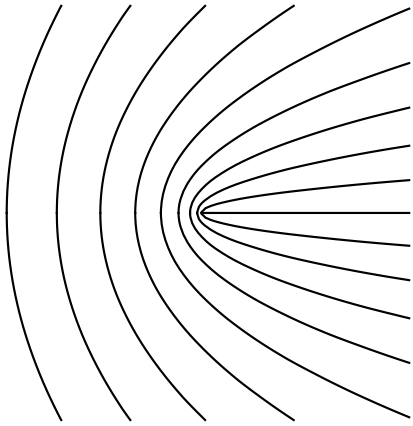


Figure 2.12 – The Lemon singularity, of index $\frac{1}{2}$.

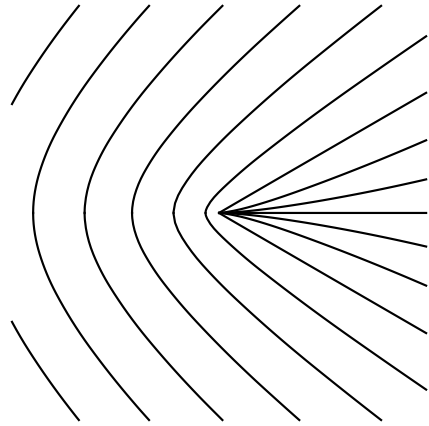


Figure 2.13 – The Monstar singularity, of index $\frac{1}{2}$.

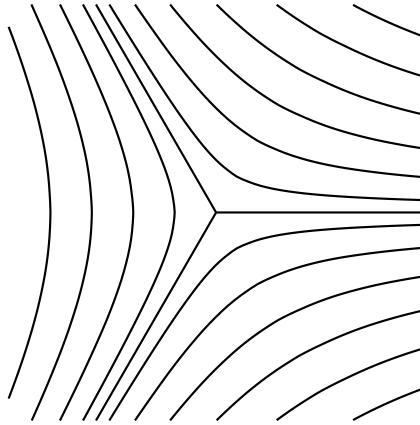


Figure 2.14 – The Star singularity, of index $-\frac{1}{2}$.

Non-mixing curves for n -level systems at conical intersections between the levels $j - 1$ and j In a neighborhood of a conical intersection $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ between the levels $j - 1$ and j ,

- There exists a smooth choice of the sign of the eigenvectors $\phi_{j-1}(u, v)$ and $\phi_j(u, v)$ such that $\chi_{j-1,j}$ defines a C^∞ vector field in a punctured neighborhood of (\bar{u}, \bar{v}) ,

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- The integral curves of $\chi_{j-1,j}$ are C^∞ and the eigenvectors ϕ_{j-1} and ϕ_j are C^∞ along them,
- For every direction η of \mathbb{R}^2 , there exists an integral curve $\gamma : [0, 1] \rightarrow \mathbb{R}^2$ of $\chi_{j-1,j}$ such that $\gamma(1) = (\bar{u}, \bar{v})$, $\lim_{t \rightarrow 1^-} \frac{\dot{\gamma}(t)}{\|\dot{\gamma}(t)\|} = \eta$.

We say that the singularity of $\chi_{j,j-1}$ has type **(N)**, for node.

Non-mixing curves for n -level systems at conical intersections between the levels j and $j+1$ (respectively $j-2$ and $j-1$) In order to complete the classification of the singularities of the non-mixing field at intersections of eigenvalues, we focus on the singularities of $\chi_{j-1,j}$ at conical intersections between the levels j and $j+1$.

Let $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ be a conical intersection between λ_j and λ_{j+1} . We introduce the following condition:

Condition (C): The vectors $P_{j,j+1}H_1\phi_{j-1}(u, v)$ and $P_{j,j+1}H_2\phi_{j-1}(u, v)$ are not colinear.

We prove the following theorem.

Theorem 2.2.9. *Let $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ be such that $\lambda_j(\bar{u}, \bar{v}) = \lambda_{j+1}(\bar{u}, \bar{v})$ is a conical intersection. Assume that Condition (C) is satisfied at (\bar{u}, \bar{v}) . Then $\chi_{j-1,j}$ has a Darbouxian singularity at (\bar{u}, \bar{v}) .*

Corollary 2.2.10. *Let $E_1, E_2, E_3 \in \mathbb{R}$ such that $E_1 < E_2 < E_3$ and $H(u, v) = \begin{pmatrix} E_1 & u & 0 \\ u & E_2 & v \\ 0 & v & E_3 \end{pmatrix}$.*

Then $\chi_{1,2}$ (respectively $\chi_{2,3}$) has Darbouxian singularities at the points $(u, v) \in \mathbb{R}^2$ such that $\lambda_2(u, v) = \lambda_3(u, v)$ (respectively, $\lambda_1(u, v) = \lambda_2(u, v)$) that are

$$(u, v) = (\pm\sqrt{(E_1 - E_3)(E_2 - E_3)}, 0) \text{ (respectively } (0, \pm\sqrt{(E_1 - E_3)(E_1 - E_2)})).$$

The plot of $\chi_{1,2}$ is made on Figure 5.18. We notice that there is a singularity of Type **(N)** at conical intersections between λ_1 and λ_2 , while there is a Star singularity at conical intersections between λ_2 and λ_3 .

2.2.3 Towards ensemble control with a single input

An important issue of quantum control is to design explicit control laws for the problem of the single input bilinear Schrödinger equation, that is

$$i\frac{d\psi}{dt} = (H_0 + uH_1)\psi \tag{2.12}$$

where ψ belongs to the unit sphere in a Hilbert space \mathcal{H} , H_0 is a self adjoint operator representing a drift term called *free Hamiltonian*, H_1 is a self-adjoint operator representing

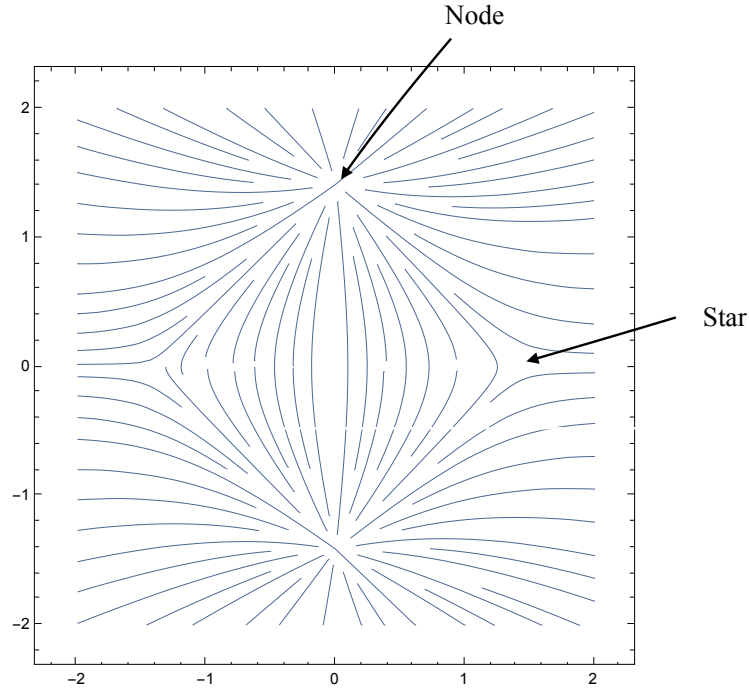


Figure 2.15 – Non mixing field between λ_1 and λ_2 for the STIRAP of Corollary 2.2.10.

the control coupling and $u : [0, T] \rightarrow \mathbb{R}$, $T > 0$. Important theoretical results of controllability have been proved with different techniques (see [7, 12, 17] and references therein). For the problem with two or more inputs, adiabatic methods are a nowadays classical way to get an explicit expression of the controls and can be used under geometric conditions on the spectrum of the controlled Hamiltonian (see the articles [10, 22, 62] and references therein), and our results about these methods are presented in Section 2.2.1 of the Introduction and are developed in Chapter 3. However, these methods are effective for inputs of dimension at least 2. Our aim is then to extend a single-input bilinear Schrödinger equation into a two-inputs bilinear Schrödinger equation in the same spirit as the Lie-extensions introduced by Sussmann and Liu in [66] and [77], then to apply the well-known adiabatic techniques to the extended system. The first step of this procedure is well known by physicists and it is called the rotating-wave approximation (RWA, for short). It is a decoupling approximation to get rid of highly oscillating terms when the system is driven by a real control. This approximation is based on a first-order averaging procedure (see [71, 77, 66, 23] for more informations about averaging of dynamical systems). This approximation is known to work well for a small detuning from the resonance frequency and a small amplitude. For a review of the RWA and its limitations see [37] and [44, 45, 51]. In [24], the mathematical framework has been set for infinite-dimensional quantum systems, formalizing what physicists call *Generalized Rabi oscillations* and showing that the RWA

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is valid for a large class of quantum systems. The adiabatic and RWA involve different time scales, and it is natural to ask whether or not they can be used in cascade. The aim of Chapter 2.2.3 is to show the validity of such an approximation under a certain condition on the time scales involved in the dynamics, using an averaging procedure. Then the well-known results of adiabatic theory (see [22, 18, 78]) can be applied in order to get transitions between the eigenstates of the free Hamiltonian. It leads us to design control laws achieving the inversion of a Spin- $\frac{1}{2}$ particule and population transfers in the STIRAP process that are robust with respect to inhomogeneities of the amplitude of the control input (see [81, 10] and Chapter 3). As a byproduct of the use of a control oscillating with a small frequency detuning, the proposed method is not expected to be robust with respect to inhomogeneities of the resonance frequencies, that is inhomogeneities of the drift term H_0 .

For such systems, when \mathcal{H} is finite dimensional, we use controls under the form

$$u_\epsilon(t) = 2\epsilon^\alpha \sum_{(j,k) \in \{1 \dots N\}^2} v_{jk}(\epsilon^{\alpha+1}t) \cos(\beta_{jk}t + \frac{1}{\epsilon} \phi_{jk}(\epsilon^{\alpha+1}t)),$$

where, for every $j, k \in \{1 \dots N\}$, $v_{jk}, \phi_{jk} \in C^\infty([0, 1], \mathbb{R})$ such that $\phi_{jk}(0) = 0$ and $\beta_{jk} \in \mathbb{R}$, $N \in \mathbb{N} \setminus \{0\}$ and we study the asymptotic behaviour of the associated quantum system (2.12) when $\epsilon \rightarrow 0$ on the interval of time $[0, \frac{1}{\epsilon^{\alpha+1}}]$. Assuming $\alpha > 1$, by a suitable choice of (v_{kj}, ϕ_{kj}) , and β_{kj} for every k, j , we show a general approximation result (see the theorems 6.1.3 and 6.2.11) that allows to explicitly design control laws that are robust with respect to inhomogeneities of the amplitude of the control input.

This result has led us to prove the following results. Let U be an open interval of \mathbb{R} containing 0.

Theorem 2.2.11. *Let $E \in \mathbb{R} \setminus \{0\}$. The equation*

$$i \frac{d\psi}{dt} = \begin{pmatrix} E & \delta u \\ \delta u & -E \end{pmatrix} \psi \tag{2.13}$$

is approximately ensemble controllable between the eigenstates of $H_0 = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$ uniformly with respect to $\delta \in [a, b] \subset (0, +\infty)$ and $u \in U$.

Theorem 2.2.12. *Let $E_1, E_2, E_3 \in \mathbb{R}$ such that $|E_k - E_q| \neq |E_j - E_l|$, for every $k, q, j, l \in \{1 \dots 3\}$ such that $(k, q) \notin \{(j, l), (l, j)\}$. The equation*

$$i \frac{d\psi}{dt} = \begin{pmatrix} E_1 & \delta_1 u & 0 \\ \delta_1 u & E_2 & \delta_2 u \\ 0 & \delta_2 u & E_3 \end{pmatrix} \psi \tag{2.14}$$

is ensemble controllable between eigenstates of $H_0 = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix} \psi$ uniformly with respect to $\delta_1 \in [a_1, b_1] \subset (0, +\infty)$ and $\delta_2 \in [a_2, b_2] \subset (0, +\infty)$ and $u \in U$.

An open question is the ensemble controllability w.r.t. $\delta \in [a, b] \subset (0, +\infty)$ of the equation

$$i \frac{d\psi}{dt} = (H_0 + \delta u H_1) \psi,$$

where $H_0, H_1 \in S_n(\mathbb{R})$, assuming that H_0, H_1 are such that Equation (2.12) is controllable. Of course a similar problem in infinite dimension would be interesting to study. Another topic of study would be to understand how to control robustly with a single input a system where the drift term has uncertainties.

2.2. *Topics of investigation*

Chapter 3

Ensemble control of quantum systems with two controls: conical case

In this Chapter we discuss how to control a parameter-dependent family of quantum systems. Our technique is based on adiabatic approximation theory and on the presence of curves of conical eigenvalue intersections of the controlled Hamiltonian. As particular cases, we recover chirped pulses for two-level quantum systems and counterintuitive solutions for three-level stimulated Raman adiabatic passages. The proposed technique works for systems evolving both in finite-dimensional and infinite-dimensional Hilbert spaces. We show that the assumptions guaranteeing ensemble controllability are structurally stable with respect to perturbations of the parameterized family of systems. The Chapter is mainly taken from [10].

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3.1 Introduction

The chapter is organized as follows: In Section 3.2 we set the ensemble controllability problem and we state our sufficient conditions for approximate ensemble controllability in finite-dimensional spaces. The proof of the sufficiency of such conditions is given in Section 3.3. The proof of the technical result on the regularity of eigenpairs is postponed to the appendix. In Section 3.4 we apply the general result to the case of two-level systems, recovering the classical results on chirped pulses. The extension to permutations within a basis of eigenvectors is studied in Section 3.5. The genericity of the conditions appearing in the sufficient conditions for approximate ensemble controllability is discussed in Section 3.6. In Section 3.7 we consider the case in which the Hamiltonian depends on more than one parameter and we illustrate our results on the STIRAP process. Finally, in Section 3.8, we discuss the extensions to the case of infinite-dimensional spaces, presenting as an example a version of the classical Eberly–Law model.

3.2 Basic definitions and statement of the main results in the finite-dimensional case

For every $n \in \mathbb{N}$, let $\llbracket 1, n \rrbracket$ denote the set of integers $\{1, \dots, n\}$. Let \mathbf{U} be an open connected subset of \mathbb{R}^d , $d \geq 2$.

We consider the controlled Schrödinger equation in \mathbb{C}^N , $N \in \mathbb{N}$,

$$i\dot{\psi} = H^z(u(t))\psi \tag{3.1}$$

where $u : \mathbb{R} \rightarrow \mathbf{U}$ is a L^∞ map. Here z is a time-independent parameter belonging to a compact interval $[z_0, z_1] \subset \mathbb{R}$. Each matrix $H^z(u)$ belongs to the set $\text{Herm}(N)$ of $N \times N$ Hermitian matrices. The map $(z, u) \mapsto H^z(u)$ is sufficiently regular, as it will be specified later on.

Denote the spectrum of $H^z(u)$ by $(\lambda_j^z(u))_{j=1}^N$ where $j \mapsto \lambda_j^z(u)$ is the nondecreasing sequence of eigenvalues of $H^z(u)$ repeated according to their multiplicities. We also write $(\phi_1^z(u), \dots, \phi_N^z(u))$ to denote an orthonormal basis of associated eigenvectors.

Definition 3.2.1. *We say that system (3.1) is ensemble approximately controllable between eigenstates if for every $\varepsilon > 0$, $j, k \in \llbracket 1, N \rrbracket$ and $u_0, u_1 \in \mathbf{U}$ such that $\lambda_j^z(u_0)$ and $\lambda_k^z(u_1)$ are simple for every $z \in [z_0, z_1]$, there exists a control $u(\cdot) : [0, T] \rightarrow \mathbf{U}$ such that for every $z \in [z_0, z_1]$ the solution of (3.1) with initial condition $\psi^z(0) = \phi_j^z(u_0)$ satisfies $\|\psi^z(T) - e^{i\theta} \phi_k^z(u_1)\| < \varepsilon$ for some $\theta \in \mathbb{R}$ (possibly depending on z and ε).*

Remark 3.2.2. The typical case of interest is when $u = 0 \in \mathbf{U}$ represents an isolated (i.e., uncontrolled) system (the so-called drift Hamiltonian) and one seeks to steer $\phi_j^z(0)$ towards $\phi_k^z(0)$ for some $j, k \in \llbracket 1, N \rrbracket$.

Definition 3.2.3. Let us fix $z \in [z_0, z_1]$. We say that $\bar{u} \in \mathbf{U}$ is a conical intersection between λ_j^z and λ_{j+1}^z if $\lambda_{j-1}^z(\bar{u}) < \lambda_j^z(\bar{u}) = \lambda_{j+1}^z(\bar{u}) < \lambda_{j+2}^z(\bar{u})$ and there exists $c > 0$ such that for every v in a neighborhood of \bar{u} in \mathbf{U} , we have

$$\|\lambda_j^z(v) - \lambda_{j+1}^z(v)\| \geq c\|\bar{u} - v\|.$$

(As example of conical intersection is shown in Figure 3.1.)

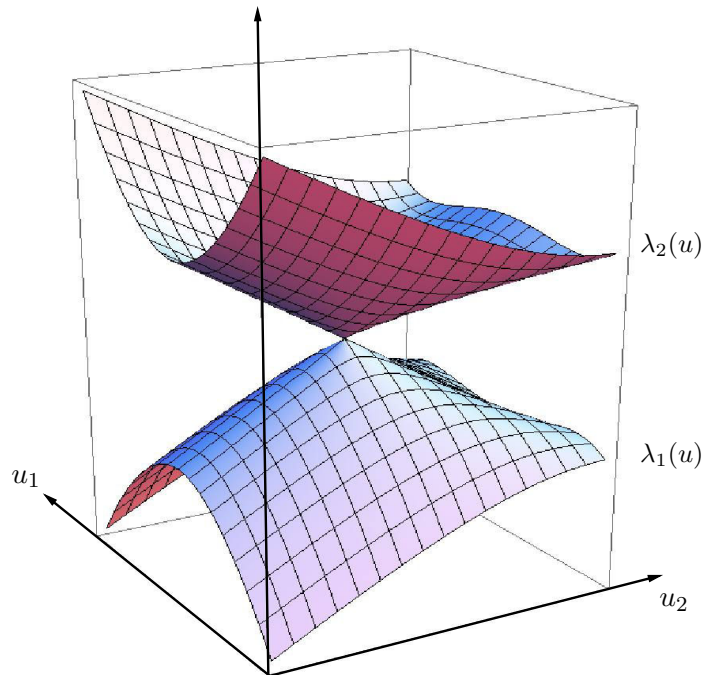


Figure 3.1 – An example of conical intersection in the case $d = N = 2$.

For $j \in \{1 \dots n\}$, let us denote by γ_j the set $\{(u, z) \in \mathbf{U} \times [z_0, z_1] \mid \lambda_j^z(u) = \lambda_{j+1}^z(u)\}$, where by convention $\gamma_0 = \gamma_n = \emptyset$. Denote the projection of $(u, z) \in \mathbb{R}^{d+1}$ onto the u -component by π .

Then $\pi(\gamma_j)$ is the projection of the set $\{(u, z) \in \mathbf{U} \times [z_0, z_1] \mid \lambda_j^z(u) = \lambda_{j+1}^z(u)\}$ onto the u -component, that is,

$$\begin{aligned} \pi(\gamma_0) &= \emptyset, \\ \pi(\gamma_j) &= \{u \in \mathbf{U} \mid \exists z \in [z_0, z_1] \text{ such that } \lambda_j^z(u) = \lambda_{j+1}^z(u)\}, \quad j \in \llbracket 1, N-1 \rrbracket, \\ \pi(\gamma_N) &= \emptyset. \end{aligned}$$

Assumption A_j . There exist a connected component $\hat{\gamma}_j$ of γ_j and a map $\beta_j : [z_0, z_1] \rightarrow \mathbf{U}$ such that β_j is a \mathcal{C}^3 embedding and

3.2. Basic definitions and statement of the main results in the finite-dimensional case

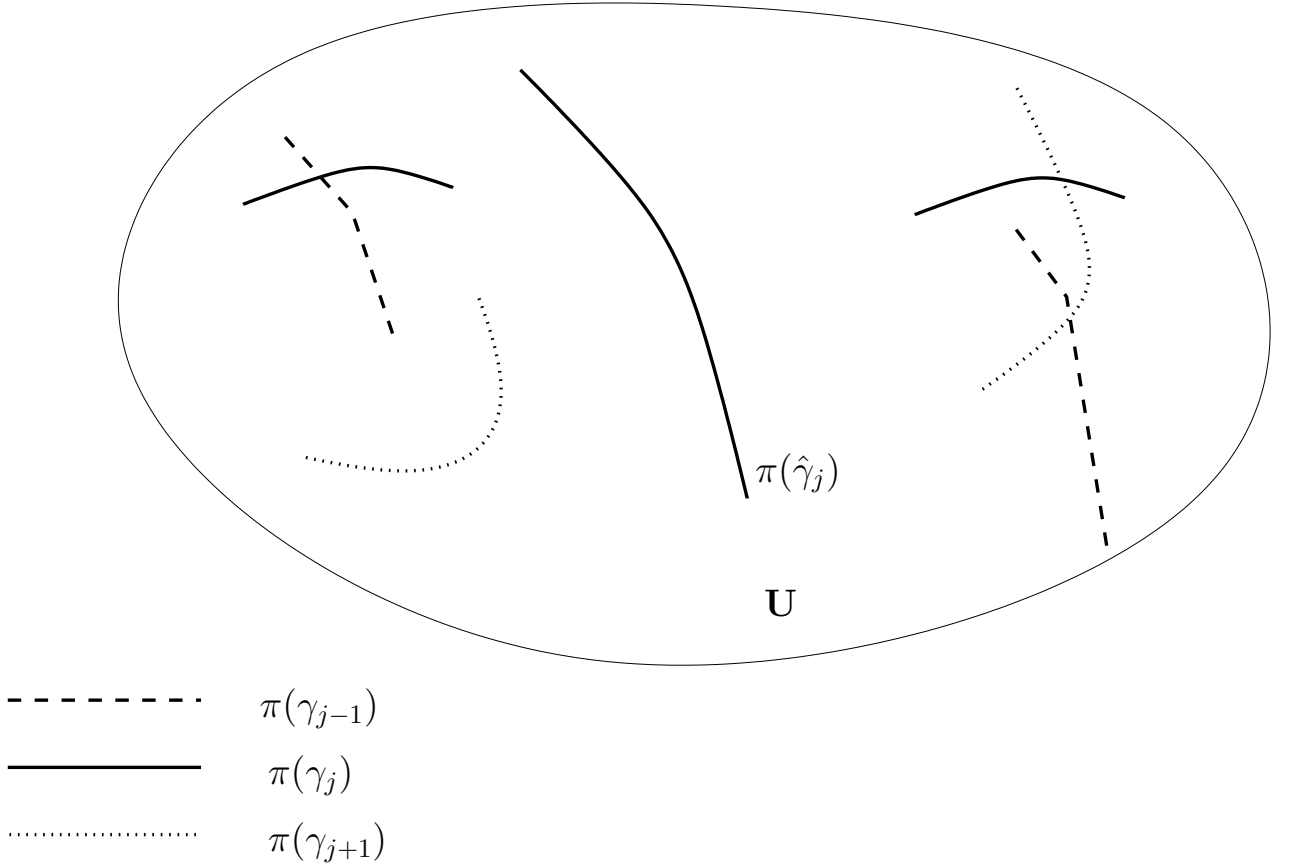


Figure 3.2 – The component $\hat{\gamma}_j$ is such that Assumption A_j is satisfied

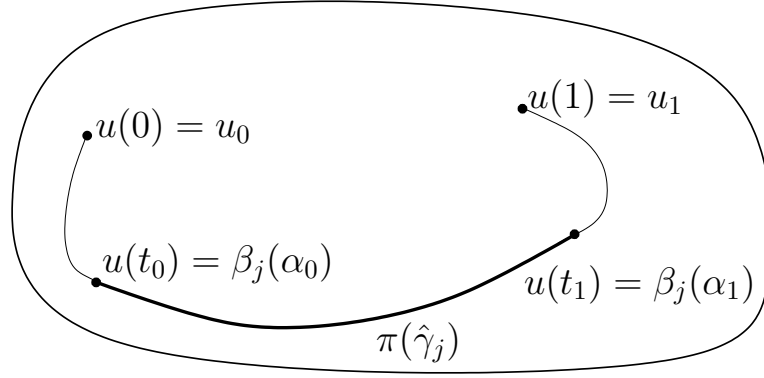
- $\pi(\hat{\gamma}_j) = \beta_j([z_0, z_1])$
- $\pi(\hat{\gamma}_j)$ is contained in $\mathbf{U} \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_{j+1}))$
- For every $z \in [z_0, z_1]$, λ_j^z and λ_{j+1}^z have a unique intersection on $\pi(\hat{\gamma}_j)$, which is conical and occurs at $\beta_j(z)$.

Moreover the set $\mathbf{U} \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_j) \cup \pi(\gamma_{j+1}))$ is pathwise connected.

Remark 3.2.4. The assumption that β_j is an embedding between the set of parameters $[z_0, z_1]$ and $\pi(\hat{\gamma}_j)$ is used here for simplicity and can be relaxed. This will be done in the general context of multi-dimensional sets of parameters in Section 3.7 (see Assumption A_j^*).

The structural stability and the genericity of Assumption A_j are discussed in Section 3.6. In the following theorem we show that the curve $\pi(\hat{\gamma}_j)$ appearing in Assumption A_j can be used to induce an adiabatic transition between the j -th and the $(j + 1)$ -th eigenstate for every z .

Theorem 3.2.5. Consider a \mathcal{C}^3 map $[z_0, z_1] \times \mathbf{U} \ni (z, u) \mapsto H^z(u) \in \text{Herm}(N)$. Let $j \in \llbracket 1, N - 1 \rrbracket$ be such that Assumption A_j is satisfied. Take $u_0, u_1 \in \mathbf{U} \setminus (\pi(\gamma_{j-1}) \cup$


 Figure 3.3 – A control $u(\cdot)$ as in the statement of Theorem 3.2.5.

$\pi(\gamma_j) \cup \pi(\gamma_{j+1})$) and consider a \mathcal{C}^3 path $u(\cdot) : [0, 1] \rightarrow \mathbf{U}$ satisfying $u(0) = u_0$, $u(1) = u_1$, and such that $u|_{[t_0, t_1]}$ is a reparameterization of β_j for some $0 < t_0 < t_1 < 1$ such that $u(t) \notin \pi(\gamma_{j-1}) \cup \pi(\gamma_j) \cup \pi(\gamma_{j+1})$ for every $t \in [0, 1] \setminus [t_0, t_1]$. (See Figure 3.3.) Assume, moreover, that $\dot{u}(t) \neq 0$ for every $t \in [0, 1]$.

Then there exists a constant $C > 0$ such that for every $z \in [z_0, z_1]$ and $\varepsilon > 0$ the solutions $\psi_\varepsilon^{z, \pm}$ of

$$i\dot{\psi}_\varepsilon^{z, \pm}(t) = H^z(u(\varepsilon t))\psi_\varepsilon^{z, \pm}(t)$$

with initial conditions

$$\psi_\varepsilon^{z, +}(0) = \phi_j^z(u_0), \quad \psi_\varepsilon^{z, -}(0) = \phi_{j+1}^z(u_0) \quad (3.2)$$

satisfy

$$\|\psi_\varepsilon^{z, +}(1/\varepsilon) - e^{i\theta^+} \phi_{j+1}^z(u_1)\| \leq C\sqrt{\varepsilon}, \quad \|\psi_\varepsilon^{z, -}(1/\varepsilon) - e^{i\theta^-} \phi_j^z(u_1)\| \leq C\sqrt{\varepsilon}, \quad (3.3)$$

for some $\theta^\pm \in \mathbb{R}$.

Remark 3.2.6. By unitarity of the evolution, if in the statement of Theorem 3.2.5 we replace the initial conditions (3.2) by

$$\|\psi_\varepsilon^{z, +}(0) - \phi_j^z(u_0)\| \leq c, \quad \|\psi_\varepsilon^{z, -}(0) - \phi_{j+1}^z(u_0)\| \leq c,$$

then the conclusion (3.3) becomes

$$\|\psi_\varepsilon^{z, +}(1/\varepsilon) - e^{i\theta^+} \phi_{j+1}^z(u_1)\| \leq C\sqrt{\varepsilon} + c, \quad \|\psi_\varepsilon^{z, -}(1/\varepsilon) - e^{i\theta^-} \phi_j^z(u_1)\| \leq C\sqrt{\varepsilon} + c.$$

Corollary 3.2.7. Consider a \mathcal{C}^3 map $[z_0, z_1] \times \mathbf{U} \ni (z, u) \mapsto H^z(u) \in \text{Herm}(N)$. Let Assumption A_j be satisfied for every $j \in \llbracket 1, N-1 \rrbracket$. Then (3.1) is ensemble approximately controllable between eigenstates.

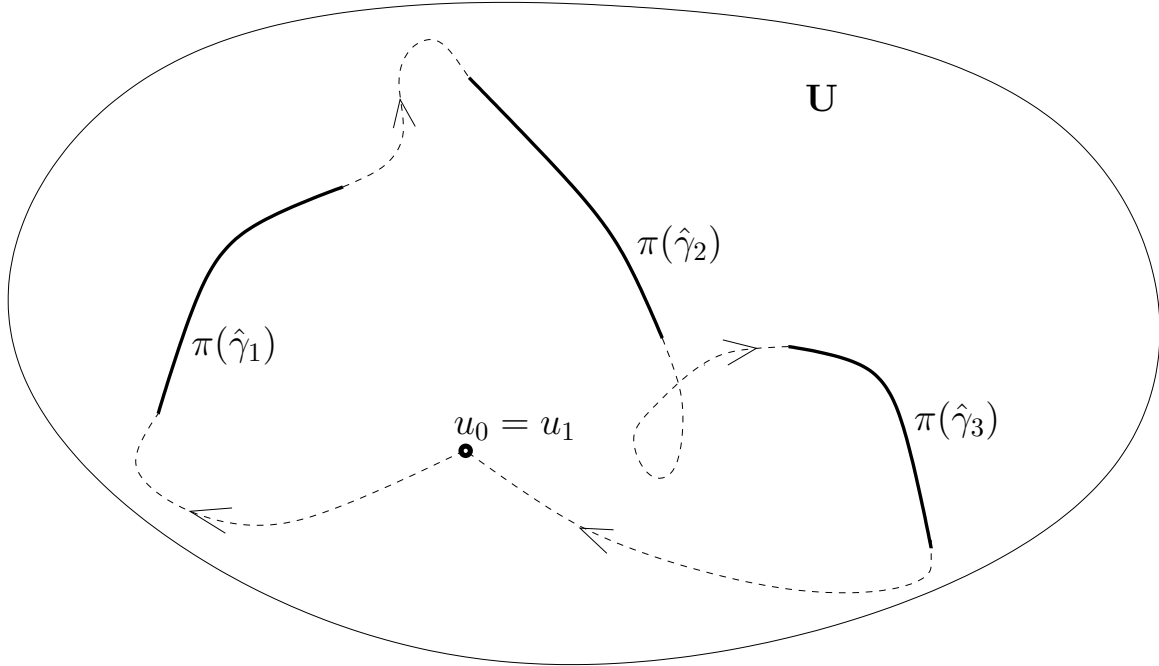


Figure 3.4 – A control realizing an ensemble transition between $\phi_1^z(u_0)$ and $\phi_4^z(u_0)$.

The corollary follows from an iterated application of Theorem 3.2.5 and its proof works by constructing a \mathcal{C}^3 control such that $u(0) = u_0$ and $u(T) = u_1$ (where u_0 and u_1 are as in Definition 3.2.1) and going through the curves $\pi(\hat{\gamma}_j)$ as in Figure 3.4. Starting from the second iteration of the application of Theorem 3.2.5, we use Remark 3.2.6 with c of order $\sqrt{\varepsilon}$ to guarantee that the adiabatic approximation after each iteration remains of order $\sqrt{\varepsilon}$.

Remark 3.2.8. *The proof of Theorem 3.2.5 is based on a uniform adiabatic theorem, which is recalled in next section (Theorem 3.3.1). Actually, under the additional hypothesis that the curves $\pi(\hat{\gamma}_j)$ are non-mixing for every $z \in [z_0, z_1]$, in the sense of [22, Section V], one can replace the factor $\sqrt{\varepsilon}$ in (3.3) and (3.4) by ε .*

3.3 Proof of the ensemble controllability result in the finite-dimensional case

Theorem 3.3.1. *Consider a \mathcal{C}^3 map $[z_0, z_1] \times \mathbf{U} \ni (z, u) \mapsto H^z(u) \in \text{Herm}(N)$. Let $u : [0, 1] \rightarrow \mathbf{U}$ be a \mathcal{C}^2 control. For every $z \in [z_0, z_1]$ and $t \in [0, 1]$, let $\Lambda_1^z(t), \dots, \Lambda_N^z(t)$ be the eigenvalues of $H^z(u(t))$ repeated according to their multiplicities and denote by $(\Phi_1^z(t), \dots, \Phi_N^z(t))$ an orthonormal basis of associated eigenvectors.*

Assume that for every $z \in [z_0, z_1]$ and every $j \in \llbracket 1, N \rrbracket$,

$$(\Lambda_j^z, \Phi_j^z) \in \mathcal{C}^2([0, 1], \mathbb{R} \times \mathbb{C}^N).$$

Let $j \in \llbracket 1, N-1 \rrbracket$ and assume that for every $z \in [z_0, z_1]$, there exists $\tau \in (0, 1)$ such that $\Lambda_j^z(t)$ and $\Lambda_{j+1}^z(t)$ are simple for every $t \in [0, 1] \setminus \{\tau\}$ and

$$\Lambda_j^z(\tau) = \Lambda_{j+1}^z(\tau) \neq \Lambda_m^z(\tau) \text{ for } m \neq j, j+1, \quad \frac{d}{dt} \Big|_{t=\tau} \Lambda_j^z(t) \neq \frac{d}{dt} \Big|_{t=\tau} \Lambda_{j+1}^z(t).$$

Then there exists $C > 0$ such that for every $z \in [z_0, z_1]$, and every $\varepsilon > 0$ the solution $\psi = \psi_\varepsilon^z$ of the equation

$$i\dot{\psi}(t) = H^z(u(\varepsilon t))\psi(t)$$

with initial condition $\psi(0) = \Phi_j^z(0)$ satisfies

$$\|\psi(1/\varepsilon) - e^{i\theta} \Phi_j^z(1)\| \leq C\sqrt{\varepsilon} \quad (3.4)$$

for some $\theta \in \mathbb{R}$.

The proof of this theorem can be obtained by applying the classical adiabatic theorem for every z , using the continuity of the corresponding constant $C(z)$ and the compactness of the interval $[z_0, z_1]$ (see for instance [52, Theorem 4] and [78, Theorem 1.2]).

In order to guarantee the regularity of eigenvalues and eigenvectors along a regular but not necessarily analytic path in the domain of admissible controls, we are going to apply the following result, whose proof is given in the appendix. (For a result in the same spirit in the infinite-dimensional setting, see [30].)

Lemma 3.3.2. *Let I be an interval in \mathbb{R} and take $H \in \mathcal{C}^{k+1}(I, \text{Herm}(N))$, $k \geq 0$. For every $t \in I$, let $\lambda_1(t) \leq \dots \leq \lambda_N(t)$ be the eigenvalues of $H(t)$, repeated according to their multiplicities. Assume that for every $\bar{t} \in I$ and every $j \in \llbracket 1, N-1 \rrbracket$ such that $\lambda_j(\bar{t}) = \lambda_{j+1}(\bar{t})$, then $\lambda_h(\bar{t}) \neq \lambda_j(\bar{t})$ for $h \neq j, j+1$ and there exist $c > 0$ and a neighborhood \bar{I} of \bar{t} in I such that*

$$\lambda_{j+1}(t) - \lambda_j(t) \geq c|t - \bar{t}|, \quad \text{for every } t \in \bar{I}. \quad (3.5)$$

Then there exist $\Lambda_1, \dots, \Lambda_N \in \mathcal{C}^{k+1}(I, \mathbb{R})$ and $\Phi_1, \dots, \Phi_N \in \mathcal{C}^k(I, \mathbb{C}^N)$ such that, for every $t \in I$, $\Lambda_1(t), \dots, \Lambda_N(t)$ are the eigenvalues of $H(t)$ repeated according to their multiplicities and $(\Phi_1(t), \dots, \Phi_N(t))$ is an orthonormal basis of corresponding eigenvectors. Moreover, Φ_1, \dots, Φ_n are $\mathcal{C}^{k+1}(I, \mathbb{C}^N)$ if all eigenvalues of H are simple along I .

Proof of Theorem 3.2.5. We are going to apply Theorem 3.3.1 on the path $u(\cdot)$. Notice that for every z the curve $u(\cdot)$ passes through exactly one point \bar{u}^z such that $\lambda_j^z(\bar{u}^z) = \lambda_{j+1}^z(\bar{u}^z)$ and through no point $v \in \mathbf{U}$ where either $\lambda_{j-1}^z(v) = \lambda_j^z(v)$ or $\lambda_{j+1}^z(v) = \lambda_{j+2}^z(v)$. Denote by t_z the time such that $u(t_z) = \bar{u}^z$.

By Lemma 3.3.2 applied to the map $t \mapsto H(u(t))$, we can assume that

$$[0, 1] \ni t \mapsto (\Lambda_j^z(t), \Phi_j^z(t)) = \begin{cases} (\lambda_j^z(u(t)), \phi_j^z(u(t))) & \text{if } t < t_z \\ (\lambda_{j+1}^z(u(t)), \phi_{j+1}^z(u(t))) & \text{if } t \geq t_z \end{cases}$$

3.4. Example 1: Two-level system driven by a chirped pulse

is \mathcal{C}^2 for every $j \in \llbracket 1, N \rrbracket$ and every $z \in [z_0, z_1]$. The application of Theorem 3.3.1 then concludes the proof of Theorem 3.2.5. \square

Remark 3.3.3. *In Theorem 3.2.5 the control $u(\cdot)$ is assumed to be \mathcal{C}^3 . The \mathcal{C}^3 regularity could actually be relaxed. The same proof would work, for instance, by assuming $u(\cdot)$ to be continuous, \mathcal{C}^3 in a neighborhood of $\pi(\hat{\gamma}_j)$ and piecewise \mathcal{C}^2 elsewhere.*

3.4 Example 1: Two-level system driven by a chirped pulse

A classical example of ensemble control by adiabatic evolution is the famous chirped pulse used in two-level systems. It is used, for instance, for controlling via magnetic fields an ensemble of spin systems with slightly different parameters. We illustrate chirped pulses on the following model

$$i \frac{d}{dt} \begin{pmatrix} \psi_1^z \\ \psi_2^z \end{pmatrix} = \begin{pmatrix} E + z & \Omega(t) \\ \Omega^*(t) & -E - z \end{pmatrix} \begin{pmatrix} \psi_1^z \\ \psi_2^z \end{pmatrix}, \quad (3.6)$$

where $E > 0$ is fixed, $\Omega(\cdot) \in L^\infty([0, T], \mathbb{C})$ is the control, $\Omega^*(t)$ denotes its complex conjugate, and z is a real parameter that can vary in a fixed range $z \in [z_0, z_1] \subset (-E, \infty)$. The quantity $E + z$ is called the *proper frequency* of system (3.6).

Chirped pulses are well studied in the literature (see [27, 74, 62]). We show here below how they naturally show up in the general framework proposed in this paper. Consider the following ensemble approximate controllability problem for (3.6): we want to construct explicitly a control steering, for every value of $z \in [z_0, z_1]$, the eigenstate $\phi_1^z(0) = (1, 0)$ to $\phi_2^z(0) = (0, 1)$ of the Hamiltonian in (3.6) corresponding to $\Omega = 0$.

Theorem 3.2.5 and Corollary 3.2.7 do not directly apply to system (3.6) since the eigenvalues of the Hamiltonian are simple for every value of $z \in [z_0, z_1]$ and $\Omega \in \mathbb{C}$.

Hence we perform a suitable time-dependent change of variables (to recast the system in interaction picture). In order to do so, we consider controls having the form

$$\Omega(t) = u_1(t)e^{-i(2Et+\Delta(t))}, \quad (3.7)$$

where $u_1(\cdot)$ and $\Delta(\cdot)$ are real-valued, and we set

$$h^z(t) = \begin{pmatrix} E + z & u_1(t)e^{-i(2Et+\Delta(t))} \\ u_1(t)e^{i(2Et+\Delta(t))} & -E - z \end{pmatrix}.$$

Let us apply the time-dependent unitary change of variable $\psi^z(t) = U(t)\Phi^z(t)$ with

$$U(t) = \begin{pmatrix} e^{-iEt} & 0 \\ 0 & e^{i(Et+\Delta(t))} \end{pmatrix}.$$

Notice that the transformation $U(t)$ preserves (up to phases) the two eigenstates $\phi_1^z(0) = (1, 0)$ and $\phi_2^z(0) = (0, 1)$.

Then Φ^z satisfies the equation $i\frac{d}{dt}\Phi^z = \mathcal{H}^z(t)\Phi^z$ with

$$\mathcal{H}^z(t) = U^{-1}(t)h^z(t)U(t) - iU^{-1}(t)\frac{dU}{dt}(t) = \begin{pmatrix} z & u_1(t) \\ u_1(t) & -z + \frac{d\Delta}{dt}(t) \end{pmatrix}.$$

Setting $u_2(t) = \frac{d\Delta}{dt}(t)$, we are then left to control the family of systems

$$i\frac{d}{dt} \begin{pmatrix} \Phi_1^z \\ \Phi_2^z \end{pmatrix} = \begin{pmatrix} z & u_1(t) \\ u_1(t) & -z + u_2(t) \end{pmatrix} \begin{pmatrix} \Phi_1^z \\ \Phi_2^z \end{pmatrix}. \quad (3.8)$$

We apply now Theorem 3.2.5 to system (3.8). To this purpose we have to check that Assumption A_1 is satisfied. Set

$$H^z(u_1, u_2) = \begin{pmatrix} z & u_1 \\ u_1 & -z + u_2 \end{pmatrix}.$$

The eigenvalues of $H^z(u_1, u_2)$ are

$$\lambda_1^z(u_1, u_2) = \frac{u_2 - \sqrt{(2z - u_2)^2 + 4u_1^2}}{2}, \quad \lambda_2^z(u_1, u_2) = \frac{u_2 + \sqrt{(2z - u_2)^2 + 4u_1^2}}{2}.$$

For any fixed $z \in [z_0, z_1]$, H^z has a unique eigenvalue intersection, which is conical and takes place at

$$(u_1, u_2) = (0, 2z).$$

In other words for each point of the set

$$\pi(\gamma_1) = \{(0, 2z) \in \mathbb{R}^2 \mid z \in [z_0, z_1]\} = \{0\} \times [2z_0, 2z_1]$$

there is exactly one system having an eigenvalue intersection at such a point, which is, moreover, conical. Assumption A_1 is then satisfied.

By applying Corollary 3.2.7 to system (3.8) we deduce the following result.

Proposition 3.4.1. *System (3.8) is ensemble approximately controllable between eigenstates.*

The controls used to achieve the controllability stated in Proposition 3.4.1 can be taken continuous, \mathcal{C}^3 in a neighborhood of $\pi(\gamma_1)$ and piecewise \mathcal{C}^2 elsewhere (see Remark 3.3.3). Notice that the same regularity holds for Ω , according to (3.7).

As a consequence of Proposition 3.4.1 we can steer (up to phases) system (3.8) (simultaneously with respect to $z \in [z_0, z_1]$) from $(1, 0)$ to an arbitrary neighborhood of $(0, 1)$, which are eigenstates of $\mathcal{H}^z(0, u_{20})$ for every $u_{20} \in \mathbb{R} \setminus [2z_0, 2z_1]$. Now, since $U(t)$

3.4. Example 1: Two-level system driven by a chirped pulse

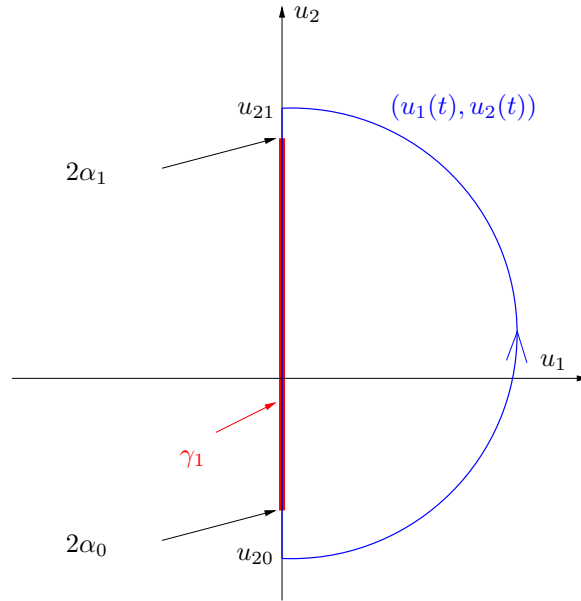


Figure 3.5 – The control $u(\cdot)$.

preserves (up to phases) $(1, 0)$ and $(0, 1)$, we can conclude that system (3.6) can be steered simultaneously by adiabatic control from $(1, 0)$ to $(0, 1)$ for every $z \in [z_0, z_1]$. Notice that the control $u = (0, u_{20})$ corresponds to $\Omega = 0$ in the original system, independently of u_{20} .

We now construct explicitly the adiabatic control realizing the transition. We start by doing this for (3.8) and then we translate the result for (3.6).

Let u_{21} be in the connected component of $\mathbb{R} \setminus [2z_0, 2z_1]$ not containing u_{20} (see Figure 3.5). Let $u : [0, 1/2] \rightarrow \mathbb{R}^2$ be a path following a curve contained in the right half-plane connecting $(0, u_{20})$ to $(0, u_{21})$. Complete the path u by letting $u : [1/2, 1] \rightarrow \mathbb{R}^2$ follow a straight segment from $(0, u_{21})$ to $(0, u_{20})$. The path $u(\cdot)$ is such that $t \mapsto u(\varepsilon t)$ yields the desired ensemble approximate transition when $\varepsilon \rightarrow 0$.

In terms of the original system, the control Ω obtained from u as in (3.7) is identically equal to zero on $[1/2, 1]$. Hence, the evolution corresponding to this portion of the control u has no effect on the dynamics and can be ignored. The original system is then controlled by

$$\Omega(\varepsilon t) = u_1(\varepsilon t) e^{-i(2Et + \frac{1}{\varepsilon} \int_0^{\varepsilon t} u_2(s) ds)}$$

with $t \in [0, \frac{1}{2\varepsilon}]$. Notice that $t \mapsto \Omega(\varepsilon t)$ is a complex function with slow-varying modulus and a phase oscillating with a frequency given by

$$\frac{d}{dt} \left(2Et + \frac{1}{\varepsilon} \int_0^{\varepsilon t} u_2(s) ds \right) = 2E + u_2(\varepsilon t).$$

Since $u_2(0) = u_{20}$ and $u_2(1/2) = u_{21}$, such a frequency slowly varies between two values, one smaller and one larger than every proper frequency $E+z$ of system (3.6) (see Figure 3.6 for an example).

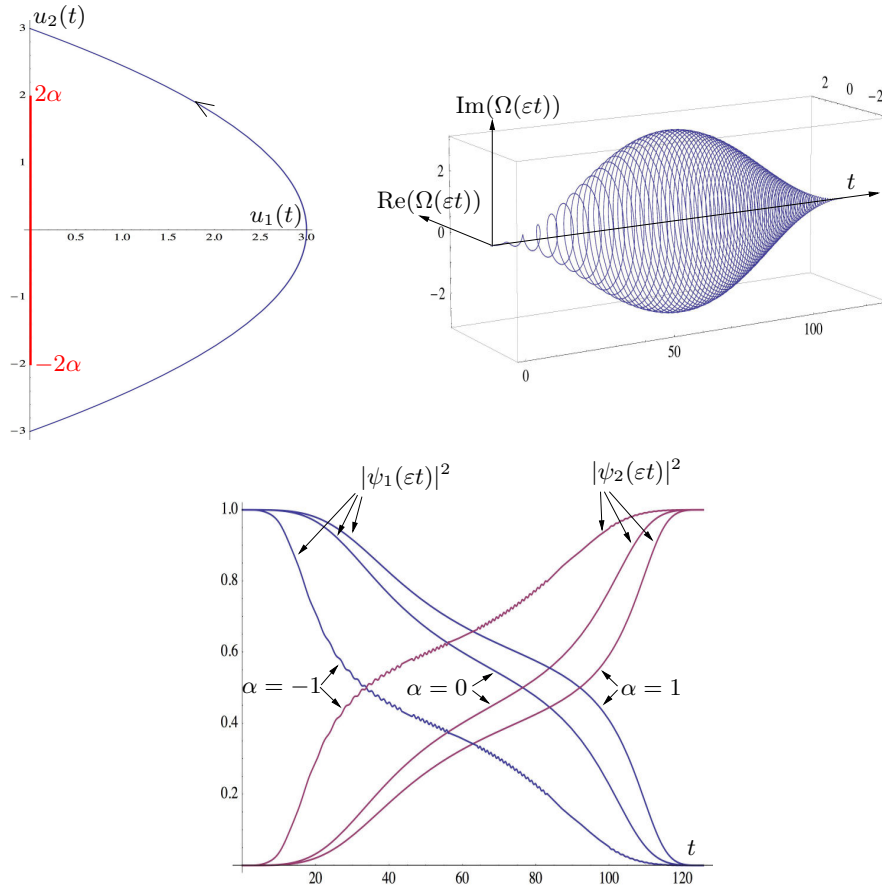


Figure 3.6 – Two-level system driven by a chirped pulse. Here $E = 2$, $z \in [-1, 1]$, $u_1(t) = \frac{3}{2}(1 - \cos(4\pi t))$, $u_2(t) = -3 \cos(2\pi t)$, for $t \in [0, \frac{1}{2}]$ and $\varepsilon = 0.004$. The frequency of the pulse is $2E + u_2(\varepsilon t) = 4 - 3 \cos(2\pi \varepsilon t)$ which varies monotonically between 1 and 7.

3.5. Permutations

Let us conclude by a remark on the precision of the adiabatic estimate. According to Theorem 3.2.5, the precision of the transition of system (3.8) corresponding to $u : [0, 1] \rightarrow \mathbb{R}^2$ is of order $\sqrt{\varepsilon}$. Taking into account, moreover, Remark 3.2.8, the precision is of order ε . For what concerns system (3.6), we are just interested, as we have seen, to the restriction of u on the interval $[0, 1/2]$ and its corresponding control Ω . Hence, since u crosses no eigenvalue intersection on $[0, 1/2]$, one can conclude that the precision of the adiabatic transition is of order ε even without recalling Remark 3.2.8.

3.5 Permutations

Inspired by [62], we refine in this section our approach in order to select adiabatic controls performing a prescribed permutation of the eigenvectors of the controlled Hamiltonian.

The set of assumptions A_j , $j \in \llbracket 1, N-1 \rrbracket$, is replaced by the slightly stronger assumption **P** below (see Figure 3.7 for an illustration).

Assumption P. For every $j \in \llbracket 1, N-1 \rrbracket$ there exist a connected component $\hat{\gamma}_j$ of γ_j and a map $\beta_j : [z_0, z_1] \rightarrow \mathbf{U}$ such that β_j is a \mathcal{C}^3 embedding and

- $\pi(\hat{\gamma}_j) = \beta_j([z_0, z_1])$.
- $\pi(\hat{\gamma}_j)$ is contained in $\mathbf{U} \setminus (\cup_{k \in \llbracket 1, N \rrbracket, k \neq j} \pi(\gamma_k))$
- For every $z \in [z_0, z_1]$, λ_j^z and λ_{j+1}^z have a unique intersection on $\hat{\gamma}_j$, which is conical and occurs at $\beta_j(z)$.

Moreover the set $\mathbf{U} \setminus (\cup_{k \in \llbracket 1, N \rrbracket} \pi(\gamma_k))$ is pathwise connected.

Under Assumption **P**, Corollary 3.2.7 can be refined as follows.

Theorem 3.5.1. Assume that **P** is satisfied. Then for every $u_0, u_1 \in \mathbf{U} \setminus (\cup_{k \in \llbracket 1, N \rrbracket} \pi(\gamma_k))$, every $p_1, \dots, p_N \in \mathbb{C}$ such that $|p_1|^2 + \dots + |p_N|^2 = 1$ and every permutation $\sigma : \llbracket 1, N \rrbracket \rightarrow \llbracket 1, N \rrbracket$, there exists a \mathcal{C}^3 path $u(\cdot) : [0, 1] \rightarrow \mathbf{U}$ satisfying $u(0) = u_0$ and $u(1) = u_1$ and a constant $C > 0$ such that for every $z \in [z_0, z_1]$ and $\varepsilon > 0$ the solution ψ_ε^z of

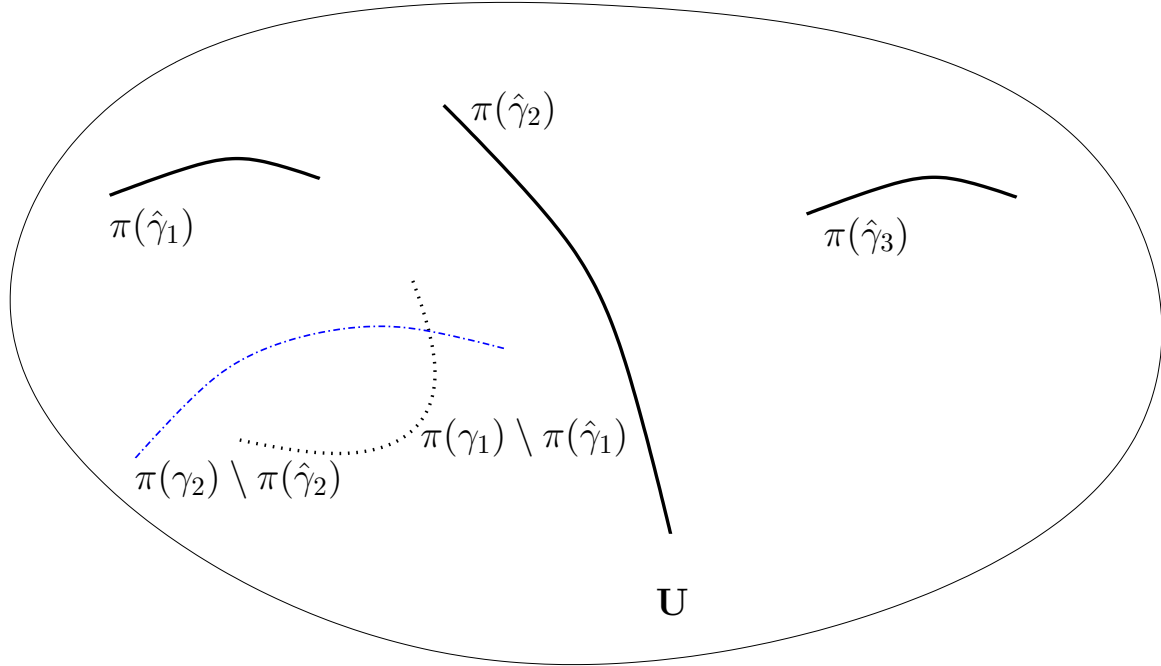
$$i\dot{\psi}_\varepsilon^z = H^z(u(\varepsilon t))\psi_\varepsilon^z$$

with initial condition $\psi_\varepsilon^z(0) = \sum_{j=1}^N p_j \phi_j^z(u_0)$, satisfies

$$\|\psi_\varepsilon^z(1/\varepsilon) - \sum_{j=1}^N p_j e^{i\theta_j} \phi_{\sigma(j)}^z(u_1)\| \leq C\sqrt{\varepsilon},$$

for some $\theta_1, \dots, \theta_N \in \mathbb{R}$.

Proof. The path $u(\cdot)$ is constructively obtained by requiring it to pass through the curves $\hat{\gamma}_j$ in a suitable order. Such an order is identified by the algorithm described below.


 Figure 3.7 – A situation in which Assumption **P** is verified.

Let $h \in \llbracket 1, N \rrbracket$. We say that the functions $f_1, \dots, f_h : [0, 1] \rightarrow \mathbb{R}$ satisfy property (Π_h) if they are continuous, piecewise affine, such that $f_j(0) = j$, $f_j(1) = \sigma(j)$ for $j \in \llbracket 1, h \rrbracket$ and, moreover, if for every $t \in (0, 1)$ and $j \neq k$, $j, k \in \llbracket 1, h \rrbracket$ such that $f_j(t) = f_k(t)$ we have

- $f_l(t) \neq f_m(t)$ for every $l \in \llbracket 1, h \rrbracket \setminus \{j, k\}$, $m \in \llbracket 1, h \rrbracket \setminus \{l\}$,
- $(f_j(t + \varepsilon) - f_k(t + \varepsilon))(f_j(t - \varepsilon) - f_k(t - \varepsilon)) < 0$ for every $\varepsilon > 0$ small enough.

We now construct recursively a set of functions f_1, \dots, f_N satisfying (Π_N) .

Let f_1 and f_2 be the affine functions uniquely determined by $f_1(0) = 1$, $f_2(0) = 2$, $f_1(1) = \sigma(1)$, $f_2(1) = \sigma(2)$. Notice that they satisfy (Π_2) .

By induction, assume to have selected f_1, \dots, f_h satisfying (Π_h) .

Let f_{h+1} be the affine function satisfying $f_{h+1}(0) = h + 1$, $f_{h+1}(1) = \sigma(h + 1)$. If (Π_{h+1}) is satisfied then the recursion step is complete. Otherwise modify f_{h+1} into a continuous function that is constantly equal to $h + 1$ in an interval $[0, \eta]$ and affine on $[\eta, 1]$, with the same boundary conditions. For every positive small enough η one has that f_1, \dots, f_{h+1} satisfy (Π_{h+1}) and this concludes the induction step.

For every $t \in [0, 1]$ let $\sigma_t : \llbracket 1, N \rrbracket \rightarrow \llbracket 1, N \rrbracket$ be a permutation such that

$$f_{\sigma_t(1)}(t) \leq f_{\sigma_t(2)}(t) \leq \dots \leq f_{\sigma_t(N)}(t).$$

Notice that $t \mapsto \sigma_t$ is piecewise constant and $\sigma_0 = \text{Id}$, $\sigma_1 = \sigma$.

Let $t_1 < t_2 < \dots < t_\mu$ be the values in $(0, 1)$ at which the graphs of the functions

3.5. Permutations

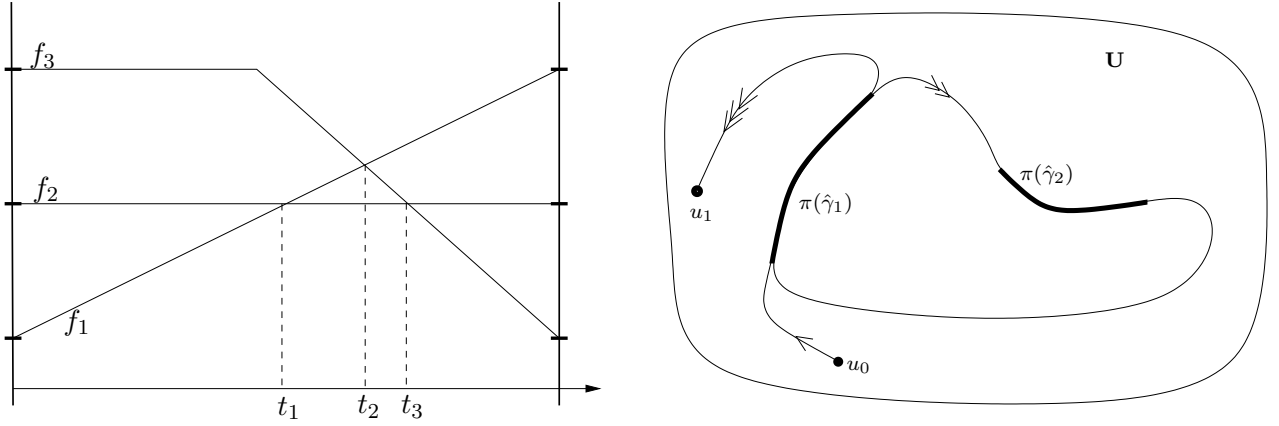


Figure 3.8 – On the left, the functions f_j and the times t_k . On the right, the control $u(\cdot)$. In this case $N = 3$, $\mu = 3$, $\tau(1) = 1$, $\tau(2) = 2$, $\tau(3) = 1$. Hence, $u(\cdot)$ passes through $\pi(\hat{\gamma}_1)$, $\pi(\hat{\gamma}_2)$, and again $\pi(\hat{\gamma}_1)$ while connecting u_0 to u_1 .

f_1, \dots, f_n intersect (see Figure 3.8). Then t_1, \dots, t_μ are the discontinuity points of $t \mapsto \sigma_t$. For every $j \in \llbracket 1, \mu \rrbracket$, let $\tau(j) \in \llbracket 1, N - 1 \rrbracket$ be defined by

$$f_{\sigma_{t_j}(\tau(j))}(t_j) = f_{\sigma_{t_j}(\tau(j)+1)}(t_j).$$

The control $u(\cdot)$ is constructed in such a way that it passes through $\pi(\hat{\gamma}_{\tau(1)}), \dots, \pi(\hat{\gamma}_{\tau(\mu)})$. More precisely let s_1, \dots, s_μ be such that $0 =: t_0 < s_0 < t_1 < s_1 < t_2 < \dots < s_{\mu-1} < t_\mu < s_\mu := 1$. Let $u(\cdot) : [0, 1] \rightarrow \mathbf{U}$ be such that $\dot{u}(t) \neq 0$ for every $t \in [0, 1]$, $u(\cdot) \in \mathcal{C}^3$, $u(0) = u_0$, $u(1) = u_1$. Moreover for every $j = 0, \dots, \mu$, the restriction $u|_{(t_j, s_j)}$ has values in $\mathbf{U} \setminus (\cup_{k \in \llbracket 1, N \rrbracket} \pi(\gamma_k))$ and for $j = 1, \dots, \mu$ the curve $u|_{[s_{j-1}, t_j]}$ is a reparameterization of $\beta_{\tau(j)}$ (see Figure 3.8).

By construction and by a repeated application of Theorem 3.2.5 and Remark 3.2.6, the solution of $i\dot{\psi}_\varepsilon^z = H^z(u(\varepsilon t))\psi_\varepsilon^z$ with initial condition $\psi_\varepsilon^z(0) = \phi_j^z(u_0)$, satisfies for every $t \in \cup_{k=0}^\mu (t_k, s_k)$

$$\|\psi_\varepsilon^z(t/\varepsilon) - e^{i\theta_j} \phi_{\sigma_{t_j}}^z(u(\varepsilon t))\| \leq C\sqrt{\varepsilon},$$

for some $\theta_j \in \mathbb{R}$. The proof of Theorem 3.5.1 is then concluded arguing by linearity. \square

Remark 3.5.2. *Let us comment on the difference between Assumption **P** and the set of hypotheses A_1, \dots, A_N appearing in the statement of Corollary 3.2.7. Assumption **P** is stronger in the sense that each $\pi(\hat{\gamma}_j)$ is required to have empty intersection not only with $\pi(\hat{\gamma}_{j-1})$ and $\pi(\hat{\gamma}_{j+1})$, but also all with $\pi(\hat{\gamma}_k)$ for $k \neq j$. Assumption **P** guarantees that while inducing a transition between the levels j and $j + 1$ the other energy levels are untouched.*

3.6 Genericity

We discuss in this section the genericity of Assumption A_j which appears in Theorem 3.2.5 and Corollary 3.2.7. Recall that, by the Wigner–von Neumann theorem [82], the set of $N \times N$ Hermitian matrices of rank equal to $N - 1$ (i.e., with one degenerate eigenvalue of multiplicity 2 and all other eigenvalues simple) is the finite union of submanifolds of codimension 3. More generally the set Υ of all $N \times N$ Hermitian matrices with degenerate eigenvalues is a Whitney stratified set (see for instance [42, Section 1.2]) of codimension 3. Similarly, symmetric real matrices with degenerate eigenvalues form a Whitney stratified set of codimension 2 of the space of all symmetric matrices. Let $d = 3$, $H : \mathbf{U} \rightarrow \text{Herm}(N)$ be a \mathcal{C}^3 map and $h = H(u) \in \text{Herm}(N)$ have rank equal to $N - 1$. Then $H(u)$ intersects Υ transversally at $h = H(u)$ if and only if u is a conical intersection. By standard transversality arguments (see, for instance, [1, Proposition 19.1] and [42, Section 1.3.2]), it follows that there exists a residual set \mathcal{R} in $\mathcal{C}^3(\mathbf{U}, \text{Herm}(N))$ such that for every $H \in \mathcal{R}$, all intersections between the eigenvalues of H are conical. (In particular for every $H \in \mathcal{R}$ and every $u \in \mathbf{U}$ such that $H(u) \in \Upsilon$, the rank of $H(u)$ is $N - 1$, since the strata of Υ corresponding to matrices of lower rank are of codimension larger than 3.)

Moreover, a conical intersection is structurally stable in the sense that, if u is a conical intersection for $H \in \mathcal{C}^3(\mathbf{U}, \text{Herm}(N))$, then any small perturbation of H has a conical intersection near u . Similar results hold for $d = 2$ in the case of real symmetric Hamiltonians.

The following two results, whose proof can be directly derived from the above considerations, establish that a small one-parameter perturbation of a Hamiltonian with conically connected spectrum satisfies the assumptions of Theorem 3.2.5 and Corollary 3.2.7. Here we impose \mathbf{U} to be bounded and the Hamiltonian H to be \mathcal{C}^3 on $\overline{\mathbf{U}}$, meaning that it admits a \mathcal{C}^3 extension on a neighborhood of $\overline{\mathbf{U}}$. We also require H not to have eigenvalue intersections on $\partial\mathbf{U}$. This prevents the occurrence of a sequence of eigenvalue intersections converging to $\partial\mathbf{U}$.

Theorem 3.6.1. *Let \mathbf{U} be an open, connected and bounded subset of \mathbb{R}^3 . Let $H : \overline{\mathbf{U}} \rightarrow \text{Herm}(N)$ be a \mathcal{C}^3 map and $(\lambda_j(u))_{j \in \llbracket 1, N \rrbracket}$ be the increasing sequence of eigenvalues of $H(u)$, $u \in \overline{\mathbf{U}}$, repeated according to their multiplicities. Fix $j \in \llbracket 1, N - 1 \rrbracket$. Assume that the levels λ_j and λ_{j+1} intersect and that all intersections between them are conical and correspond to controls $u \in \mathbf{U}$. If $j > 1$ (respectively, $j < N - 1$), assume, moreover, that all intersections between the levels λ_{j-1} and λ_j (respectively, λ_{j+1} and λ_{j+2}) are conical and correspond to controls $u \in \mathbf{U}$.*

Let us define

$$\Xi = \{h \in \mathcal{C}^3(\overline{\mathbf{U}} \times \mathbb{R}, \text{Herm}(N)) \mid h(\cdot, 0) = H(\cdot)\}$$

3.7. Multidimensional set of parameters

endowed with the \mathcal{C}^3 Whitney topology induced by $\mathcal{C}^3(\overline{\mathbf{U}} \times \mathbb{R}, \text{Herm}(N))$.

Then there exists an open and dense subset $\hat{\Xi}$ of Ξ , such that for every $h \in \hat{\Xi}$, the restriction $h : \mathbf{U} \times [-\delta, \delta] \rightarrow \text{Herm}(N)$ satisfies Assumption A_j for some $\delta > 0$.

Corollary 3.6.2. *Let \mathbf{U} be an open, connected and bounded subset of \mathbb{R}^3 . Let $H : \overline{\mathbf{U}} \rightarrow \text{Herm}(N)$ be a \mathcal{C}^3 map and $(\lambda_j(u))_{j \in \llbracket 1, N \rrbracket}$ be the increasing sequence of eigenvalues of $H(u)$, $u \in \overline{\mathbf{U}}$, repeated according to their multiplicities. Assume that all eigenvalue intersections are conical and correspond to controls $u \in \mathbf{U}$. Assume moreover that, for every $j \in \llbracket 1, N - 1 \rrbracket$, λ_j and λ_{j+1} intersect.*

Let Ξ be defined as in Theorem 3.6.1. Then there exists a open and dense subset $\hat{\Xi}$ of Ξ , such that for every $h \in \hat{\Xi}$, the restriction $h : \mathbf{U} \times [-\delta, \delta] \rightarrow \text{Herm}(N)$ satisfies Assumption \mathbf{P} for some $\delta > 0$ (and, in particular, Assumption A_j every $j \in \llbracket 1, N \rrbracket$).

As a consequence of Corollary 3.2.7 and Theorem 3.5.1, every h in the set $\hat{\Xi}$ of parameter-dependent Hamiltonians appearing in the statement of Corollary 3.6.2 defines, when restricted to $\mathbf{U} \times [-\delta, \delta]$, a system which is ensemble approximately controllable between eigenstates and which satisfies the conclusion of Theorem 3.5.1.

The same conclusions as those of Theorem 3.6.1 and Corollary 3.6.2 hold when $d = 2$ (i.e., \mathbf{U} is a subset of \mathbb{R}^2) and the Hamiltonians H and h take values in the set of symmetric $N \times N$ real matrices.

3.7 Multidimensional set of parameters

We consider in this section the situation in which the parameter on which the Hamiltonian depends varies in a set of dimension larger than one. Our technique still applies when the set of eigenvalue intersections projects onto a one-dimensional curve in the space of controls. Even if this situation is not generic, it however shows up in several physical examples, as we illustrate in Sections 3.7.1 and 3.7.2.

Let Σ be the set of parameters, contained in \mathbb{R}^m for some $m \in \mathbb{N}$. We consider the ensemble controllability problem for the Schrödinger equation on \mathbb{C}^N , $N \in \mathbb{N}$,

$$i\dot{\psi} = H^z(u(t))\psi, \quad z \in \Sigma. \quad (3.9)$$

Denote by $(\lambda_j^z(u))_{j=1}^N$ the nondecreasing sequence of eigenvalues of $H^z(u)$ repeated according to their multiplicities and by $(\phi_1^z(u), \dots, \phi_N^z(u))$ an orthonormal basis of associated eigenvectors. Let us define

$$\begin{aligned} \gamma_0 &= \emptyset, \\ \gamma_j &= \{(u, z) \in \mathbf{U} \times \Sigma \mid \text{such that } \lambda_j^z(u) = \lambda_{j+1}^z(u)\}, \quad j \in \llbracket 1, N - 1 \rrbracket, \\ \gamma_N &= \emptyset. \end{aligned}$$

Denote the projection of $(u, z) \in U \times \Sigma$ onto the u -component by π .

Assumption A_j^* . *There exists a connected component $\hat{\gamma}_j$ of γ_j such that*

- *There exists an interval $[z_0, z_1] \subset \mathbb{R}$ and a \mathcal{C}^3 embedding $\beta_j : [z_0, z_1] \rightarrow \mathbf{U}$ such that $\pi(\hat{\gamma}_j) = \beta_j([z_0, z_1])$;*
- *$\pi(\hat{\gamma}_j)$ is contained in $\mathbf{U} \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_{j+1}))$;*
- *For every $z \in \Sigma$, there exists a unique $u \in \pi(\hat{\gamma}_j)$ such that λ_j^z and λ_{j+1}^z have an intersection at u , which is conical.*

Moreover the set $\mathbf{U} \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_j) \cup \pi(\gamma_{j+1}))$ is pathwise connected.

Theorem 3.2.5 and Corollary 3.2.7 hold true by replacing $[z_0, z_1] \times \mathbf{U} \ni (z, u) \mapsto H^z(u) \in \text{Herm}(N)$ by $\Sigma \times \mathbf{U} \ni (z, u) \mapsto H^z(u) \in \text{Herm}(N)$ and A_j by A_j^* . The same proof works without major modifications.

3.7.1 Chirped pulses for two-level systems with two parameters

We consider here below an extension of the example studied in Section 3.4, in which we add an uncertain parameter also in the coupling between the control and the system. Consider the controlled equation

$$i \frac{d}{dt} \begin{pmatrix} \psi_1^z \\ \psi_2^z \end{pmatrix} = \begin{pmatrix} E + \alpha & \beta \Omega(t) \\ \beta \Omega^*(t) & -E - \alpha \end{pmatrix} \begin{pmatrix} \psi_1^z \\ \psi_2^z \end{pmatrix}, \quad (3.10)$$

where $z = (\alpha, \beta) \in [\alpha_0, \alpha_1] \times [\beta_0, \beta_1] \subset \mathbb{R} \times (0, +\infty)$. As before, $E > 0$ is fixed and we want to steer the system from $\phi_1^z(0) = (1, 0)$ to $\phi_2^z(0) = (0, 1)$, up to phases.

The same change of variables as in Section 3.4 and the control transformation

$$\Omega(t) = u_1(t) e^{-i(2Et + \Delta(t))}, \quad u_2(t) = \frac{d\Delta}{dt}(t),$$

yield the equivalent system $i \frac{d}{dt} \Phi^z = \mathcal{H}^z(t) \Phi^z$ with

$$\mathcal{H}^z(t) = \begin{pmatrix} \alpha & \beta u_1(t) \\ \beta u_1(t) & -\alpha + u_2(t) \end{pmatrix}.$$

Since the eigenvalue intersections of \mathcal{H}^z only depend on α and not on β , the entire discussion of Section 3.4 still applies in the presence of the parameter β . This underlines once more the robustness of the chirped pulse strategy for two-level systems.

3.7.2 Example 2: STIRAP

Consider the three-level system with controlled Hamiltonian

$$H^{(\alpha_1, \alpha_3, \beta_1, \beta_2)}(u_1, u_2) = \begin{pmatrix} E_1 + \alpha_1 & \beta_1 u_1 & 0 \\ \beta_1 u_1 & E_2 & \beta_2 u_2 \\ 0 & \beta_2 u_2 & E_3 + \alpha_3 \end{pmatrix}$$

3.7. Multidimensional set of parameters

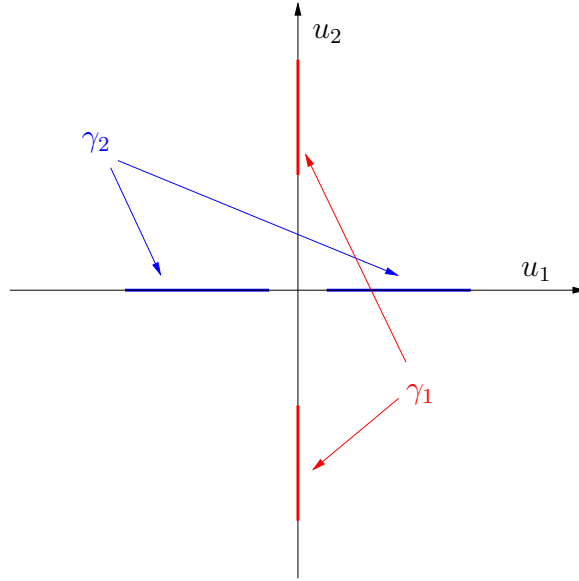


Figure 3.9 – The sets $\pi(\gamma_1)$ and $\pi(\gamma_2)$ for the STIRAP process.

with $\alpha_j \in [\alpha_{j0}, \alpha_{j1}]$, $j = 1, 3$, $\beta_j \in [\beta_{j0}, \beta_{j1}]$, $j = 1, 2$, $\beta_{10}, \beta_{20} > 0$ and α_{j0}, α_{j1} such that $E_1 + \alpha_1 < E_2 < E_3 + \alpha_3$. (One could clearly add a further parameter uncertainty in the level E_2 , which is not relevant, since the trace of the matrix can always be shifted without modifying the dynamical properties of the system.) The controls u_1 and u_2 are real-valued.

Denote $z = (\alpha_1, \alpha_3, \beta_1, \beta_2)$ and

$$\Sigma = [\alpha_{10}, \alpha_{11}] \times [\alpha_{30}, \alpha_{31}] \times [\beta_{10}, \beta_{11}] \times [\beta_{20}, \beta_{21}].$$

The eigenvalue intersections of $H^z(u_1, u_2)$ occur on the axes u_1 and u_2 . More precisely,

$$\begin{aligned} \pi(\gamma_1) &= \left\{ \left(0, -\frac{\sqrt{(E_1 + \alpha_1 - E_3 - \alpha_3)(E_1 + \alpha_1 - E_2)}}{\beta_2} \right) \mid z \in \Sigma \right\} \cup \\ &\quad \left\{ \left(0, \frac{\sqrt{(E_1 + \alpha_1 - E_3 - \alpha_3)(E_1 + \alpha_1 - E_2)}}{\beta_2} \right) \mid z \in \Sigma \right\}, \\ \pi(\gamma_2) &= \left\{ \left(-\frac{\sqrt{(E_1 + \alpha_1 - E_3 - \alpha_3)(E_2 - E_3 - \alpha_3)}}{\beta_1}, 0 \right) \mid z \in \Sigma \right\} \cup \\ &\quad \left\{ \left(\frac{\sqrt{(E_1 + \alpha_1 - E_3 - \alpha_3)(E_2 - E_3 - \alpha_3)}}{\beta_1}, 0 \right) \mid z \in \Sigma \right\}. \end{aligned}$$

In particular, $\pi(\gamma_1)$ and $\pi(\gamma_2)$ are both unions of two segments (see Figure 3.9), hence they are 1-dimensional smooth embedded manifolds. All hypotheses of Corollary 3.2.7 (in the multi-dimensional parameter extension discussed above) are satisfied and we conclude

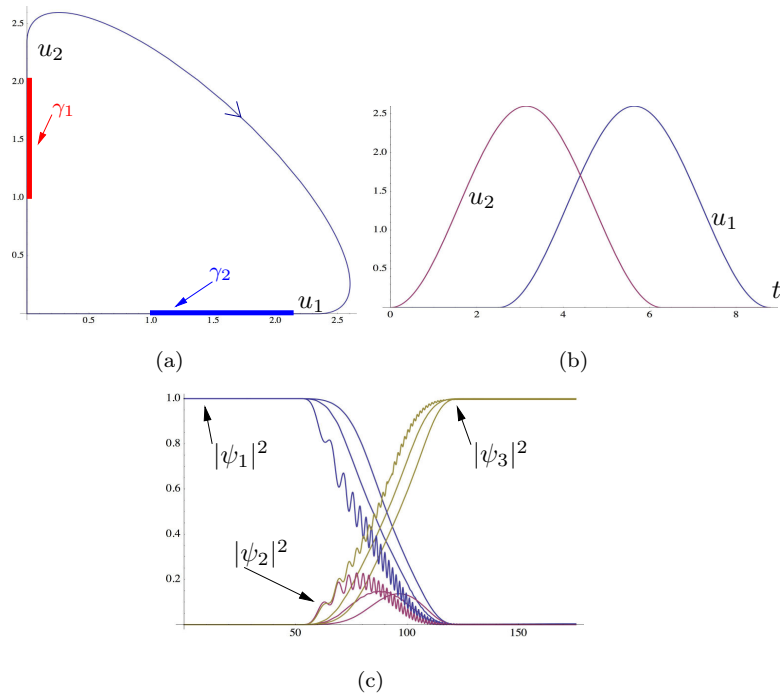


Figure 3.10 – Example of STIRAP process with $E_1 = -1$, $E_2 = 0$, $E_3 = 1$, $\alpha_1, \alpha_3 \in [-0.1, 0.1]$, $\beta_1, \beta_2 \in [0.8, 1.2]$. In (a) we give the parametric plot of the control, in (b) the shape of its components as functions of time and in (c) the components of the wave function for the three choices of parameters $(\alpha_1, \alpha_3, \beta_1, \beta_2) = (0, 0, 1, 1), (0.1, -0.1, 0.8, 1.2), (-0.1, 0.1, 1.2, 0.8)$. For this simulation we used $\varepsilon = 0.05$.

that the system is ensemble approximately controllable between eigenstates. Moreover, according to Remark 3.2.8, the precision of the transition described in Theorem 3.2.5 can be made of order ε , where ε is the velocity at which we follow the adiabatic path.

For instance, in order to steer system (3.9) from $\phi_1^z = (1, 0, 0)$ to $\phi_3^z = (0, 0, 1)$ we can follow the path in Figure 3.10a.

In Figure 3.10b we plot the two components of the control realising the transition. Notice that such controls are in the celebrated *counter-intuitive order*, meaning that, in order to go from state 1 to state 3, one first activates the control u_2 , responsible for the transition $2 \rightarrow 3$, and then the control u_1 , responsible for the transition $1 \rightarrow 2$ (creating the so-called *dark state*). The approach presented in this paper gives a complete mathematical explanation of why the counter-intuitive order works and why it is so robust with respect to parameter fluctuations.

3.8 Extension to the infinite-dimensional case

The results of the previous sections extend, under some suitable regularity assumptions, to the case where \mathbb{C}^N is replaced by an infinite-dimensional complex separable Hilbert space \mathcal{H} .

In order to avoid excessive technicalities, we present this extension in the case where the Hamiltonian H depends affinely on the controls and where the controlled Hamiltonians are bounded. (For the general nonlinear case, one could follow the approach in [30].)

We then consider a Hamiltonian of the type

$$H^z(u) = H_0^z + \sum_{j=1}^d u_j H_j^z,$$

with the parameter z belonging to $\Sigma \subset \mathbb{R}^m$ for some $m \in \mathbb{N}$, and with H_j^z , $j = 0, \dots, d$, satisfying the following assumption.

(H_∞) Fix $z_0 \in \Sigma$ and assume that:

- $H_0^{z_0}$ is self-adjoint and bounded from below;
- $H_0^z - H_0^{z_0}, H_1^z, \dots, H_d^z$ are bounded for all $z \in \Sigma$;
- the map $(z, u) \mapsto H_0^{z_0} - H^z(u)$ is \mathcal{C}^3 from $\Sigma \times \mathbf{U}$ to the Banach space of bounded self-adjoint operators endowed with the operator norm;
- for all $(z, u) \in \Sigma \times \mathbf{U}$ the eigenvalues $\lambda_1^z(u) \leq \dots \leq \lambda_N^z(u)$ of $H^z(u)$ are such that
 - $\text{spectrum}(H^z(u)) \cap [\lambda_1^z(u), \lambda_N^z(u)] = \{\lambda_1^z(u), \dots, \lambda_N^z(u)\}$ and $\lambda_j^z(u)$ has finite multiplicity for every $j \in \llbracket 1, N \rrbracket$,
 - $\text{dist}(\text{spectrum}(H^z(u)) \setminus [\lambda_1^z(u), \lambda_N^z(u)], \{\lambda_1^z(u), \lambda_N^z(u)\}) \geq \Gamma$,
 with $\Gamma > 0$ independent of (z, u) (see Figure 3.11).

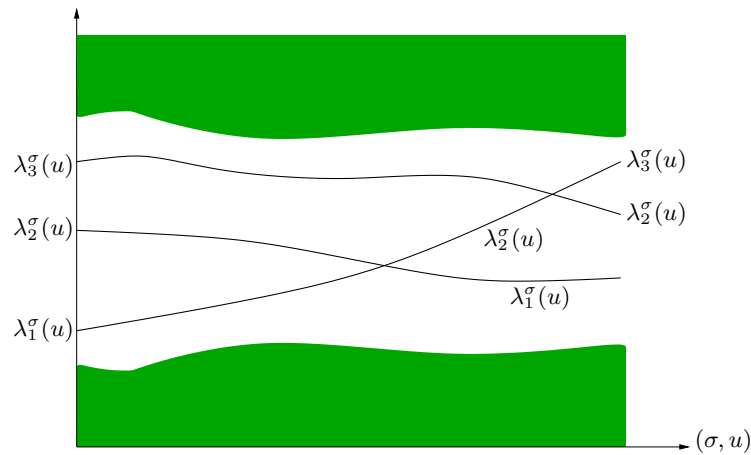


Figure 3.11 – The eigenvalues $\lambda_1^z(u) \leq \lambda_2^z(u) \leq \lambda_3^z(u)$ of $H^z(u)$ separated from the rest of the spectrum (which is contained in the shaded regions).

Under the hypothesis (\mathbf{H}_∞) , for every continuous control $u : [0, T] \rightarrow \mathbf{U}$ and every initial condition, the equation

$$i\dot{\psi} = H^z(u(t))\psi \quad (3.11)$$

admits a unique solution [78, Proposition 2.1].

Let $P^{z,u} : \mathcal{H} \rightarrow \mathcal{H}$ be the orthogonal projector onto the sum of the eigenspaces corresponding to $\lambda_1^z(u), \dots, \lambda_N^z(u)$. Without loss of generality this space is of complex dimension N . Then (see, for instance, [68]), for every $(\bar{z}, \bar{u}) \in \Sigma \times \mathbf{U}$ and every (z, u) in a neighborhood of (\bar{z}, \bar{u}) ,

$$P^{z,u} = -\frac{1}{2\pi i} \int_{\gamma} (H^z(u) - c)^{-1} dc,$$

where γ is a Jordan curve in \mathbb{C} separating $\lambda_1^z(\bar{u}), \dots, \lambda_N^z(\bar{u})$ and $\text{spectrum}(H^z(\bar{u})) \setminus [\lambda_1^z(\bar{u}), \lambda_N^z(\bar{u})]$. Hence $(z, u) \mapsto P^{z,u}$ is \mathcal{C}^3 as a map from $\Sigma \times \mathbf{U}$ to the Banach space of bounded operators on \mathcal{H} endowed with the operator norm.

Let $I^{z,u} : \mathbb{C}^N \rightarrow \mathcal{H}$ be a linear map such that $I^{z,u}$ is unitary between \mathbb{C}^N and the image of $P^{z,u}$.

Assume for now that $(z, u) \mapsto I^{z,u}$ is globally \mathcal{C}^3 on $\Sigma \times \mathbf{U}$. We denote by $(I^{z,u})^{-1}$ the inverse of $I^{z,u}$ on the image of $P^{z,u}$. The Hamiltonian $(z, u) \mapsto \widehat{H}^z(u) = (I^{z,u})^{-1} H^z(u) I^{z,u} \in \text{Herm}(N)$ is \mathcal{C}^3 and its eigenvalues are $\lambda_1^z(u), \dots, \lambda_N^z(u)$.

When $(z, u) \mapsto I^{z,u}$ cannot be globally defined as a \mathcal{C}^3 map, the same arguments can be applied in local charts leading to the following generalization of Theorem 3.2.5 and Corollary 3.2.7

As in the previous section, the sets $\pi(\gamma_j)$ are defined as

$$\begin{aligned} \pi(\gamma_0) &= \emptyset, \\ \pi(\gamma_j) &= \{u \in \mathbf{U} \mid \exists z \in \Sigma \text{ such that } \lambda_j^z(u) = \lambda_{j+1}^z(u)\}, \quad j \in \llbracket 1, N-1 \rrbracket, \\ \pi(\gamma_N) &= \emptyset. \end{aligned}$$

Theorem 3.8.1. *Assume that (H_∞) holds true. Let $j \in \llbracket 1, N-1 \rrbracket$ be such that Assumption A_j^* of Section 3.7 is satisfied. Take $u_0, u_1 \in \mathbf{U} \setminus (\gamma_{j-1} \cup \gamma_j \cup \gamma_{j+1})$ and consider a \mathcal{C}^3 path $u(\cdot) : [0, 1] \rightarrow \mathbf{U}$ satisfying $u(0) = u_0$, $u(1) = u_1$, and such that $u|_{[t_0, t_1]}$ is a reparameterization of β_j for some $0 < t_0 < t_1 < 1$ such that $u(t) \notin \gamma_{j-1} \cup \gamma_j \cup \gamma_{j+1}$ for every $t \in [0, 1] \setminus [t_0, t_1]$. Assume, moreover, that $\dot{u}(t) \neq 0$ for every $t \in [0, 1]$.*

Then there exists a constant $C > 0$ such that for every $z \in \Sigma$ and $\varepsilon > 0$ the solutions $\psi_\varepsilon^{z,\pm}$ of

$$i\dot{\psi}_\varepsilon^{z,\pm}(t) = H^z(u(\varepsilon t))\psi_\varepsilon^{z,\pm}(t)$$

with initial conditions

$$\psi_\varepsilon^{z,+}(0) = \phi_j^z(u_0), \quad \psi_\varepsilon^{z,-}(0) = \phi_{j+1}^z(u_0)$$

3.8. Extension to the infinite-dimensional case

satisfy

$$\|\psi_\varepsilon^{z,+}(1/\varepsilon) - e^{i\theta^+} \phi_{j+1}^z(u_1)\| \leq C\sqrt{\varepsilon}, \quad \|\psi_\varepsilon^{z,-}(1/\varepsilon) - e^{i\theta^-} \phi_j^z(u_1)\| \leq C\sqrt{\varepsilon},$$

for some $\theta^\pm \in \mathbb{R}$.

Proof. An adiabatic decoupling theorem (see Theorem 3.9.1 in appendix) states that, given a \mathcal{C}^2 path $u : [0, 1] \rightarrow \mathbf{U}$ as defined in the statement of the theorem and $\hat{\psi}_0 \in \mathbb{C}^N$, the solutions $\psi(\cdot)$ and $\hat{\psi}(\cdot)$ of, respectively, $i\dot{\psi}(t) = H^z(u(\varepsilon t))\psi(t)$, $\psi(0) = I^{z,u(0)}\hat{\psi}_0$, and $i\dot{\hat{\psi}}(t) = \hat{H}^z(u(\varepsilon t))\hat{\psi}(t)$, $\hat{\psi}(0) = \hat{\psi}_0$, are such that $\psi(1/\varepsilon)$ is $\sqrt{\varepsilon}$ -close, up to phases, to $I^{z,u(1)}\hat{\psi}(1/\varepsilon)$, uniformly w.r.t. $z \in \Sigma$. The result follows by applying Theorem 3.2.5 to the equation $i\dot{\psi}(t) = \hat{H}^z(u(\varepsilon t))\hat{\psi}(t)$. \square

Corollary 3.8.2. *Assume that (H_∞) holds true. Let Assumption A_j^* be satisfied for every $j \in \llbracket 1, N-1 \rrbracket$. Then (3.11) is ensemble approximately controllable between the eigenstates $\{\phi_1^z(u), \dots, \phi_N^z(u)\}$ in the sense that for every $\varepsilon > 0$, $j, k \in \llbracket 1, N \rrbracket$ and $u_0, u_1 \in \mathbf{U}$ such that $\lambda_j^z(u_0)$ and $\lambda_k^z(u_1)$ are simple for every $z \in \Sigma$, there exists a control $u(\cdot) : [0, T] \rightarrow \mathbf{U}$ such that for every $z \in \Sigma$ the solution of (3.11) with initial condition $\psi^z(0) = \phi_j^z(u_0)$ satisfies $\|\psi^z(T) - e^{i\theta} \phi_k^z(u_1)\| < \varepsilon$ for some $\theta \in \mathbb{R}$.*

Remark 3.8.3. *When Σ is one-dimensional, genericity results similar to those in Section 3.6 can be obtained. For related structural stability and genericity considerations, see [22].*

3.8.1 Example 3: Eberly–Law-like models

We study in this section a model for coupled spin-oscillator dynamics (see [61, 84, 15]). For other spin-boson models, see [20, 56, 67] and references therein. The state space is the tensor product of the state spaces of an harmonic oscillator and of a spin- $\frac{1}{2}$ particle. The system has two control parameters that we assume to be real, the first one, u_1 , coupling the two levels of the spin system and the other one, u_2 , producing simultaneous spin transitions and vibrational phonon excitations.

We let ω be the gap between the levels of the harmonic oscillator and δ be the internal gap of the spin system, α (respectively, β) the coupling strength between u_1 (respectively, u_2) and the system. The vector $z = (\alpha, \beta, \omega, \delta)$ will be considered as a set of parameters whose uncertainty will be tackled by the technique proposed in the previous sections.

The model can then be represented by the infinite-dimensional controlled quantum system

$$i\dot{\psi} = H^z(u)\psi, \quad \psi \in \ell^2,$$

where $u = (u_1, u_2) \in \mathbb{R}^2$, $z \in [\alpha_0, \alpha_1] \times [\beta_0, \beta_1] \times [\omega_0, \omega_1] \times [\delta_0, \delta_1] = \Sigma$, and

$$H^z(u) = \begin{pmatrix} 0 & \alpha u_1 & 0 & 0 & 0 & \cdots \\ \alpha u_1 & \delta & \beta u_2 & 0 & 0 & \ddots \\ 0 & \beta u_2 & \omega & \alpha u_1 & 0 & \ddots \\ 0 & 0 & \alpha u_1 & \omega + \delta & \beta u_2 & \ddots \\ 0 & 0 & 0 & \beta u_2 & 2\omega & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \quad (3.12)$$

We assume that $\alpha_0, \beta_0, \omega_0, \delta_0 > 0$. For simplicity, we also assume that $\omega_0 > \delta_1$, that is, the diagonal of $H^z(u)$ is a strictly increasing sequence. Further conditions on $\alpha_j, \beta_j, \omega_j, \delta_j$, $j = 0, 1$, will be imposed below (see (3.13)).

The Hamiltonian $H^z(u)$ is self-adjoint, has purely discrete spectrum, and, if both u_1 and u_2 are different from zero, then all eigenvalues of $H^z(u)$ are non-degenerate (see [2]).

In order to apply our general strategy, let us describe the eigenvalue intersections of $H^z(u)$. This is quite simple, since, for $u_1 = 0$ or $u_2 = 0$, the matrix describing $H^z(u)$ is block-diagonal.

Let us first consider intersections along the axis $u_2 = 0$. The eigenvalues of $H^z(u_1, 0)$ as a function of u_1 are shown in Figure 3.12. A simple computation shows that the smallest value of $|u_1|$ for which $H^z(u_1, 0)$ has degenerate eigenvalues is $u_1^* = \frac{\sqrt{\omega^2 - \delta^2}}{2\alpha}$ and the second-smallest value is $\bar{u}_1 = \frac{\sqrt{4\omega^2 - \delta^2}}{2\alpha}$.

We reason similarly along the axis $u_1 = 0$ and we get that the smallest value of $|u_2|$ for which $H^z(0, u_2)$ has degenerate eigenvalues different from zero is $u_2^* = \frac{\sqrt{\delta(2\omega - \delta)}}{2\beta}$ and the second-smallest value is $\bar{u}_2 = \frac{\sqrt{\delta(2\omega - \delta) + 3\omega^2}}{2\beta}$. The smallest value of $|u_2|$ for which 0 is a degenerate eigenvalue for $H^z(0, u_2)$ is $u_{20}^* = \frac{\sqrt{\delta\omega}}{\beta}$ and the second-smallest value is $\bar{u}_{20} = \frac{\sqrt{2\omega(\delta + \omega)}}{\beta}$.

We assume in the following that

$$\max_{z \in \Sigma} u_1^* < \min_{z \in \Sigma} \bar{u}_1, \quad \max_{z \in \Sigma} u_2^* < \min_{z \in \Sigma} \bar{u}_2, \quad \max_{z \in \Sigma} u_{20}^* < \min_{z \in \Sigma} \bar{u}_{20}. \quad (3.13)$$

Let $U = [-\eta, \eta + \max_{z \in \Sigma} u_1^*] \times [-\eta, \eta + \max_{z \in \Sigma} u_{20}^*]$ with $\eta > 0$ small. Then Assumptions A_j^* , $j \geq 1$, introduced in Section 3.7, hold true with

$$\begin{aligned} \pi(\hat{\gamma}_1) &= \{0\} \times [\min_{z \in \Sigma} u_{20}^*, \max_{z \in \Sigma} u_{20}^*], \\ \pi(\hat{\gamma}_{2j+1}) &= \{0\} \times [\min_{z \in \Sigma} u_2^*, \max_{z \in \Sigma} u_2^*], & j \geq 1, \\ \pi(\hat{\gamma}_{2j}) &= [\min_{z \in \Sigma} u_1^*, \max_{z \in \Sigma} u_1^*] \times \{0\}, & j \geq 1. \end{aligned}$$

In particular, all eigenvalue intersections in $\hat{\gamma}_j$, $j \geq 1$, are conical. Condition (3.13) also implies that, for every $n \in \mathbb{N}$, Assumption (\mathbf{H}_∞) is satisfied by the first $2n + 1$ eigenvalues

3.8. Extension to the infinite-dimensional case

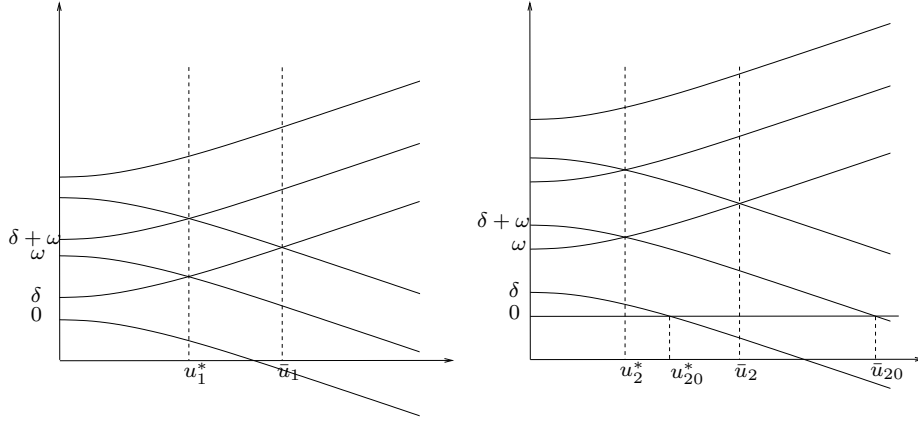


Figure 3.12 – The eigenvalues of $H^z(u_1, 0)$ (left) and $H^z(0, u_2)$ (right).

with $\mathbf{U} = U \cap \{u_2 < u_1 + \eta\}$, by the first 2 eigenvalues λ_1^z, λ_2^z with $\mathbf{U} = U \cap \{u_1 < u_2 + \eta\}$ and by the eigenvalues $\lambda_3^z, \dots, \lambda_{2n}^z$ with $\mathbf{U} = U \cap \{u_1 < u_2 + \eta, u_2 < \max_{z \in \Sigma} u_2^* + \eta\}$.

Henceforth, ensemble approximate controllability between eigenvectors holds true. Figure 3.13 shows a path in the space of controls leading to an ensemble transfer from $\phi_1^z(0)$ to $\phi_4^z(0)$. The path is a loop starting and ending at $u = 0$ that goes through $\pi(\hat{\gamma}_1)$, $\pi(\hat{\gamma}_2)$, and $\pi(\hat{\gamma}_3)$.

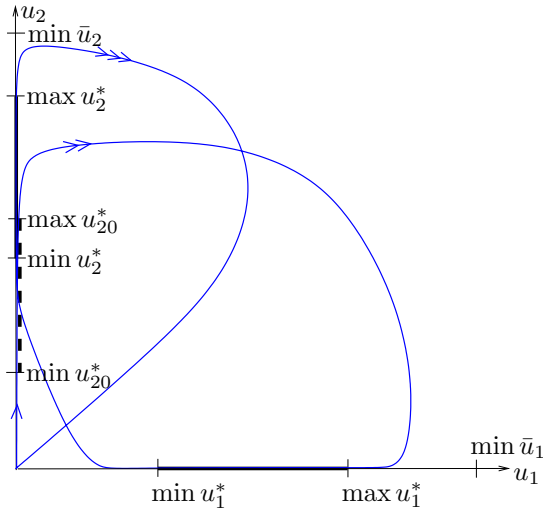


Figure 3.13 – A loop in the plane (u_1, u_2) inducing a population transfer from the first to the fourth eigenstate of the drift Hamiltonian.

3.9 Appendix

Regularity of eigenvalues and eigenvectors In this section we prove Lemma 3.3.2, which states that a time-dependent Hamiltonian $H \in \mathcal{C}^{k+1}(I, \text{Herm}(N))$ whose eigenvalues intersections are all conical has \mathcal{C}^{k+1} eigenvalues and \mathcal{C}^k eigenvectors.

Proof of Lemma 3.3.2. For each $j \in \llbracket 1, N \rrbracket$, consider the function

$$\ell_j : \text{Herm}(N) \rightarrow \mathbb{R}$$

that associates with a Hermitian matrix its j -th eigenvalue, where eigenvalues are counted according to their multiplicities, in such a way that $\ell_1 \leq \dots \leq \ell_N$. By Rellich theorem [69], each map ℓ_j is analytic on

$$\text{Herm}_j(N) = \{h \in \text{Herm}(N) \mid \ell_j(h) \text{ is a simple eigenvalue of } h\}.$$

Moreover, for every $h \in \text{Herm}_j(N)$, there exist a neighborhood \mathcal{V}_h of h in $\text{Herm}_j(N)$ and an analytic function $\varphi_j : \mathcal{V}_h \rightarrow \mathbb{C}^N$ such that $\varphi_j(g)$ is a norm 1 eigenvector of g of eigenvalue $\ell_j(g)$ for every $g \in \mathcal{V}_h$. Hence, for every $j \in \llbracket 1, N \rrbracket$, the j -th eigenvalue and a choice of a corresponding eigenvector of norm 1 are \mathcal{C}^{k+1} on

$$\{t \in I \mid \ell_j(H(t)) \text{ is a simple eigenvalue of } H(t)\}.$$

We are left to assess the regularity of eigenpairs in a neighborhood of a time $\bar{t} \in I$ such that $H(\bar{t}) \notin \text{Herm}_j(N)$.

Let J be a neighborhood of \bar{t} in I such that for every $t \in J \setminus \{\bar{t}\}$ both $\ell_j(H(t))$ and $\ell_{j+1}(H(t))$ are simple. For every $t \in J$, let $P^t : \mathbb{C}^N \rightarrow \mathbb{C}^N$ be the orthogonal projector on the sum of the eigenspaces corresponding to $\ell_j(H(t))$ and $\ell_{j+1}(H(t))$.

Then (see, for instance, [68]),

$$P^t = -\frac{1}{2\pi i} \int_{\gamma} (H(t) - c)^{-1} dc$$

where γ is a Jordan curve in \mathbb{C} separating $\ell_j(H(t))$, $\ell_{j+1}(H(t))$ and

$$\text{spectrum}(H(t)) \setminus \{\ell_j(H(t)), \ell_{j+1}(H(t))\}.$$

Up to taking a smaller J if necessary, the curve γ can be taken independently of $t \in J$.

Hence $t \mapsto P^t$ is \mathcal{C}^{k+1} as a map from J to the space of linear operators on \mathbb{C}^N . Then there exists a linear map $I^t : \mathbb{C}^2 \rightarrow \mathbb{C}^N$, depending \mathcal{C}^{k+1} on t , such that I^t is unitary between \mathbb{C}^2 and the image of P^t . We denote by $(I^t)^{-1}$ the inverse of I^t on the image of P^t .

The Hamiltonian $h(t) = (I^t)^{-1}H(t)I^t : \mathbb{C}^2 \rightarrow \mathbb{C}^2$ is well defined on J , depends \mathcal{C}^{k+1} on t , and has $\ell_j(H(t))$ and $\ell_{j+1}(H(t))$ as eigenvalues. If, moreover, v is an eigenvector of

3.9. Appendix

$h(t)$, then $I^t v$ is an eigenvector of $H(t)$. We are therefore left to prove the result for the eigenpairs of $h(t)$.

Without loss of generality we can consider the case where the trace of $h(t)$ is zero for every $t \in J$. Hence, $h(t)$ has the form

$$h(t) = \begin{pmatrix} a(t) & b(t) + ic(t) \\ b(t) - ic(t) & -a(t) \end{pmatrix},$$

where $a(\cdot)$, $b(\cdot)$, $c(\cdot)$ are real-valued \mathcal{C}^{k+1} functions on J .

Moreover, since $h(\bar{t})$ has a double eigenvalue, we have $a(\bar{t}) = b(\bar{t}) = c(\bar{t}) = 0$. Without loss of generality $\bar{t} = 0$.

Let $\alpha, \beta, \gamma : J \rightarrow \mathbb{R}$ be \mathcal{C}^k functions such that

$$a(t) = t\alpha(t), \quad b(t) = t\beta(t), \quad c(t) = t\gamma(t), \quad t \in J.$$

Hypothesis (3.5) guarantees that $\alpha(0) \neq 0$ or $\beta(0) \neq 0$ or $\gamma(0) \neq 0$. Notice that, up to applying a unitary change of variables in \mathbb{C}^2 and restricting J , we can assume that $\beta(t) \neq 0$ for every $t \in J$.

The eigenvalues of $h(t)$ are $\pm \sqrt{a(t)^2 + b(t)^2 + c(t)^2} = \pm |t| \sqrt{\alpha(t)^2 + \beta(t)^2 + \gamma(t)^2}$. The function

$$t \mapsto \begin{cases} -\sqrt{a(t)^2 + b(t)^2 + c(t)^2} & \text{if } t < 0 \\ \sqrt{a(t)^2 + b(t)^2 + c(t)^2} & \text{if } t \geq 0 \end{cases}$$

is then equal to $t\sqrt{\alpha(t)^2 + \beta(t)^2 + \gamma(t)^2}$ which is \mathcal{C}^{k+1} on J . Indeed, the only term of the $(k+1)$ -th derivative of $t\sqrt{\alpha(t)^2 + \beta(t)^2 + \gamma(t)^2}$ involving the $(k+1)$ -th derivative of α , β , and γ is

$$\frac{t(\alpha^{(k+1)}(t)\alpha(t) + \beta^{(k+1)}(t)\beta(t) + \gamma^{(k+1)}(t)\gamma(t))}{\sqrt{\alpha(t)^2 + \beta(t)^2 + \gamma(t)^2}}.$$

Now, since $a(t) = t\alpha(t)$ is \mathcal{C}^{k+1} , the term $t\alpha^{(k+1)}(t)$ is continuous. The same argument holds for β and γ and the \mathcal{C}^{k+1} regularity of $t\sqrt{\alpha(t)^2 + \beta(t)^2 + \gamma(t)^2}$ is proved.

For what concerns the unit eigenvectors, a simple calculation shows that, up to phases and scaling, they are equal to

$$\left(\frac{-a(t) \pm \sqrt{a(t)^2 + b(t)^2 + c(t)^2}}{b(t) - ic(t)}, 1 \right) = \left(\frac{-\alpha(t) \pm \text{sign}(t)\sqrt{\alpha(t)^2 + \beta(t)^2 + \gamma(t)^2}}{\beta(t) - i\gamma(t)}, 1 \right)$$

for $t \neq 0$. As above, connecting suitably the two branches, we can rewrite the eigenvectors as

$$\left(\frac{-\alpha(t) \pm \sqrt{\alpha(t)^2 + \beta(t)^2 + \gamma(t)^2}}{\beta(t) - i\gamma(t)}, 1 \right),$$

which are \mathcal{C}^k on J . □

Adiabatic decoupling of dimension n . We present here a result of adiabatic decoupling. It is adapted from [78], and is interesting because the adiabatic structure is preserved for the local n -levels dynamics. The proof is similar to the proofs of the theorems 4.6.4 and 4.6.5 of Section 4.6.2.

Theorem 3.9.1 (Adiabatic decoupling for parametric systems). *Assume that the Hamiltonian H is such that (H_∞) holds true as in Section 3.8. Assume moreover that*

$$\{\lambda_j(H^z(u)) \mid j \in K\},$$

with $K = \{q \dots q'\} \subset \mathbb{N}$ where $q, q' \in \mathbb{N}$, is separated from

$$\text{Spectrum}(H^z(u)) \setminus \{\lambda_j(H^z(u)) \mid j \in K\},$$

for u in a neighborhood W of 0 in \mathbb{R}^k and $z \in [z_0, z_1]$. Define, for every $(u, z) \in W \times [z_0, z_1]$, $I^{u,z}$ and $\widehat{H}^z(u)$ as in section 3.8. Consider a C^2 regular path $u : [0, 1] \rightarrow W$ and $\tilde{\psi}_0^z \in \mathbb{C}^2$, for every $z \in [z_0, z_1]$. Let $\ell \in \mathbb{N}$ and assume that for every $z \in [z_0, z_1]$, there exist C^ℓ functions $\Lambda_j^z : [0, 1] \rightarrow \mathbb{R}$ for every $j \in K$ such that for every $t \in [0, 1]$, $\{\Lambda_j^z(t), \mid j \in K\} = \{\lambda_j^z(u(t)), \mid j \in K\}$ and that, for every $z \in [z_0, z_1]$, $\widehat{H}^z(u(\cdot))$ admits C^2 eigenvectors $(\Phi_j^z(\cdot))_{j \in K}$ such that $(t, z) \mapsto \frac{d\Phi_j^z(t)}{dt}$ and $(t, z) \mapsto \frac{d^2\Phi_j^z(t)}{dt^2}$ are bounded uniformly with respect to $(t, z) \in [0, 1] \times [z_0, z_1]$, for every $j \in K$. Assume that there exists $c > 0$ such that

$$\left| \int_0^t e^{\frac{i}{\epsilon} \int_0^s (\Lambda_{j+1}^z(x) - \Lambda_j^z(x)) dx} ds \right| \leq c\epsilon^{1/(\ell+1)}, \quad \forall t \in [0, 1], \quad \forall z \in [z_0, z_1], \quad \forall j \in K. \quad (3.14)$$

Then the solutions ψ_ϵ^z and $\tilde{\psi}_\epsilon^z$ of, respectively, $i \frac{d\psi^z}{dt} = H^z(u(\epsilon t))\psi^z, \psi^z(0) = I^{u(0),z}\tilde{\psi}_0^z$, and $i \frac{d\tilde{\psi}^z}{dt} = \widehat{H}^z(u(\epsilon t))\tilde{\psi}^z, \tilde{\psi}^z(0) = \tilde{\psi}_0^z$ are such that $\psi^z(1/\epsilon)$ is $O(\epsilon^{\frac{1}{\ell+1}})$ -close, up to phases, to $I^{u(1),z}\tilde{\psi}^z(1/\epsilon)$, uniformly w.r.t. $z \in [z_0, z_1]$.

3.9. *Appendix*

Ensemble control of quantum systems with two controls: non-conical case

In Chapter 3 we proposed a framework for the adiabatic ensemble control of a continuum of n -level systems with real Hamiltonian, driven by two controls and having conical intersections between the eigenvalues. The method works under the assumption that for all values of the parameter eigenvalue intersections remain conical and describe a smooth curve. These assumptions are satisfied for generic small parametric perturbations, however, for generic large perturbations it may happen that conicity of eigenvalue intersections is lost at isolated points of the curve. The goal of this chapter is to extend the analysis to this case. In particular, we

- characterize typical non-conical intersections and give normal forms for them;
- study the evolution of the system corresponding to adiabatic paths in the space of controls passing through such intersections;
- conclude on the ensemble controllability of generic 1-parameter systems presenting typical intersections (conical and non-conical).

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4.1 Introduction

Consider a two-level system driven by a zero trace real Hamiltonian, that is, an equation of the form

$$i\frac{d\psi}{dt}(t) = H(u(t), v(t))\psi(t), \quad \psi(t) \in \mathbb{C}^2, \quad (u(t), v(t)) \in \mathbb{R}^2, \quad (4.1)$$

with

$$H(u, v) = \begin{pmatrix} f_1(u, v) & f_2(u, v) \\ f_2(u, v) & -f_1(u, v) \end{pmatrix}, \quad f = (f_1, f_2) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2).$$

As in Chapter 3, we restrict our attention to real Hamiltonians, which are relevant in many physical systems, for instance for Galerkin approximations of the Schrödinger equation $i\partial_t\psi(x, t) = (-\Delta + V(x) + u(t)W(x))\psi(x, t)$, where x belongs to a bounded set of \mathbb{R}^n and V, W are regular enough real functions. The spectrum of $H(u, v)$ is $\{\pm\sqrt{f_1(u, v)^2 + f_2(u, v)^2}\}$ and, in particular, it is degenerate if and only if $f(u, v) = (0, 0)$. Denote by $\lambda^+(u, v)$ the largest eigenvalue of $H(u, v)$, that is, $\lambda^+(u, v) = \sqrt{f_1(u, v)^2 + f_2(u, v)^2}$. Notice that the

gap (denoted $\text{Gap}(u, v)$) between the two eigenvalues of $H(u, v)$ is equal to $2\lambda^+(u, v)$ and that $\lambda^+(u, v) = 0$ if and only if $f(u, v) = 0$, that is, if (u, v) is an *eigenvalue intersection*. Such a point is said to be *conical* if

$$\chi(f) := \det(\nabla f_1, \nabla f_2)$$

is nonzero at (u, v) , where ∇ denotes the gradient with respect to the variables u and v . An eigenvalue intersection (u, v) is said to be *semi-conical* if $\nabla f_1(u, v)$ and $\nabla f_2(u, v)$ are collinear, are not both zero, and the directional derivative $\partial_\eta \chi(f)$ along

$$\eta = (-\partial_2 f_j(u, v), \partial_1 f_j(u, v))$$

is nonzero if $j \in \{1, 2\}$ is such that $\eta \neq 0$. The direction spanned by η is called the *non-conical direction* at (u, v) . If (u, v) is a conical intersection, then

$$\frac{1}{C} \|(u', v') - (u, v)\| \leq \text{Gap}(u', v') \leq C \|(u', v') - (u, v)\| \quad (4.2)$$

for some $C > 0$ and for all (u', v') in a neighborhood of (u, v) . If, instead, (u, v) is a semi-conical intersection, then an inequality of the type (4.2) holds along any line passing through (u, v) in a direction transversal to the non-conical direction. Along the non-conical direction η we have

$$\frac{1}{C} t^2 \leq \text{Gap}((u, v) + t\eta) \leq C t^2$$

for some $C > 0$ and for all t in a neighborhood of 0.

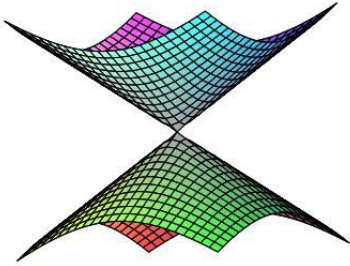


Figure 4.1 – Conical intersection as a function of the controls $(u, v) \in \mathbb{R}^2$.

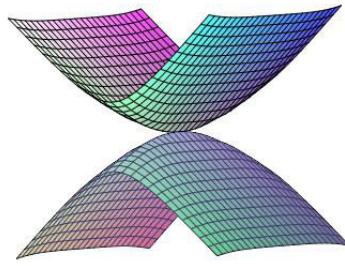


Figure 4.2 – Semi-conical intersection of eigenvalues as a function of the controls $(u, v) \in \mathbb{R}^2$.

We are now considering a one-parameter family of two-level systems as above, that is, the *Ensemble Schrödinger Equation*

$$i \frac{d\psi}{dt}(t) = H(u(t), v(t), z)\psi(t), \quad \psi(t) \in \mathbb{C}^2, \quad (u(t), v(t)) \in \mathbb{R}^2, \quad (4.3)$$

4.1. Introduction

with

$$H(u, v, z) = \begin{pmatrix} f_1(u, v, z) & f_2(u, v, z) \\ f_2(u, v, z) & -f_1(u, v, z) \end{pmatrix}, \quad f = (f_1, f_2) \in C^\infty(\mathbb{R}^3, \mathbb{R}^2),$$

the spectrum of $H(u, v, z)$ is $\{\pm\sqrt{f_1(u, v, z)^2 + f_2(u, v, z)^2}\}$ and, in particular, it is degenerate if and only if $f(u, v, z) = (0, 0)$. In order to extend the definition of conical and semi-conical intersections for a one-parameter Hamiltonian, we need to add to the previous definitions some regularity assumptions with respect to the perturbation parameter z . Let (u, v, z) be a point such that $f(u, v, z) = (0, 0)$. It is said to be conical for the family (*F-conical*) if (u, v) is conical for $f(\cdot, \cdot, z)$ and $\partial_3 f(u, v, z) \neq (0, 0)$. It is said to be semi-conical for the family (*F-semi-conical*) if it is semi-conical for $f(\cdot, \cdot, z)$ and f is a submersion at (u, v, z) . The requirement that f is a submersion guarantees that the set

$$Z(f) = \{(u, v, z) \mid f(u, v, z) = (0, 0)\}$$

is a smooth curve in the neighborhood of a semi-conical point. The gap $\text{Gap}(u, v, z)$ between the two eigenvalues of $H(u, v, z)$ is equal to $2\lambda^+(u, v, z) = 2\sqrt{f_1(u, v, z)^2 + f_2(u, v, z)^2}$ and we have $\text{Gap}(u, v, z) = 0$ if and only if $(u, v, z) \in Z(f)$. In the following we denote by $Z_{\text{nc}}(f)$ the set of non-conical intersections in $Z(f)$.

Lemma 4.1.1. *Let $(\bar{u}, \bar{v}, \bar{z})$ be a F-semi-conical intersection. Then $(\bar{u}, \bar{v}, \bar{z})$ is isolated in $Z_{\text{nc}}(f)$, $Z(f)$ is locally a smooth curve near $(\bar{u}, \bar{v}, \bar{z})$, and its tangent is not vertical. Moreover, the non-conical direction corresponding to $(\bar{u}, \bar{v}, \bar{z})$ is tangent to the projection on the plane (u, v) of such a curve at (\bar{u}, \bar{v}) .*

We focus in what follows on generic properties for systems of the type (4.3). This means that we look for properties which hold for all f in a “large” subset of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. For a precise definition of genericity as we intend it in this chapter, we refer to Section 4.2.1.

Theorem 4.1.2. *Generically with respect to $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$, for any connected component γ of $Z(f)$,*

- (i) γ is a one-dimensional submanifold of \mathbb{R}^3 ;
- (ii) The projection $\pi(\gamma)$ of γ on the plane (u, v) is a C^∞ embedded curve of \mathbb{R}^2 ;
- (iii) $(Z(f) \setminus Z_{\text{nc}}(f)) \cap \gamma$ is made of F-conical intersections and $Z_{\text{nc}}(f) \cap \gamma$ is made of F-semi-conical intersections only.

The following theorem resumes the main properties of the control strategy that we study in the chapter.

Theorem 4.1.3. *Assume that $Z(f)$ has a single connected component γ . Assume moreover that*

1. γ satisfies properties (i)–(iii) of Theorem 4.1.2;
2. $\pi(\gamma)$ has no self-intersections.

Take two conical intersections $(u_0, v_0, z_0), (u_1, v_1, z_1)$ in γ with $z_0 < z_1$. Consider a regular C^4 path $(u, v) : [0, 1] \rightarrow \mathbb{R}^2$ such that $(u, v)(t_0) = (u_0, v_0), (u, v)(t_1) = (u_1, v_1)$ for some $0 < t_0 < t_1 < 1$. Assume, moreover, that $(u, v)(0) = (u, v)(1) =: (\bar{u}, \bar{v})$, that $(u, v)(t) \in \pi(\gamma)$ if and only if $t \in [t_0, t_1]$, that $z \in [z_0, z_1]$ for every z and t such that $(u(t), v(t), z) \in \gamma$. For every $z \in [z_0, z_1]$, let ϕ_-^z and ϕ_+^z be two normalized eigenvectors of $H(\bar{u}, \bar{v}, z)$ corresponding to $\lambda^-(\bar{u}, \bar{v}, z)$ and $\lambda^+(\bar{u}, \bar{v}, z)$, respectively. Then there exists $C > 0$ such that for every $z \in [z_0, z_1]$ and every $\epsilon > 0$, the solution ψ of $i\dot{\psi}(t) = H_f(u(\epsilon t), v(\epsilon t), z)\psi(t), \psi(0) = \phi_-^z$, satisfies

$$\left\| \psi\left(\frac{1}{\epsilon}\right) - e^{i\xi} \phi_+^z \right\| < C\epsilon^{\frac{1}{3}},$$

for some $\xi \in \mathbb{R}$, possibly depending on ϵ and z .

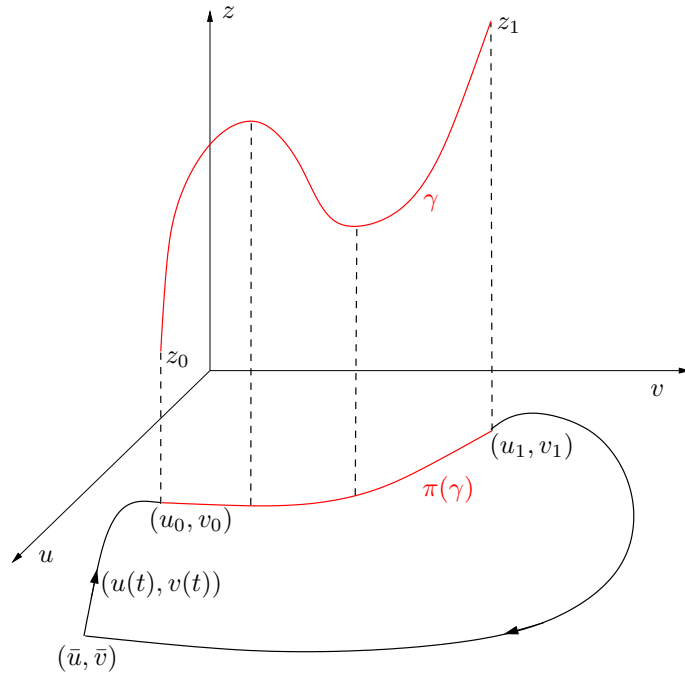


Figure 4.3 – A curve (u, v) as in the statement of Theorem 4.1.3

The chapter is organized as follows: In Section 4.2, we set the generic hypothesis on the Hamiltonians and provide the normal forms for the different types of systems briefly exposed in the introduction. In Section 4.3, we prove Theorem 4.1.2 and we study the singularities of the projection $\pi(f)$ of $Z(f)$ on the control plane. In Section 4.4, we study the dynamical properties of an isolated semi-conical intersection of eigenvalues and we prove Theorem 4.1.3. Then, in Section 4.6, we extend Theorem 4.1.3 for higher dimensional systems.

4.2 Basic facts and normal forms

4.2.1 Generic families of 2-level Hamiltonians

Define the smooth function $f = (f_1, f_2) : \mathbb{R}^k \times \mathbb{R}^l \rightarrow \mathbb{R}^2$. Denote by (e_1, \dots, e_{k+l}) the canonical basis of \mathbb{R}^{k+l} . Given a vector $\eta \in \mathbb{R}^{k+l}$ and a smooth function $g : \mathbb{R}^{k+l} \rightarrow \mathbb{R}^q$, $q \in \mathbb{N}$, we write $\partial_\eta g$ for the directional derivative of g in the direction v and ∂_i for ∂_{e_i} , $i = 1, \dots, k+l$. For $x \in \mathbb{R}^{k+l}$ and $h \in T_x \mathbb{R}^{k+l} \approx \mathbb{R}^{k+l}$, denote the differential of f at x applied to h by $Df_x(h)$.

In the following, we study generic situations in the cases $k = 2, l = 0$ and $k = 2, l = 1$. The coordinates (x_1, x_2) play the role of controls, and are denoted by (u, v) , while—in the case $l = 1$ —the coordinate x_3 is a parameter and is denoted by z . The space $C^\infty(\mathbb{R}^{2+l}, \mathbb{R}^2)$ is endowed in what follows with the C^∞ -Whitney topology.

We say that a property satisfied by $f \in C^\infty(\mathbb{R}^{2+l}, \mathbb{R}^2)$ is generic if it is satisfied in an open and dense subset of the space $C^\infty(\mathbb{R}^{2+l}, \mathbb{R}^2)$ endowed in what follows with the C^∞ -Whitney topology.

The single system case $k = 2, l = 0$

Consider a 2-dimensional real Hamiltonian of the form

$$H_f(u, v) = \begin{pmatrix} f_1(u, v) & f_2(u, v) \\ f_2(u, v) & -f_1(u, v) \end{pmatrix},$$

where $f_1, f_2 : \mathbb{R}^2 \rightarrow \mathbb{R}$ are smooth functions depending on 2 control variables (u, v) . Define the smooth function $f = (f_1, f_2) : \mathbb{R}^2 \rightarrow \mathbb{R}^2$. Denote by $\chi(f)(u, v)$ the Jacobian of f . By a slight abuse of notations, we will confound $\chi(f)$ and $\chi(H_f)$. Notice that the eigenvalues of H_f are $\lambda^+ = \sqrt{f_1^2 + f_2^2}$ and $\lambda^- = -\sqrt{f_1^2 + f_2^2}$. Define $\text{Gap} = \lambda^+ - \lambda^- = 2\sqrt{f_1^2 + f_2^2}$.

Definition 4.2.1. *Let $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ be such that $f(\bar{u}, \bar{v}) = (0, 0)$. We say that (\bar{u}, \bar{v}) is conical in direction $\nu \in \mathbb{R}^2$ if $\partial_\nu f(\bar{u}, \bar{v}) \neq (0, 0)$.*

Definition 4.2.2. *Let us consider $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. Let (\bar{u}, \bar{v}) be such that $f(\bar{u}, \bar{v}) = (0, 0)$.*

- *We say that (\bar{u}, \bar{v}) is conical for f if $\chi(f)(\bar{u}, \bar{v}) \neq 0$.*
- *We say that (\bar{u}, \bar{v}) is semi-conical if $\nabla f_1(\bar{u}, \bar{v})$ and $\nabla f_2(\bar{u}, \bar{v})$ are collinear, are not both zero, and the directional derivative $\partial_\eta \chi(f)(\bar{u}, \bar{v})$ along $\eta = (-\partial_2 f_j(\bar{u}, \bar{v}), \partial_1 f_j(\bar{u}, \bar{v}))$ is nonzero if $j \in \{1, 2\}$ is such that $\eta \neq 0$. The direction spanned by η is called the non-conical direction at (\bar{u}, \bar{v}) .*

Remark 4.2.3. *The definition of conical intersection for $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ given above is equivalent the one used in [22], namely, a point (\bar{u}, \bar{v}) such that $f(\bar{u}, \bar{v}) = (0, 0)$ and there exists $c > 0$ such that, for every $\eta \in \mathbb{R}^2$ of norm 1 and $\delta > 0$ small enough, we have $\frac{\text{Gap}((\bar{u}, \bar{v}) + \delta \eta)}{\delta} \geq c$*

The following proposition states that semi-conical points are isolated zeros of f . The proof can be deduced quite easily from the definition, for simplicity the proof can be deduced directly from the normal forms given in Section 4.2.3.

Proposition 4.2.4 (Semi-conical intersections are isolated). *Consider a semi-conical point (\bar{u}, \bar{v}) for f . Then there exists a neighborhood V of (\bar{u}, \bar{v}) in \mathbb{R}^2 such that for every $(u, v) \in V \setminus \{(\bar{u}, \bar{v})\}$, $f(u, v) \neq (0, 0)$.*

We recall here that conical intersections are generic. Denote by $J^{n_1}(\mathbb{R}^{n_2}, \mathbb{R}^{n_3})$ the set of n_1 -order jets of functions from \mathbb{R}^{n_2} to \mathbb{R}^{n_3} . Define

$$S_r = \{j^1(f)(0) \in J^1(\mathbb{R}^2, \mathbb{R}^2) \mid f(0) = 0, \text{rank}(Df(0)) = r\}, \quad r = 0, 1.$$

It is easy to check that S_0, S_1 are two submanifolds of $J^1(\mathbb{R}^2, \mathbb{R}^2)$ of codimension 6 and 3, respectively. One can easily show that the algebraic subset $S_0 \cup S_1$ of $J^1(\mathbb{R}^2, \mathbb{R}^2)$ admits a Whitney stratification (see [42] Part I, Chapter 1) whose strata have codimension strictly larger than the dimension of \mathbb{R}^2 . By Thom's transversality theorem (see, e.g., [41]) used in combination with [42, §1.3.2],

$$\begin{aligned} U &= \{f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2) \mid j^1(f)(\mathbb{R}^2) \cap (S_1 \cup S_2) = \emptyset\} \\ &= \{f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2) \mid j^1(f)(\mathbb{R}^2) \cap S_1 = \emptyset\} \cap \{f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2) \mid j^1(f)(\mathbb{R}^2) \cap S_2 = \emptyset\} \end{aligned}$$

is an open and dense subset of $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$.

The parametric case $k = 2, l = 1$

Consider a 2-dimensional real Hamiltonian of the form

$$H_f(u, v, z) = \begin{pmatrix} f_1(u, v, z) & f_2(u, v, z) \\ f_2(u, v, z) & -f_1(u, v, z) \end{pmatrix},$$

where $f_1, f_2 : \mathbb{R}^3 \rightarrow \mathbb{R}$ are smooth functions depending on two control variables (u, v) and one parameter z . Define the smooth function $f = (f_1, f_2) : \mathbb{R}^3 \rightarrow \mathbb{R}^2$. An *eigenvalue intersection* is a point (u, v, z) such that $f(u, v, z) = (0, 0)$.

Definition 4.2.5. For $i, j \in \{1, \dots, 3\}$, let $\chi_{ij}(f)$ be the Jacobian of the restriction of f to the plane parallel to $\text{span}(e_i, e_j)$, i.e.,

$$\chi_{ij}(f)(u, v, z) = \begin{vmatrix} \partial_i f_1(u, v, z) & \partial_j f_1(u, v, z) \\ \partial_i f_2(u, v, z) & \partial_j f_2(u, v, z) \end{vmatrix}.$$

By a slight abuse of notation, we set $\chi(f) = \chi_{12}(f)$.

4.2. Basic facts and normal forms

In order to extend the definition of conical and semi-conical intersections for a parametrized Hamiltonian, we need to add to the previous definitions some regularity assumptions with respect to the parameter z .

Definition 4.2.6. *Let (u, v, z) be a point such that $f(u, v, z) = (0, 0)$. It is said to be conical for the family (F-conical) if (u, v) is conical for $f(\cdot, \cdot, z)$ and $\partial_3 f(u, v, z) \neq (0, 0)$. It is said to be semi-conical for the family (F-semi-conical) if it is semi-conical for $f(\cdot, \cdot, z)$ and f is a submersion at (u, v, z) .*

Proposition 4.2.7. *Generically with respect to $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$, f is a submersion at every point of $Z(f)$ and the set $Z(f) = \{(u, v, z) \in \mathbb{R}^3 \mid f(u, v, z) = 0\}$ is a submanifold of \mathbb{R}^3 of dimension 1.*

Proof. Define

$$\Sigma_r = \{j^1(f)(0) \in J^1(\mathbb{R}^3, \mathbb{R}^2) \mid f(0) = 0, \text{rank}(Df(0)) = r\}, \quad r = 0, 1.$$

Notice that Σ_0 and Σ_1 are smooth submanifolds of $J^1(\mathbb{R}^3, \mathbb{R}^2)$ of codimensions 8 and 4, respectively. One can easily show that the algebraic subset $\Sigma_0 \cup \Sigma_1$ of $J^1(\mathbb{R}^3, \mathbb{R}^2)$ admits a Whitney stratification (see [42] Part I, Chapter 1) whose strata have codimension strictly larger than 3. By Thom's transversality theorem (see, e.g., [41]) used in combination with [42, §1.3.2], $U = \{f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2) \mid j^1(f)(\mathbb{R}^3) \cap (\Sigma_0 \cup \Sigma_1) = \emptyset\}$ is an open and dense subset of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. Hence, f is generically a submersion at every point $(u, v, z) \in Z(f)$. The proposition is proved. \square

In the next two propositions we provide a geometric description of the curve $Z(f)$ and we show its links with the conicity properties of f .

Proposition 4.2.8. *A point $(\bar{u}, \bar{v}, \bar{z}) \in Z(f)$ is conical for $f(\cdot, \cdot, \bar{z})$ if and only if f is a submersion at $(\bar{u}, \bar{v}, \bar{z})$ such that $Z(f)$ is locally near $(\bar{u}, \bar{v}, \bar{z})$ a one dimensional submanifold transversal to the plane of \mathbb{R}^3 of equation $z = \bar{z}$.*

Proof. Let $(\bar{u}, \bar{v}, \bar{z}) \in Z(f)$ be conical for $f(\cdot, \cdot, \bar{z})$. By definition, we have $\chi(f)(\bar{u}, \bar{v}, \bar{z}) \neq 0$, hence f is a submersion at $(\bar{u}, \bar{v}, \bar{z})$. It follows that $Z(f)$ is locally near $(\bar{u}, \bar{v}, \bar{z})$ a one dimensional submanifold of \mathbb{R}^3 . Fix a local smooth regular parametrization $c(t) = (u(t), v(t), z(t))_{t \in \mathbb{R}}$ of $c \subset Z(f)$ such that $c(\bar{t}) = (\bar{u}, \bar{v}, \bar{z})$. Assume for the sake of contradiction that $\dot{z}(\bar{t}) = 0$ where $\bar{t} \in \mathbb{R}$. Differentiating the condition $f(c(t)) = 0$ for every $t \in \mathbb{R}$, we have

$$\begin{cases} \dot{u}(\bar{t})\partial_1 f_1(\bar{u}, \bar{v}, \bar{z}) + \dot{v}(\bar{t})\partial_2 f_1(\bar{u}, \bar{v}, \bar{z}) = 0 \\ \dot{u}(\bar{t})\partial_1 f_2(\bar{u}, \bar{v}, \bar{z}) + \dot{v}(\bar{t})\partial_2 f_2(\bar{u}, \bar{v}, \bar{z}) = 0 \end{cases} \quad (4.4)$$

Hence $\chi(f)(\bar{u}, \bar{v}, \bar{z}) = 0$, that is impossible.

Conversely, consider a submersion f at $(\bar{u}, \bar{v}, \bar{z})$ such that $Z(f)$ is locally near $(\bar{u}, \bar{v}, \bar{z})$ a one dimensional submanifold transversal to the plane of \mathbb{R}^3 of equation $z = \bar{z}$. For the sake of contradiction, assume that $(\bar{u}, \bar{v}, \bar{z})$ is non conical for $f(\cdot, \cdot, \bar{z})$. By definition, there exists a direction $\eta \in \mathbb{R}^2$ such that $\partial_{(\eta, 0)} f(\bar{u}, \bar{v}, \bar{z}) = 0$. Fix a local smooth regular parametrization $c(t) = (u(t), v(t), z(t))_{t \in \mathbb{R}}$ of $c \subset Z(f)$ such that $c(\bar{t}) = (\bar{u}, \bar{v}, \bar{z})$ where $\bar{t} \in \mathbb{R}$. Differentiating the condition $f(c(t)) = 0$ for every $t \in \mathbb{R}$, we have $(\dot{u}(\bar{t}), \dot{v}(\bar{t}), \dot{z}(\bar{t})) \in \ker Df_{(\bar{u}, \bar{v}, \bar{z})}$. f being a submersion at $(\bar{u}, \bar{v}, \bar{z})$, we can deduce that $(\dot{u}(\bar{t}), \dot{v}(\bar{t}), \dot{z}(\bar{t}))$ is colinear to $(\eta, 0)$. Hence we get $\dot{z}(\bar{t}) = 0$, that is impossible. \square

Proposition 4.2.9. *Assume that f is a submersion locally near $(\bar{u}, \bar{v}, \bar{z})$ and that $(\bar{u}, \bar{v}, \bar{z})$ is non-conical for $f(\cdot, \cdot, \bar{z})$ in the direction $\eta \in \mathbb{R}^2 \setminus \{(0, 0)\}$. Fix a local smooth regular parametrization $c(t) = (u(t), v(t), z(t))_{t \in \mathbb{R}}$ of $c \subset Z(f)$ such that $c(\bar{t}) = (\bar{u}, \bar{v}, \bar{z})$ and $\dot{z}(\bar{t}) = 0$ where $\bar{t} \in \mathbb{R}$. Then we have the equivalence*

$$\ddot{z}(\bar{t}) = 0 \iff \partial_{(\eta, 0)} \chi(f)(\bar{u}, \bar{v}, \bar{z}) = 0.$$

In particular, if $(\bar{u}, \bar{v}, \bar{z})$ is F -semi-conical for f then $\ddot{z}(\bar{t}) \neq 0$.

Proof. Without loss of generality, we can assume $(\bar{u}, \bar{v}, \bar{z}) = (0, 0, 0)$. Under the assumption that f is a submersion, we have $(\partial_1 f_1(0), \partial_2 f_1(0)) \neq (0, 0)$ or $(\partial_1 f_2(0), \partial_2 f_2(0)) \neq (0, 0)$. Without loss of generality, assume $\partial_1 f_1(0) = r \cos(\theta)$ and $\partial_2 f_1(0) = r \sin(\theta)$ where

$r > 0$ and $\theta \in [0, 2\pi]$. Define the matrix $R_\theta = \begin{pmatrix} -\sin(\theta) & -\cos(\theta) & 0 \\ \cos(\theta) & -\sin(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix}$. For every

$(u, v, z) \in \mathbb{R}^3$, define $\tilde{f}(u, v, z) = (f \circ R_\theta)(u, v, z)$. By simple computations, we have $\partial_1 \tilde{f}(0) = 0$. Moreover, differentiating at order 2, we see that for every $(u, v, z) \in \mathbb{R}^3$, $\partial_1 \chi(\tilde{f})(u, v, z) = \partial_{(\eta, 0)} \chi(f)(u, v, z)$. Hence, it is sufficient to prove the proposition for $\eta = (1, 0)$.

Assume $\partial_1 f_1(0) = \partial_1 f_2(0) = 0$. Fix a local smooth regular parametrization $c(t) = (u(t), v(t), z(t))_{t \in \mathbb{R}}$ of $c \subset Z(f)$ such that $c(\bar{t}) = 0$ and $\dot{z}(\bar{t}) = 0$. For every t in $[0, 1]$, the equality $\frac{d}{dt} f(c(t)) = 0$ provides $\dot{c}(\bar{t})$ is colinear to e_1 . The equality $\frac{d^2}{dt^2} f(c(t)) = 0$ can be rewritten as

$$Df_{c(t)}(\ddot{c}(t)) + D^2 f_{c(t)}(\dot{c}(t), \dot{c}(t)) = 0,$$

that is

$$\begin{cases} \ddot{y}(\bar{t}) \partial_2 f_1(0) + \ddot{z}(\bar{t}) \partial_3 f_1(0) + \partial_{11} f_1(0) = 0 \\ \ddot{y}(\bar{t}) \partial_2 f_2(0) + \ddot{z}(\bar{t}) \partial_3 f_2(0) + \partial_{11} f_2(0) = 0 \end{cases}. \quad (4.5)$$

Assume $\ddot{z}(\bar{t}) = 0$. Using Equation (4.5), the linear system $\begin{cases} u \partial_2 f_1(0) + v \partial_{11} f_1(0) = 0 \\ u \partial_2 f_2(0) + v \partial_{11} f_2(0) = 0 \end{cases}$ has a non null solution in (u, v) . It implies its determinant is 0. By direct computa-

4.2. Basic facts and normal forms

tions, we have, for every (u, v, z) in \mathbb{R}^3 , $\partial_1 \chi(f)(u, v, z) = \begin{vmatrix} \partial_{11} f_1(u, v, z) & \partial_2 f_1(u, v, z) \\ \partial_{11} f_2(u, v, z) & \partial_2 f_2(u, v, z) \end{vmatrix} + \begin{vmatrix} \partial_1 f_1(u, v, z) & \partial_{21} f_1(u, v, z) \\ \partial_1 f_2(u, v, z) & \partial_{21} f_2(u, v, z) \end{vmatrix}$. Using the hypothesis $\partial_1 f_1(0) = \partial_1 f_2(0) = 0$, we get $\partial_1 \chi(f)(0) = 0$.

Conversely, assume $\partial_1 \chi(f)(0) = 0$. By definition of the determinant, $(\partial_{11} f_1(0), \partial_{11} f_2(0))$ is colinear to $Df_0(e_2)$. Assume $\ddot{z}(\bar{t}) \neq 0$. Equation (4.5) provides $Df_0(e_3)$ is colinear to $Df_0(e_2)$. It is impossible under the assumption that f is a submersion near 0. \square

Remark 4.2.10. *We have the following*

- *If $(\bar{u}, \bar{v}, \bar{z})$ is F -conical and $(u(t), v(t), z(t))_{t \in \mathbb{R}}$ such that $(u(\bar{t}), v(\bar{t}), z(\bar{t})) = (\bar{u}, \bar{v}, \bar{z})$ is a smooth and regular local parametrization of $Z(f)$ then $\dot{z}(\bar{t}) \neq 0$.*
- *Similarly, if $(\bar{u}, \bar{v}, \bar{z})$ is F -semi-conical, then $\dot{z}(\bar{t}) = 0$ and $\ddot{z}(\bar{t}) \neq 0$.*

In particular, F -semi-conical intersections are isolated in \mathbb{R}^3 .

Using the notations of the previous proposition, we are going to see that, for a generic f in $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$, the height function $t \mapsto z(t)$ of the submanifold $c \subset Z(f)$ may admit non-degenerate singular points that do not disappear by small perturbations of f . The following propositions guarantee that for a generic f , all intersections are either F -conical or F -semi-conical.

Proposition 4.2.11. *For a generic smooth function $f : \mathbb{R}^3 \rightarrow \mathbb{R}^2$, for every $(u, v, z) \in \mathbb{R}^3$ such that (u, v, z) is a conical intersection for $f(\cdot, \cdot, z)$, we have that (u, v, z) is a F -conical intersection for f .*

Proof. The set $Q = \{j^1(f)(0) \in J^1(\mathbb{R}^3, \mathbb{R}^2) \mid f(0) = 0, \partial_3 f(0) = 0\}$ is a Whitney stratified subset of $J^1(\mathbb{R}^3, \mathbb{R}^2)$ of codimension 4. By Thom's transversality theorem (see, e.g., [41]) used in combination with [42, §1.3.2], the set $\{f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2) \mid j^1(f)(\mathbb{R}^3) \cap Q = \emptyset\}$ is an open and dense subset of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. \square

Proposition 4.2.12. *For a generic smooth function $f : \mathbb{R}^3 \rightarrow \mathbb{R}^2$, for every $(u, v, z) \in \mathbb{R}^3$ such that (u, v, z) is a non-conical intersection for $f(\cdot, \cdot, z)$, we have that (u, v, z) is a F -semi-conical intersection for f .*

Proof. Set

$$S_j = \{j^2(f)(0) \in J^2(\mathbb{R}^3, \mathbb{R}^2) \mid f(0) = (0, 0), \partial_1 f_j(0) = \partial_2 f_j(0) = 0\}, \quad j = 0, 1.$$

Then S_0 and S_1 are smooth subspaces of $J^2(\mathbb{R}^3, \mathbb{R}^2)$ of codimension 4. Define

$$\eta = (-\partial_2 f_1(0), \partial_1 f_1(0), 0),$$

$$S_2 = \{j^2(f)(0) \in J^2(\mathbb{R}^3, \mathbb{R}^2) \mid f(0) = 0, (\partial_1 f_1(0), \partial_2 f_1(0)) \neq 0, \chi(f)(0) = 0, \partial_\eta \chi(f)(0) = 0\}$$

and

$$\tilde{S}_2 = \{j^2(f)(0) \in J^2(\mathbb{R}^3, \mathbb{R}^2) \mid f(0) = 0, \chi(f)(0) = 0, \partial_\eta \chi(f)(0) = 0\}.$$

We are going to prove that S_2 is a smooth submanifold of $J^2(\mathbb{R}^3, \mathbb{R}^2)$ of codimension 4, that is, that the equalities $f(0) = 0$, $\chi(f)(0) = 0$ and $\partial_\eta \chi(f)(0) = 0$ define independent equations in $J^2(\mathbb{R}^3, \mathbb{R}^2)$ under the condition $(\partial_1 f_1(0), \partial_2 f_1(0)) \neq 0$. The equality $f(0) = 0$ is clearly independent from the two others. Using the property that $\partial_1 f_1(0) \neq 0$ or $\partial_2 f_1(0) \neq 0$, one easily establishes that $\chi(f)(0) = 0$ and $\partial_\eta \chi(f)(0) = 0$ define independent equations in $J^2(\mathbb{R}^3, \mathbb{R}^2)$.

One then can easily prove that the algebraic subset $S = S_0 \cup S_1 \cup \tilde{S}_2 = S_0 \cup S_1 \cup S_2$ of $J^2(\mathbb{R}^3, \mathbb{R}^2)$ admits a Whitney stratification whose strata have a codimension strictly larger than 3. By Thom's transversality theorem (see, e.g., [41]) used in combination with [42, §1.3.2], we get that $O = \{f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2) \mid j^2(f)(\mathbb{R}^3) \cap S = \emptyset\}$ is an open and dense subset of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. \square

Considering $G = U \cap R \cap O$ where U , R , and O are defined respectively in Propositions 4.2.7, 4.2.11, and 4.2.12, G is an open and dense subset of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$.

4.2.2 Admissible transformations

The aim of this section is to define admissible transformations in order to get normal forms for the Hamiltonians H_f defined for $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ by $H_f(u, v) = \begin{pmatrix} f_1(u, v) & f_2(u, v) \\ f_2(u, v) & -f_1(u, v) \end{pmatrix}$ and for $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ by $H_f(u, v, z) = \begin{pmatrix} f_1(u, v, z) & f_2(u, v, z) \\ f_2(u, v, z) & -f_1(u, v, z) \end{pmatrix}$. Consider the *Schrödinger Equation*, defined for $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ by

$$i \frac{d\psi(t)}{dt} = H_f(u(t), v(t))\psi(t), \quad (4.6)$$

where $\psi(t) \in \mathbb{C}^2$, and the *Ensemble Schrödinger Equation*, defined for $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ by

$$i \frac{d\psi(t)}{dt} = H_f(u(t), v(t), z)\psi(t), \quad (4.7)$$

where $\psi(t) \in \mathbb{C}^2$. The control functions u, v are in $L^\infty(\mathbb{R}, \mathbb{R})$ and the perturbation z belongs to $[z_0, z_1]$ where $z_0, z_1 \in \mathbb{R}$.

The three transformations correspond to equivalent representations of the dynamical systems (4.6) and (4.7) achieved, respectively, by time-reparameterization, state-space diffeomorphism, and independent diffeomorphic transformations of both the space of controls and the space of perturbations.

Definition 4.2.13. *We say that two elements f and \tilde{f} of $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ (respectively, $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$) are time-equivalent at 0 if there exists a nowhere-vanishing function $\xi \in$*

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$C^\infty(\mathbb{R}^2, \mathbb{R})$ such that $\tilde{f}(u, v) = \xi(u, v)f(u, v)$ (respectively, $\tilde{f}(u, v, z) = \xi(u, v)f(u, v, z)$) in a neighborhood of 0.

Remark 4.2.14. A time-equivalence as introduced in Definition 4.2.13 with $\xi > 0$ corresponds to a time-change in Equation (4.6). As for the case $\xi < 0$, consider $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, $\psi_0, \psi_1 \in \mathbb{C}^2$ and a control path $(u(\cdot), v(\cdot))$ such that the solution $\psi(\cdot)$ of Equation (4.6) such that $\psi(0) = \psi_0$ satisfies $\psi(T) = \psi_1$ where $T > 0$. Then the solution $\tilde{\psi}$ of Equation (4.6) associated with $(u(T - \cdot), v(T - \cdot))$ such that $\tilde{\psi}(0) = \bar{\psi}_1$ satisfies $\tilde{\psi}(T) = \bar{\psi}_0$ (where we denote by \bar{x} the complex-conjugate of $x \in \mathbb{C}^2$). Hence the equations (4.6) and

$$i \frac{d\psi(t)}{dt} = -H_f(u(t), v(t))\psi(t), \quad (7-)$$

where $\psi(t) \in \mathbb{C}^2$ have the same controllability properties. Hence time-equivalence can be defined rigorously for a function $\xi \in C^\infty(\mathbb{R}^2, (-\infty, 0))$. The same argument is also valid for $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$.

Definition 4.2.15. We say that two elements f and \tilde{f} of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ or $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ are left-equivalent if there exists $P \in O_2(\mathbb{R})$ independent of u, v, z such that $H_{\tilde{f}} = PH_fP^{-1}$.

Remark 4.2.16. Let f be in $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ or $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. Considering

$$P_{\theta, \zeta} = \begin{pmatrix} \cos(\theta) & -\zeta \sin(\theta) \\ \sin(\theta) & \zeta \cos(\theta) \end{pmatrix} \in O_2(\mathbb{R}),$$

where $\zeta = \pm 1$, the associated left-equivalence transforms $f = (f_1, f_2)$ into

$$\tilde{f} = (\cos(2\theta)f_1 - \zeta \sin(2\theta)f_2, \zeta \cos(2\theta)f_2 + \sin(2\theta)f_1).$$

Remark 4.2.17. Let f be in $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ or $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. If $t \mapsto \psi(t)$ is a solution of Equation (4.6) or (4.7) associated with f and with initial condition $\psi(0) = \psi_0$, then $t \mapsto Y(t) = P\psi(t)$ is a solution of Equation (4.7) associated with \tilde{f} satisfying $Y(0) = P\psi_0$. Hence, transitions for Y between the eigenstates of $H_{\tilde{f}} = PH_fP^{-1}$ correspond to transitions for ψ between the eigenstates of H_f .

Definition 4.2.18. We say that two elements f and \tilde{f} of $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ are right-equivalent at 0 if there exists a diffeomorphism $\phi \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ such that $\phi(0) = 0$ and $\tilde{f} = f \circ \phi$ in a neighborhood of 0.

Definition 4.2.19. We say that two elements f and \tilde{f} of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ are right-equivalent at 0 if there exists a diffeomorphism $\phi \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$ of the form

$$\phi : (u, v, z) \mapsto (\phi_1(u, v), \phi_2(u, v), \phi_3(z)),$$

where $\phi_1, \phi_2 \in C^\infty(\mathbb{R}^2, \mathbb{R})$ and $\phi_3 \in C^\infty(\mathbb{R}, \mathbb{R})$, satisfying $\phi(0) = 0$ and $\tilde{f} = f \circ \phi$ in a neighborhood of 0.

Combining the previous three definitions we introduce the following notion of equivalence.

Definition 4.2.20. *We say that two elements f and \tilde{f} of $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ are equivalent at 0 if there exists $(\phi, \theta, \xi) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2) \times [-\pi, \pi] \times C^\infty(\mathbb{R}^2, \mathbb{R} \setminus \{0\})$ with ϕ as in Definition 4.2.19, and $\zeta = \pm 1$ such that for every (u, v, z) in a neighborhood of 0,*

$$\begin{cases} \tilde{f}_1(u, v) = \xi(u, v)(\cos(2\theta)f_1 \circ \phi(u, v) - \zeta \sin(2\theta)f_2 \circ \phi(u, v)), \\ \tilde{f}_2(u, v) = \xi(u, v)(\sin(2\theta)f_1 \circ \phi(u, v) + \zeta \cos(2\theta)f_2 \circ \phi(u, v)). \end{cases}$$

Definition 4.2.21. *We say that two elements f and \tilde{f} of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ are equivalent at 0 if there exists $(\phi, \theta, \xi) \in C^\infty(\mathbb{R}^3, \mathbb{R}^3) \times [-\pi, \pi] \times C^\infty(\mathbb{R}^2, \mathbb{R} \setminus \{0\})$ with ϕ as in Definition 4.2.19, and $\zeta = \pm 1$ such that for every (u, v, z) in a neighborhood of 0,*

$$\begin{cases} \tilde{f}_1(u, v, z) = \xi(u, v)(\cos(2\theta)f_1 \circ \phi(u, v, z) - \zeta \sin(2\theta)f_2 \circ \phi(u, v, z)), \\ \tilde{f}_2(u, v, z) = \xi(u, v)(\sin(2\theta)f_1 \circ \phi(u, v, z) + \zeta \cos(2\theta)f_2 \circ \phi(u, v, z)). \end{cases}$$

An essential feature of admissible transformations is the following proposition

Proposition 4.2.22. — *Let $f, \tilde{f} \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ be equivalent. Then 0 is conical for f if and only if it is conical for \tilde{f} and 0 is semi-conical for f if and only if it is semi-conical for \tilde{f} .*
 — *Let $f, \tilde{f} \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ be equivalent. Then 0 is F -conical for f if and only if it is F -conical for \tilde{f} and 0 is F -semi-conical for f if and only if it is F -semi-conical for \tilde{f} .*

In order to prove the proposition, we first obtain the following lemma.

Lemma 4.2.23. *Let $f, \tilde{f} \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ be equivalent. Then, for every $(u, v) \in \mathbb{R}^2$ in a neighborhood of 0, $\chi(f)(u, v) \neq 0$ if and only if $\chi(\tilde{f})(\phi(u, v)) \neq 0$.*

Proof. Notice that it is sufficient to prove the result separately for each of the three type of equivalence: time-equivalence, left-equivalence, and right-equivalence.

- For a time-equivalence \tilde{f} of f associated with ξ in $C^\infty(\mathbb{R}^2, \mathbb{R})$, we have by direct computations of the determinant, $\chi(\tilde{f})(u, v) = \xi(u, v)^2 \chi(f)(u, v)$ where ξ is non-vanishing.
- For a left-equivalence \tilde{f} of f , we have

$$\nabla \tilde{f}_1 = \cos(2\theta) \nabla f_1 - \zeta \sin(2\theta) \nabla f_2, \quad \nabla \tilde{f}_2 = \cos(2\theta) \nabla f_2 + \zeta \sin(2\theta) \nabla f_1,$$

where $\zeta = \pm 1$. Hence, we obtain that, for every $(u, v) \in \mathbb{R}^2$, $\chi(\tilde{f})(u, v) = \zeta \chi(f)(u, v)$.

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- For a right-equivalence $\tilde{f} = f \circ \phi$ of f associated with ϕ , we have for every $X = (u, v) \in \mathbb{R}^2$ in a neighborhood of $(0, 0)$, and for $i \in \{1, 2\}$,

$$\nabla(f_i \circ \phi)(u, v) = \begin{pmatrix} \partial_1 f_i(\phi(X)) \partial_1 \phi_1(X) + \partial_2 f_i(\phi(X)) \partial_1 \phi_2(X) \\ \partial_1 f_i(\phi(X)) \partial_2 \phi_1(X) + \partial_2 f_i(\phi(X)) \partial_2 \phi_2(X) \end{pmatrix}.$$

Hence,

$$\begin{aligned} \chi(f \circ \phi)(X) &= \det(\nabla(f_1 \circ \phi)(X), \nabla(f_2 \circ \phi)(X)) \\ &= \partial_1 f_1(\phi(X)) \partial_2 f_2(\phi(X)) \partial_1 \phi_1(X) \partial_2 \phi_2(X) - \partial_1 f_2(\phi(X)) \partial_2 f_1(\phi(X)) \partial_1 \phi_1(X) \partial_2 \phi_2(X) \\ &\quad + \partial_2 f_1(\phi(X)) \partial_1 f_2(\phi(X)) \partial_1 \phi_2(X) \partial_2 \phi_1(X) - \partial_2 f_2(\phi(X)) \partial_1 f_1(\phi(X)) \partial_1 \phi_2(X) \partial_2 \phi_1(X). \end{aligned}$$

We deduce that

$$\chi(f \circ \phi)(X) = \chi(f)(\phi(X)) \begin{vmatrix} \partial_1 \phi_1(X) & \partial_2 \phi_1(X) \\ \partial_1 \phi_2(X) & \partial_2 \phi_2(X) \end{vmatrix},$$

where ϕ is a diffeomorphism in a neighborhood of $(0, 0, 0)$ satisfying $\partial_1 \phi_3(0) = \partial_2 \phi_3(0) = 0$, we obtain $\begin{vmatrix} \partial_1 \phi_1(0) & \partial_2 \phi_1(0) \\ \partial_1 \phi_2(0) & \partial_2 \phi_2(0) \end{vmatrix} \neq 0$. □

By similar arguments, we have the following lemma.

Lemma 4.2.24. *Let $f, \tilde{f} \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ be equivalent. Then, for every $(u, v, z) \in \mathbb{R}^3$ in a neighborhood of 0, $\chi(f)(u, v, z) \neq 0$ if and only if $\chi(\tilde{f})(\phi(u, v, z)) \neq 0$.*

Proof. (Proof of Proposition 4.2.22) We prove the first claim. Consider $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. For a right-equivalence \tilde{f} of f , Lemma 4.2.23 proves that 0 is conical for f if and only if 0 is conical for \tilde{f} . Now assume that 0 is semi-conical for $f \in C^\infty$. With the previous computations, we have seen in the proof of Lemma 4.2.23 that for every right-equivalence $\tilde{f} = f \circ \phi$ where $\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^2$, we have, for every $(u, v) \in \mathbb{R}^2$ in a neighborhood of $(0, 0)$,

$$\chi(\tilde{f})(u, v) = \chi(f)(\phi(u, v)) \begin{vmatrix} \partial_1 \phi_1(u, v) & \partial_2 \phi_1(u, v) \\ \partial_1 \phi_2(u, v) & \partial_2 \phi_2(u, v) \end{vmatrix}.$$

Hence denoting by η the non-conical direction, we get $\partial_\eta \chi(f)(u, v) \neq 0$ if and only if $\partial_{\tilde{\eta}} \chi(\tilde{f})(\phi(u, v)) \neq 0$ where $\tilde{\eta} = D\phi_{\phi(u, v)}^{-1}(\eta)$. By the computations made in Lemma 4.2.23, we get that, if \tilde{f} is a left or right equivalence of f , then $\nabla \tilde{f}_1(0) = \nabla \tilde{f}_2(0) = 0$ if and only if $\nabla f_1(0) = \nabla f_2(0) = 0$, and $\chi(\tilde{f})(0) \neq 0$ if and only if $\chi(f)(0) \neq 0$. Then we get the expected equivalence.

By similar computations and noticing for the F-conical case that if two elements of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ are equivalent then $\partial_3 f(0) \neq 0$ if and only if $\partial_3 \tilde{f}(0) \neq 0$ and for the F-semi-conical case that f is a submersion at 0 if and only if \tilde{f} is a submersion at 0, we prove the second claim concerning $f, \tilde{f} \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. □

4.2.3 Normal forms for the non parametric case

Conical intersection

Define $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ such that $\chi(f)(0) \neq 0$. In this case, f is a diffeomorphism in a neighborhood of 0. Hence f is right-equivalent to $\text{Id} : \mathbb{R}^2 \rightarrow \mathbb{R}^2$. The normal form provides the well-known Hamiltonian $H(u, v) = \begin{pmatrix} u & v \\ v & -u \end{pmatrix}$, for $u, v \in \mathbb{R}^2$.

Semi-conical intersection

The main result of this section is the following theorem.

Theorem 4.2.25. *Assume that 0 is semi-conical for $f \in C^\infty(\mathbb{R}^2, \mathbb{R})$. Then f is equivalent to $(u, v) \mapsto \begin{pmatrix} h(u)u \\ u + v^2 \end{pmatrix}$ where $h : \mathbb{R} \rightarrow \mathbb{R}$ is a smooth function satisfying $h(0) = 1$.*

The **algorithm** that we will refer as **(A)** to get the normal form is the following:

- **STEP 1:** By a left-equivalence we transform f_1 and f_2 into two functions \tilde{f}_1 and \tilde{f}_2 such that $\nabla \tilde{f}_1(0) = \nabla \tilde{f}_2(0) \neq 0$.
- **STEP 2:** By a right-equivalence, we bring the non-conical direction to $\text{span}(e_2)$.
- **STEP 3:** By a right-equivalence and using Lemma 4.7.11, we transform the functions f_1 and f_2 into a suitable form.

Proof of Theorem 4.2.25: STEP 1

Proposition 4.2.26. *Consider $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ having a semi-conical intersection at 0. Then there exists \tilde{f} left-equivalent to f such that $\nabla \tilde{f}_1(0) = \nabla \tilde{f}_2(0) \neq 0$.*

Proof. Without loss of generality, we can assume $\nabla f_1(0) \neq 0$. Define $\alpha \in \mathbb{R}$ such that $\nabla f_2(0) = \alpha \nabla f_1(0)$.

Denote by \tilde{f} the function obtained by applying to f the left-equivalence associated with $\theta \in [-\pi, \pi]$ and $\zeta = 1$ as in Remark 4.2.16. Hence,

$$\nabla \tilde{f}_1 = \cos(2\theta) \nabla f_1 - \sin(2\theta) \nabla f_2, \quad \nabla \tilde{f}_2 = \cos(2\theta) \nabla f_2 + \sin(2\theta) \nabla f_1.$$

We have $\nabla \tilde{f}_1(0) = \nabla \tilde{f}_2(0)$ if and only if $\left\langle \begin{pmatrix} \cos(2\theta) \\ \sin(2\theta) \end{pmatrix}, \begin{pmatrix} 1 - \alpha \\ -(1 + \alpha) \end{pmatrix} \right\rangle = 0$. It is clearly possible to choose $\theta \in [-\pi, \pi]$ satisfying the previous condition, the proposition is proved.

□

Until the end of this section, we assume that 0 is semi-conical for $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$.

Proof of Theorem 4.2.25: STEP 2

Proposition 4.2.27. *Assume that 0 is semi-conical for $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. There exists a right-equivalence $\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ of f such that $\tilde{f} = f \circ \phi$ satisfies*

$$\partial_2 \tilde{f}_1(0, 0) = \partial_2 \tilde{f}_2(0, 0) = 0.$$

Moreover, if $\nabla f_1(0, 0) \neq 0$ and $\nabla f_2(0, 0) \neq 0$, then we have

$$\partial_1 \tilde{f}_1(0, 0) \neq 0, \quad \partial_1 \tilde{f}_2(0, 0) \neq 0.$$

Proof. Consider $r_1, r_2 \in [0, +\infty)$ and $\beta_1 \in [0, 2\pi]$ such that

$$\partial_2 f_1(0, 0) = r_1 \cos(\beta_1), \quad \partial_1 f_1(0, 0) = r_1 \sin(\beta_1), \quad \partial_2 f_2(0, 0) = r_2 \cos(\beta_1), \quad \partial_1 f_2(0, 0) = r_2 \sin(\beta_1).$$

Introducing the right-equivalence $\phi(u, v) = \begin{pmatrix} -\sin(\beta_1) & \cos(\beta_1) \\ -\cos(\beta_1) & -\sin(\beta_1) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}$ and $\tilde{f} = (f \circ \phi)$,

we have $D\tilde{f}(0, 0) = \begin{pmatrix} -r_1 & 0 \\ -r_2 & 0 \end{pmatrix}$. If we assume $\nabla f_1(0, 0) \neq 0$ and $\nabla f_2(0, 0) \neq 0$, then we can choose r_1 and r_2 which are non-zero, and we get the result.

□

For $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, the propositions 4.2.26 and 4.2.27 lead us to consider the next condition that we will refer to as condition **(SC2)**,

$$f(0) = 0, \quad \partial_2 f(0) = 0, \quad \partial_1 f_1(0) = \partial_1 f_2(0) \neq 0, \quad \partial_2 \chi(f)(0) \neq 0. \quad (\mathbf{SC2})$$

Proof of Theorem 4.2.25: STEP 3

Proposition 4.2.28. *Let $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ satisfy Condition **(SC2)**. Then there exists $h \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfying $h(0) = 1$ such that f is right-equivalent to $(u, v) \mapsto \begin{pmatrix} h(u)u \\ u + v^2 \end{pmatrix}$ or $(u, v) \mapsto \begin{pmatrix} h(u)u \\ u - v^2 \end{pmatrix}$.*

Proof. Because of the condition $\partial_1 f_1(0) \neq 0$, the map $\Phi : (u, v) \mapsto (f_1(u, v), v)$ is a diffeomorphism in a neighborhood of 0 and $g = f \circ \Phi^{-1}$ is right-equivalent to f . Locally near 0 we have

$$g_1(u, v) = u, \quad g_2(u, v) = f_2(G(u, v), v),$$

where G is a smooth function satisfying $\partial_1 G(u, v) = \frac{1}{\partial_1 f_1(G(u, v), v)}$ and $\partial_2 G(u, v) = -\frac{\partial_2 f_1(G(u, v), v)}{\partial_1 f_1(G(u, v), v)}$. Hence,

$$\begin{aligned}\partial_1 g_2(u, v) &= \partial_1 f_2(G(u, v), v) \partial_1 G(u, v), \\ \partial_2 g_2(u, v) &= \partial_1 f_2(G(u, v), v) \partial_2 G(u, v) + \partial_2 f_2(G(u, v), v).\end{aligned}$$

The condition $\partial_1 f_1(0) \neq 0 \neq \partial_1 f_2(0)$ implies that $\partial_1 g_2(0) \neq 0$. Moreover,

$$\begin{aligned}\partial_{22} g_2(u, v) &= \partial_{22} G(u, v) \partial_1 f_2(G(u, v), v) + \partial_{22} f_2(G(u, v), v) \\ &\quad + \partial_2 G(u, v)^2 \partial_{11} f_2(G(u, v), v) + 2\partial_2 G(u, v) \partial_{12} f_2(G(u, v), v).\end{aligned}$$

Evaluating at 0 and noticing that $\partial_1 G(0) = \frac{1}{\partial_1 f_1(0)}$ and $\partial_2 G(0) = 0$, we get $\partial_2 g_2(0) = 0$ and

$$\partial_{22} g_2(0) = \partial_{22} G(0) \partial_1 f_2(0) + \partial_{22} f_2(0) = \frac{\partial_2 \chi(f)(0)}{\partial_1 f_1(0)} \neq 0,$$

since f satisfies Condition **(SC2)**. By the Implicit Function Theorem, $\partial_2 g_2(u, v)$ vanishes on a smooth curve $v = \eta(u)$ in a neighborhood of 0. By Lemma 4.7.11, there exist two smooth functions $m \in C^\infty(\mathbb{R}^2, \mathbb{R})$ and $f_0 \in C^\infty(\mathbb{R}, \mathbb{R})$ such that $g_2(u, v) = (v - \eta(u))^2 m(u, v) + f_0(u)$ in a neighborhood of 0. The conditions $\partial_1 g_2(0) \neq 0$ and $\partial_{22} g_2(0) \neq 0$ yield $f_0'(0) \neq 0$ and $m(0) \neq 0$, respectively. Applying first the right-equivalence $(u, v) \mapsto \begin{pmatrix} u \\ (v - \eta(u)) \sqrt{|m(u, v)|} \end{pmatrix}$ and then $(u, v) \mapsto \begin{pmatrix} f_0(u) \\ v \end{pmatrix}$, we deduce that f is right-equivalent to $(u, v) \mapsto \begin{pmatrix} h(u)u \\ (u + \text{sign}(m(0, 0))v^2) \end{pmatrix}$, for some smooth function h obtained by inversion of f_0 . Noticing that the quantity $\frac{\partial_1 f_1(0)}{\partial_1 f_2(0)}$ is invariant by right-equivalence, this provides $h(0) = \frac{\partial_1 f_1(0)}{\partial_1 f_2(0)} = 1$. \square

Proof. (Proof of Theorem 4.2.25) We start the proof by showing that

$$f : (u, v) \mapsto \begin{pmatrix} h(u)u \\ u - v^2 \end{pmatrix}$$

is right-time-equivalent to

$$(u, v) \mapsto \begin{pmatrix} \tilde{h}(u)u \\ u + v^2 \end{pmatrix},$$

where \tilde{h} is in $C^\infty(\mathbb{R}, \mathbb{R})$. Indeed, we can apply the right-equivalence $(u, v) \mapsto (-u, v)$, then the time-equivalence associated with $\xi \equiv -1$. The result follows defining $\tilde{h}(u) = h(-u)$. Theorem 4.2.25 then follows from Propositions 4.2.27 and 4.2.28. \square

Conditions that guarantee $h'(0) \neq 0$

In this section, we show that we can define the Algorithm **(A)** such we can define a surjective mapping $f \mapsto h_f$ from the set of functions in $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ having a semi-conical intersection at 0 to the set of functions in $C^\infty(\mathbb{R}, \mathbb{R})$ that are equal to 1 at 0, where for every f , h_f corresponds to the function h obtained by the Algorithm **(A)**. Then we show that

$$V_M = \{j^2(f)(0,0) \in J^2(\mathbb{R}^2, \mathbb{R}^2) \mid 0 \text{ is a semi-conical intersection for } f, h'_f(0) = 0\}$$

is a closed Whitney stratified set of codimension 4.

For the first step of the Algorithm **(A)**, consider a function $f = (f_1, f_2) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ having a semi-conical intersection at 0. Without loss of generality, we can assume $\nabla f_1(0) \neq 0$. Define $\alpha \in \mathbb{R}$ as in 4.2.26 as the unique real number such that $\nabla f_2(0) = \alpha \nabla f_1(0)$, and consider the function $\tilde{f} \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, left-equivalent to f , defined by

$$\begin{aligned} \tilde{f}_1(u, v) &= \frac{1}{\sqrt{2 + 2\alpha^2}} ((1 + \alpha)f_1(u, v) - (1 - \alpha)f_2(u, v)) \\ \tilde{f}_2(u, v) &= \frac{1}{\sqrt{2 + 2\alpha^2}} ((1 + \alpha)f_2(u, v) + (1 - \alpha)f_1(u, v)), \end{aligned}$$

for every $(u, v) \in \mathbb{R}^2$. Consider the coordinates $(x_{jk} = \partial_j f_k(0))_{j,k \in \{1,2\}}$, $(\tilde{x}_{jk} = \partial_j \tilde{f}_k(0))_{j,k \in \{1,2\}}$, $(y_{jk}^l = \partial_{jk}^2 f_l(0))_{j,k,l \in \{1,2\}}$, and $(\tilde{y}_{jk}^l = \partial_{jk}^2 \tilde{f}_l(0))_{j,k,l \in \{1,2\}}$ in $J^2(\mathbb{R}^2, \mathbb{R}^2)$. Notice that the first order derivatives of f at 0 are uniquely determined by $\nabla f_1(0)$ and α , and that we have $\tilde{x}_{12} = \tilde{x}_{11}$ and $\tilde{x}_{22} = \tilde{x}_{21}$. Hence we can consider the mapping

$$F : ((x_{j1})_{j \in \{1,2\}}, (y_{jk}^l)_{j,k,l \in \{1,2\}}, \alpha) \mapsto ((\tilde{x}_{j1})_{j \in \{1,2\}}, (\tilde{y}_{jk}^l)_{j,k,l \in \{1,2\}}).$$

We prove that F is a submersion from $(\mathbb{R}^2 \setminus \{(0,0)\}) \times \mathbb{R}^7$ to $(\mathbb{R}^2 \setminus \{(0,0)\}) \times \mathbb{R}^6$, so that if S is a codimension k submanifold of \mathbb{R}^8 , then $F^{-1}(S)$ is a codimension k submanifold of \mathbb{R}^9 . To get this, we notice that for every (u, v) ,

$$\begin{pmatrix} \tilde{f}_1(u, v) \\ \tilde{f}_2(u, v) \end{pmatrix} = M(\alpha) \begin{pmatrix} f_1(u, v) \\ f_2(u, v) \end{pmatrix},$$

where $M(\alpha)$ is an invertible 2×2 matrix depending only on α . Hence it is sufficient to prove that the mapping

$$((x_{j1})_{j \in \{1,2\}}, \alpha) \mapsto ((\tilde{x}_{j1})_{j \in \{1,2\}})$$

is a submersion from $(\mathbb{R}^2 \setminus \{(0,0)\}) \times \mathbb{R}$ to $\mathbb{R}^2 \setminus \{(0,0)\}$. For every $(x_{11}, x_{21}, \alpha) \in \mathbb{R}^2 \setminus \{(0,0)\} \times \mathbb{R}$, and for every $j \in \{1,2\}$, we have by definition of α , $\tilde{x}_{j1} = \frac{\sqrt{1+\alpha^2}}{\sqrt{2}} x_{j1}$. We can conclude by direct computations.

For the second step of the Algorithm **(A)**, for every $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, define the right-equivalence of f as in Proposition 4.2.27 by $\hat{f}(u, v) = f(\partial_1 f_1(0)u - \partial_2 f_1(0)v, -\partial_2 f_1(0)u +$

$\partial_1 f_1(0)v$). Consider the coordinates $(x_{jk} = \partial_j f_k(0))_{j,k \in \{1,2\}}$, $(\hat{x}_{jk} = \partial_j \hat{f}_k(0))_{j,k \in \{1,2\}}$, $(y_{jk}^l = \partial_{jk}^2 f_l(0))_{j,k,l \in \{1,2\}}$, and $(\hat{y}_{jk}^l = \partial_{jk}^2 \hat{f}_l(0))_{j,k,l \in \{1,2\}}$ in $J^2(\mathbb{R}^2, \mathbb{R}^2)$. Notice that we have $\hat{x}_{21} = 0$. By direct computations, we can show that the mapping

$$\hat{F} : ((x_{jk})_{j,k \in \{1,2\}}, (y_{jk}^l)_{j,k,l \in \{1,2\}}) \mapsto ((\hat{x}_{jk})_{(j,k) \in \{1,2\}^2 \setminus \{(2,1)\}}, (\hat{y}_{jk}^l)_{j,k,l \in \{1,2\}})$$

is a submersion from \mathbb{R}^{10} to \mathbb{R}^9 .

For the third step of the Algorithm **(A)**, for every $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ satisfying Condition **(SC2)**, we apply the same right-transformation as in Proposition 4.2.28, and we get a function $h \in C^\infty(\mathbb{R}, \mathbb{R})$ such that $h(0) = 1$.

Concatenating the three steps, we define a surjective mapping $f \mapsto h_f$ from the set of functions in $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ having a semi-conical intersection at 0 to the set of functions in $C^\infty(\mathbb{R}, \mathbb{R})$ that are equal to 1 at 0, where for every f , h_f corresponds to the function h obtained by the Algorithm **(A)**.

We prove the following result concerning the third step of the Algorithm **(A)**.

Lemma 4.2.29. *For a function $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ satisfying Condition **(SC2)**, consider the function $(u, v) \mapsto \begin{pmatrix} uh(u) \\ u + v^2 \end{pmatrix}$ obtained from f by the same right-equivalence as in the proof of Proposition 4.2.28, where $h \in C^\infty(\mathbb{R}, \mathbb{R})$ is such that $h(0) = 1$. Then we have $h'(0) = 0$ if and only if*

$$(\partial_{11} f_2(0,0) \partial_1 f_1(0,0) - \partial_1 f_2(0,0) \partial_{11} f_1(0,0)) \partial_2 \chi(f)(0,0) = (\partial_1 \chi(f)(0,0))^2. \quad (4.8)$$

Proof. By using the functions f_0 and g_2 and G as in the proof of Proposition 4.2.28, the following equivalences hold.

$$\begin{aligned} h'(0) = 0 &\iff f_0''(0) = 0 \\ &\iff \partial_{11} g_2(0,0) \partial_{22} g_2(0,0) = (\partial_{12} g_2(0,0))^2. \end{aligned} \quad (\text{E})$$

Now recall that $\forall(u, v)$, $g_2(u, v) = f_2(G(u, v), v)$. Moreover, we have

$$\begin{aligned} \partial_2 g_2(0,0) &= 0 \\ \partial_{22} g_2(0,0) &= \frac{\partial_2 \chi(f)(0,0)}{\partial_1 f_1(0,0)} \\ \partial_{12} g_2(0,0) &= \frac{\partial_1 f_2(0,0)}{\partial_1 f_1(0,0)}. \end{aligned}$$

We can show that

$$\begin{aligned} \partial_{12} g_2(0,0) &= \frac{\partial_1 \chi(f)(0,0)}{(\partial_1 f_1(0,0))^2} \\ \partial_{11} g_2(0,0) &= \frac{\partial_{11} f_2(0,0) \partial_1 f_1(0,0) - \partial_1 f_2(0,0) \partial_{11} f_1(0,0)}{(\partial_1 f_1(0,0))^3}. \end{aligned}$$

Replacing these expressions in Equation (E), we get the result. \square

4.2. Basic facts and normal forms

Notice that Equality (4.8) is clearly independent from Condition **(SC2)**. Using Lemma 4.2.29 and the fact that F and \hat{F} are submersions, we can conclude that

$$V_M = \{j^2(f)(0, 0) \in J^2(\mathbb{R}^2, \mathbb{R}^2) \mid 0 \text{ is a semi-conical intersection for } f, h'_f(0) = 0\}$$

is a closed Whitney stratified set of codimension 4.

Consider now the set $V_S = \{j^2(F)(0, 0, 0) \in J^2(\mathbb{R}^3, \mathbb{R}^2) \mid j^2(F(\cdot, \cdot, 0))(0, 0) \in V_M\}$ where $j^2(F(\cdot, \cdot, 0))$ is the 2-jet of $f(\cdot, \cdot) = F(\cdot, \cdot, 0)$ related to the variables u and v . By Thom's transversality theorem (see, e.g., [41]) used in combination with [42, §1.3.2], we can deduce that

$$\tilde{O} = \{F \in C^\infty(\mathbb{R}^3, \mathbb{R}^2), j^2F(\mathbb{R}^3) \cap V_S = \emptyset\}$$

is an open and dense subset of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$.

4.2.4 Normal forms for the parametric case

Proposition 4.2.30. *For every $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ such that 0 is F -conical or F -semi-conical for f and $\partial_3 f_2(0) \neq 0$, let $\beta(f) = \frac{\partial_3 f_1}{\partial_3 f_2}(0)$. Then $\beta(f)$ is invariant by right-equivalence.*

Proof. Let \tilde{f} be right-equivalent to f and let $\phi_1 \in C^\infty(\mathbb{R}^2, \mathbb{R}), \phi_2 \in C^\infty(\mathbb{R}^2, \mathbb{R}), \phi_3 \in C^\infty(\mathbb{R}, \mathbb{R})$ be such that $\phi(u, v, z) = (\phi_1(u, v), \phi_2(u, v), \phi_3(z))$ is a right-equivalence between f and \tilde{f} . Differentiating w.r.t. z , we have

$$\frac{\partial_3 \tilde{f}_1}{\partial_3 \tilde{f}_2}(0) = \frac{\partial_3 f_1(0) \phi'_3(0)}{\partial_3 f_2(0) \phi'_3(0)} = \beta(f),$$

using the fact $\phi'_3(0) \neq 0$ because ϕ is a diffeomorphism. □

Conical case

Theorem 4.2.31. *Let $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. Then 0 is F -conical for f if and only if there exist $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R})$ satisfying $h_1(0) = h_2(0) = 1$, such that f is equivalent to*

$$(u, v, z) \mapsto \begin{pmatrix} h_1(u, v, z)(z - u) \\ h_2(u, v, z)(z - v) \end{pmatrix}.$$

Proof. By the same argument as in the proof of Proposition 4.2.26, there exists \tilde{f} left-equivalent to f such that $\partial_3 \tilde{f}_1(0) \neq 0, \partial_3 \tilde{f}_2(0) \neq 0$ and $\beta(\tilde{f}) = 1$. Using the fact that $\tilde{f}(0) = 0$, we deduce that \tilde{f}_1 and \tilde{f}_2 vanish respectively on two smooth surfaces whose equations are of the form $z = \eta_1(u, v)$ and $z = \eta_2(u, v)$, where η_1, η_2 are smooth functions vanishing at $(0, 0)$. By Lemma 4.7.10, there exist two smooth scalar functions $(u, v, z) \mapsto \phi_1(u, v, z), (u, v, z) \mapsto \phi_2(u, v, z)$ such that

$$\tilde{f}_1(u, v, z) = \phi_1(u, v, z)(z - \eta_1(u, v)), \quad \tilde{f}_2(u, v, z) = \phi_2(u, v, z)(z - \eta_2(u, v)).$$

Differentiating these expressions and evaluating them at 0 we get that

$$\chi(\tilde{f})(0) = \phi_1(0)\phi_2(0)\chi(\eta)(0),$$

where $\eta = (\eta_1, \eta_2)$. Hence, by F-conicity of 0, $\phi_1(0) \neq 0$, $\phi_2(0) \neq 0$, and $\chi(\eta)(0) \neq 0$. In particular, η is a diffeomorphism in a neighborhood of $(0, 0)$. Then \tilde{f} is right-equivalent to

$$\tilde{f} \circ \mu^{-1}(u, v, z) = \begin{pmatrix} h_1(u, v, z)(u - z) \\ h_2(u, v, z)(v - z) \end{pmatrix},$$

where $\mu : (u, v, z) \mapsto (\eta_1(u, v), \eta_2(u, v), z)$ and $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R})$ satisfy $h_1(0) \neq 0$ and $h_2(0) \neq 0$. By Proposition 4.2.30, $\frac{h_1(0)}{h_2(0)} = \beta(\tilde{f}) = 1$. By applying a time equivalence associated with $\xi \equiv \frac{1}{h_1(0)}$, we conclude the proof of the theorem. \square

Semi-conical case

Theorem 4.2.32. *Let $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. Then 0 is F-semi-conical for $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ if and only if there exist $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ satisfying $h_1(0) = h_2(0) = 1$ and $m \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfying $m(0) \notin \{-1, 0\}$ such that f is equivalent to*

$$(u, v, z) \mapsto \begin{pmatrix} h_1(u, v, z)(z - m(u)u) \\ h_2(u, v, z)(z + u + v^2) \end{pmatrix}.$$

Before proving the theorem, let us make some general considerations and provide an intermediate result in Proposition 4.2.33.

First remark that, up to a left-equivalence, we can assume that

$$\partial_1 f_1(0) \neq 0, \partial_1 f_2(0) \neq 0, \partial_3 f_1(0) = \partial_3 f_2(0) \neq 0.$$

In particular, $\beta(f) = 1$. In order to impose the non-conical direction to be in the $\text{span}(e_2)$ -direction, we use the same right-equivalence of the plane (u, v) as in the first step of the algorithm **(A)** in Section 4.2.3 (see Proposition 4.2.27). As a result, we end up with \hat{f} equivalent to f and such that

$$\begin{aligned} f(0) = 0, \partial_2 f(0) = 0, \partial_1 f_1(0) \neq 0, \partial_1 f_2(0) \neq 0, \partial_3 f_1(0) = \partial_3 f_2(0) \neq 0, \\ \chi_{13}(f)(0) \neq 0, \partial_2 \chi(f)(0) \neq 0. \end{aligned} \tag{SC2P}$$

Notice that the condition $\chi_{13}(f)(0) \neq 0$ can then be rewritten as $\partial_1 f_1(0) \neq \partial_1 f_2(0)$. The proof of the theorem is based on the following result.

Proposition 4.2.33. *Let $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ satisfy (SC2P) at 0. Then there exist $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R})$ non-vanishing at 0 and $m \in C^\infty(\mathbb{R}, \mathbb{R})$ such that $\frac{h_1(0)}{h_2(0)} = 1$, $m(0) = -\frac{\partial_1 f_1(0)}{\partial_1 f_2(0)} \notin \{-1, 0\}$, and f is right-equivalent to*

$$(u, v, z) \mapsto \begin{pmatrix} h_1(u, v, z)(z - m(u)u) \\ h_2(u, v, z)(z + u \pm v^2) \end{pmatrix},$$

where the sign depends on f .

4.2. Basic facts and normal forms

Proof. Using the fact that $f(0) = 0$ and the conditions $\partial_3 f_1(0) \neq 0 \neq \partial_3 f_2(0)$, we can deduce that f_1 and f_2 are smooth functions vanishing, in the neighborhood of the origin, on two smooth surfaces whose equations are, respectively, $z = \eta_1(u, v)$ and $z = \eta_2(u, v)$, where $\eta_1, \eta_2 : \mathbb{R}^2 \rightarrow \mathbb{R}$ are smooth functions vanishing at 0. By Lemma 4.7.10, there exist two smooth functions $\phi_1, \phi_2 : \mathbb{R}^3 \rightarrow \mathbb{R}$ such that

$$f_1(u, v, z) = \phi_1(u, v, z)(z - \eta_1(u, v)), \quad f_2(u, v, z) = \phi_2(u, v, z)(z - \eta_2(u, v)).$$

Differentiating these expressions with respect to z , we deduce that $\phi_1(0) \neq 0 \neq \phi_2(0)$. Differentiating f_1 and f_2 with respect to y , we get then from (SC2P) that $\partial_1 \eta_1(0) \neq 0 \neq \partial_1 \eta_2(0)$ and $\partial_2 \eta_1(0) = \partial_2 \eta_2(0) = 0$. Applying the right-equivalence associated with the inverse of $(u, v) \mapsto \begin{pmatrix} \eta_1(u, v) \\ v \end{pmatrix}$, we get that f is right-equivalent to

$$(u, v, z) \mapsto \begin{pmatrix} \phi_1(G(u, v), v, z)(z - u) \\ \phi_2(G(u, v), v, z)(z - \eta_2(G(u, v), v)) \end{pmatrix},$$

for some smooth function G such that $\partial_1 G(0) \neq 0$. Set $\tilde{\eta}(u, v) = \eta_2(G(u, v), v)$. Then $\tilde{\eta}(0) = 0$ and

$$\partial_1 \tilde{\eta}(u, v) = \partial_1 G(u, v) \partial_1 \eta_2(G(u, v), v), \quad \partial_2 \tilde{\eta}(u, v) = \partial_1 \eta_2(G(u, v), v) \partial_2 G(u, v) + \partial_2 \eta_2(G(u, v), v).$$

Evaluating at zero, we get that $\partial_1 \tilde{\eta}(0) \neq 0$ and $\partial_2 \tilde{\eta}(0) = 0$. Differentiating once more and using the hypothesis $\partial_2 \chi(f)(0) \neq 0$, we have $\partial_{22} \tilde{\eta}(0) \neq 0$. By the same arguments as in the proof of Theorem 4.2.25, f is right-equivalent to

$$(u, v, z) \mapsto \begin{pmatrix} h_1(u, v, z)(z - m(u)u) \\ h_2(u, v, z)(z + u \pm v^2) \end{pmatrix}$$

where $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R})$ and $m \in C^\infty(\mathbb{R}, \mathbb{R})$. Noticing that the quantities $\frac{\partial_1 f_1(0)}{\partial_1 f_2(0)}$ and $\beta(f)$ are invariant by right-equivalence, we get $\frac{h_1(0)}{h_2(0)} = \beta(f) = 1$ and $m(0) = -\frac{\partial_1 f_1(0)}{\partial_1 f_2(0)} \notin \{-1, 0\}$ because f satisfies .(SC2P) at 0. □

Proof of Theorem 4.2.32. First notice that if f is of the form

$$f : (u, v, z) \mapsto \begin{pmatrix} h_1(u, v, z)(z - m(u)u) \\ h_2(u, v, z)(z + u - v^2) \end{pmatrix}$$

then there exist $\tilde{h}_1, \tilde{h}_2 \in C^\infty(\mathbb{R}^3, \mathbb{R})$ and $\tilde{m} \in C^\infty(\mathbb{R}, \mathbb{R})$ such that f is right-time equivalent to

$$(u, v, z) \mapsto \begin{pmatrix} \tilde{h}_1(u, v, z)(z - \tilde{m}(u)u) \\ \tilde{h}_2(u, v, z)(z + u + v^2) \end{pmatrix}.$$

Indeed, applying the right-equivalence $(u, v, z) \mapsto (-u, v, -z)$ and the time-equivalence associated with $\xi : (u, v) \mapsto -1$ the claim follows with $\tilde{h}_i(u, v, z) = h_i(-u, v, -z)$, $i \in \{1, 2\}$, and $\tilde{m}(u) = m(-u)$. Theorem 4.2.32 hence follows from Proposition 4.2.33. □

4.3 Generic global properties of the singular locus

4.3.1 Proof of Lemma 4.1.1 and Theorem 4.1.2

Let $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$, $Z(f) = \{(u, v, z) \mid f(u, v, z) = (0, 0)\}$, and denote by $Z_{\text{nc}}(f)$ the set of non-conical intersections in $Z(f)$. Let $\pi(f)$ be the orthogonal projection of $Z(f)$ onto the plane (u, v) .

Proposition 4.3.1. *Assume that $(\bar{u}, \bar{v}, \bar{z})$ is a F -semi-conical intersection for $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. Then $\pi(f)$ is tangent at (\bar{u}, \bar{v}) to the non-conical direction of f at $(\bar{u}, \bar{v}, \bar{z})$.*

Proof. By Proposition 4.2.8, $Z(f)$ is locally near $(\bar{u}, \bar{v}, \bar{z})$ a smooth curve that we parameterize by $c(t) = (u(t), v(t), z(t))_{t \in \mathbb{R}}$, with $c(0) = (\bar{u}, \bar{v}, \bar{z})$ and $\dot{z}(0) = 0$. The condition $f(c(t)) \equiv 0$ implies that $Df_{c(t)}(\dot{c}(t)) \equiv 0$. In particular, $(\dot{u}(0), \dot{v}(0))$ is colinear to $\eta = \begin{pmatrix} -\partial_2 f_1(\bar{u}, \bar{v}, \bar{z}) \\ \partial_1 f_1(\bar{u}, \bar{v}, \bar{z}) \end{pmatrix}$, which is the non-conical direction of f at $(\bar{u}, \bar{v}, \bar{z})$. \square

Proposition 4.3.2. *Assume that $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ is a submersion at every point of $Z(f)$. Then $\pi(f)$ has no cuspidal point.*

Proof. Fix a local smooth regular parametrization $c(t) = (u(t), v(t), z(t))_{t \in \mathbb{R}}$ of $c \subset Z(f)$. It is sufficient to show that there exist no $t \in \mathbb{R}$ such that $\dot{u}(t) = \dot{v}(t) = 0$. By the same arguments as those used in the proof of Proposition 4.2.8, we get that $\dot{u}(t) = 0$ implies that $\begin{vmatrix} \partial_2 f_1(c(t)) & \partial_3 f_1(c(t)) \\ \partial_2 f_2(c(t)) & \partial_3 f_2(c(t)) \end{vmatrix} = 0$, while $\dot{v}(t) = 0$ implies that $\begin{vmatrix} \partial_1 f_1(c(t)) & \partial_3 f_1(c(t)) \\ \partial_1 f_2(c(t)) & \partial_3 f_2(c(t)) \end{vmatrix} = 0$. If the two determinants simultaneously vanish then f is not a submersion at $c(t)$. \square

Propositions 4.3.1 and 4.3.2, together with Remark 4.2.10, prove Lemma 4.1.1. As for Theorem 4.1.2, it follows from Proposition 4.3.2 together with Propositions 4.2.7, 4.2.11, and 4.2.12.

Remark 4.3.3. *Condition (ii) in Theorem 4.1.2 is essential for the control applications by adiabatic methods. It guarantees that the only possible singularities for the curve $\pi(f)$ in \mathbb{R}^2 are self-intersections.*

4.3.2 Generic self-intersections of $\pi(f)$

We aim at studying more precise generic properties of $\pi(f)$. Following the notations in [41], let X and Y be two smooth manifolds and denote by $J^k(X, Y)$ the set of k -jets from X to Y . Set $X^s = X \times \dots \times X$ (s -times) and

$$X^{(s)} = \{(x_1, \dots, x_s) \in X^s \mid x_i \neq x_j \text{ for } 1 \leq i < j \leq s\}.$$

4.4. Adiabatic control through a semi-conical intersection of eigenvalues

Let $\alpha : J^k(X, Y) \rightarrow X$ be the source map and denote by $\alpha^s : J^k(X, Y) \rightarrow X^s$ its natural extension. The set $J_s^k(X, Y) = (\alpha^s)^{-1}(X^{(s)})$ is called the s -fold k -jet bundle. We associate with a smooth function $f : X \rightarrow Y$ the map

$$\begin{aligned} j_s^k f : X^{(s)} &\longrightarrow J_s^k(X, Y), \\ (x_1, \dots, x_s) &\mapsto (j^k f(x_1), \dots, (j^k f(x_s))). \end{aligned}$$

Theorem 4.3.4. ([41, §4, Theorem 4.13] and [42, §1.3.2]) *Let X and Y be smooth manifolds and W be an algebraic submanifold of $J_s^k(X, Y)$. Let*

$$T_W = \{f \in C^\infty(X, Y) \mid j_s^k f \pitchfork W\}.$$

Then T_W is open and dense in $C^\infty(X, Y)$.

Proposition 4.3.5. *Generically with respect to $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$,*

1. $\pi(f)$ has no triple points;
2. Let (u, v) and (\tilde{u}, \tilde{v}) be two double points of $\pi(f)$ and let $z_1 \neq z_2$ and $\tilde{z}_1 \neq \tilde{z}_2$ be such that $f(u, v, z_1) = f(u, v, z_2) = f(\tilde{u}, \tilde{v}, \tilde{z}_1) = f(\tilde{u}, \tilde{v}, \tilde{z}_2) = 0$. Then $z_i \neq \tilde{z}_j$ for every $i, j \in \{1, 2\}$;
3. Let (u, v) and $z \neq \tilde{z}$ satisfy $f(u, v, z) = f(u, v, \tilde{z}) = 0$. Then (u, v, z) and (u, v, \tilde{z}) are F -conical for f ;
4. Let (u, v, z) and $(\tilde{u}, \tilde{v}, \tilde{z})$ be two non-conical intersections for f . Then $z \neq \tilde{z}$.

Proof. Here we prove the first claim, similar arguments leading to the other claims. A point (u, v) is a triple point of $\pi(f)$ if and only if there exist z_1, z_2, z_3 pairwise distinct such that $f(u, v, z_1) = f(u, v, z_2) = f(u, v, z_3) = 0$. Define the subspace W of $J_3^1(\mathbb{R}^3, \mathbb{R}^2)$ by

$$\begin{aligned} W = \{j_3^1 f(X_1, X_2, X_3) \mid f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2), X_1, X_2, X_3 \in \mathbb{R}^3, \pi(X_1) = \pi(X_2) = \pi(X_3), \\ f(X_1) = f(X_2) = f(X_3) = 0\}. \end{aligned}$$

Then W is a codimension $10 > 9 = \dim(X^{(3)})$ algebraic submanifold of $J_3^1(X, Y)$. Theorem 4.3.4 then implies that $T_W = \{f \in C^\infty(X, Y) \mid j_3^1 f \cap W = \emptyset\}$ is an open and dense subset of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. \square

4.4 Adiabatic control through a semi-conical intersection of eigenvalues

We consider $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ and the associated Hamiltonian $H_f = \begin{pmatrix} f_1 & f_2 \\ f_2 & -f_1 \end{pmatrix}$.

Consider a control path $(u(t), v(t))_{t \in [0,1]}$. Denote by

$$\lambda^-(u(t), v(t)) = -\sqrt{f_1(u(t), v(t))^2 + f_2(u(t), v(t))^2}$$

and

$$\lambda^+(u(t), v(t)) = \sqrt{f_1(u(t), v(t))^2 + f_2(u(t), v(t))^2}$$

the smallest and largest eigenvalue of H_f , respectively.

In the following, we denote by $\phi_-(u(t), v(t))$ (respectively, $\phi_+(u(t), v(t))$) a real normalized eigenvector of H_f at $(u(t), v(t))$ associated with $\lambda_-(u(t), v(t))$ (respectively, $\lambda_+(u(t), v(t))$). If $f(u(t), v(t)) \neq 0$ then $\lambda_-(u(t), v(t))$ and $\lambda_+(u(t), v(t))$ are simple and the choice of $\phi_{\pm}(u(t), v(t))$ is unique up to multiplication by -1 . If $(u(t), v(t))_{t \in [0,1]}$ does not cross $Z(f)$ then $t \mapsto \phi_-(u(t), v(t))$, $t \mapsto \phi_+(u(t), v(t))$ and $t \mapsto \lambda^-(u(t), v(t))$, $t \mapsto \lambda^+(u(t), v(t))$ can be chosen with the same regularity as $(u(t), v(t))_{t \in [0,1]}$. It is a classical fact that this may not be the case when $(u(t), v(t))_{t \in [0,1]}$ crosses $Z(f)$. However, we are going to prove the existence of a C^k basis of eigendirections of H_f along a C^{k+2} path $(u(t), v(t))_{t \in [0,1]}$ passing through a semi-conical intersection in a conical or a non-conical direction.

4.4.1 Adiabatic dynamics

Let $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. Consider a smooth regular control path $(u(t), v(t))_{t \in [0,1]}$ such that there exist $P \in C^2([0, 1], \text{SO}_2(\mathbb{R}))$ and $\lambda \in C^k([0, 1], \mathbb{R})$ such that $\{\lambda(t), -\lambda(t)\}$ is the spectrum of $H_f(u(t), v(t))$, and the columns of P form a basis of eigenvectors of $H_f(u(t), v(t))$ for every $t \in [0, 1]$. We can write, for every $t \in [0, 1]$, $P(t) = \begin{pmatrix} \cos(\theta(t)) & -\sin(\theta(t)) \\ \sin(\theta(t)) & \cos(\theta(t)) \end{pmatrix}$ where $\theta \in C^2([0, 1], \mathbb{R})$.

Let us study the dynamics of

$$i \frac{d\psi_\epsilon(t)}{dt} = H_f(u(\epsilon t), v(\epsilon t))\psi_\epsilon(t), \quad \psi_\epsilon(0) = \tilde{\psi}_0, \quad (4.9)$$

where $t \in [0, \frac{1}{\epsilon}]$ and $\tilde{\psi}_0$ is independent of ϵ .

Defining $Y_\epsilon(\tau) = P(\tau)\psi_\epsilon(\frac{\tau}{\epsilon})$ for every $\tau \in [0, 1]$, we have

$$i \frac{dY_\epsilon(\tau)}{d\tau} = \left(\frac{1}{\epsilon} \begin{pmatrix} \lambda(\tau) & 0 \\ 0 & -\lambda(\tau) \end{pmatrix} + \begin{pmatrix} 0 & i\dot{\theta}(\tau) \\ -i\dot{\theta}(\tau) & 0 \end{pmatrix} \right) Y_\epsilon(\tau). \quad (4.10)$$

Thanks to the further change of variables $\tilde{Y}_\epsilon(\tau) = \begin{pmatrix} e^{\frac{i}{\epsilon} \int_0^\tau \lambda(s) ds} & 0 \\ 0 & e^{-\frac{i}{\epsilon} \int_0^\tau \lambda(s) ds} \end{pmatrix} Y_\epsilon(\tau)$, the dynamics are transformed into

$$\frac{d\tilde{Y}_\epsilon(\tau)}{d\tau} = \begin{pmatrix} 0 & i\dot{\theta}(\tau) e^{\frac{2i}{\epsilon} \int_0^\tau \lambda(s) ds} \\ -i\dot{\theta}(\tau) e^{-\frac{2i}{\epsilon} \int_0^\tau \lambda(s) ds} & 0 \end{pmatrix} \tilde{Y}_\epsilon(\tau). \quad (4.11)$$

Based on Corollaries 4.7.3 and 4.7.7, one gets the following result.

4.4. Adiabatic control through a semi-conical intersection of eigenvalues

Theorem 4.4.1 (Adiabatic Theorem). *Let $k \in \mathbb{N}$ and assume that $\lambda : [0, 1] \rightarrow \mathbb{R}$ is C^k and $\theta : [0, 1] \rightarrow \mathbb{R}$ is C^2 . Let $\psi_\epsilon : [0, 1] \rightarrow \mathbb{C}^2$ be the solution of Equation (5.3). Assume that there exists $c > 0$ such that*

$$\left| \int_0^t e^{\frac{2i}{\epsilon} \int_0^s \lambda(x) dx} ds \right| \leq c\epsilon^{1/(k+1)}, \quad \forall t \in [0, 1]. \quad (4.12)$$

Then $\tilde{Y}_\epsilon(\tau) = \tilde{Y}_\epsilon(0) + O(\epsilon^q)$ uniformly w.r.t. $\tau \in [0, 1]$. In particular, if $\tilde{\psi}_0 = \begin{pmatrix} \cos(\theta(0)) \\ \sin(\theta(0)) \end{pmatrix}$, then $\psi_\epsilon(\frac{1}{\epsilon}) = e^{i\eta} \begin{pmatrix} \cos(\theta(1)) \\ \sin(\theta(1)) \end{pmatrix} + O(\epsilon^{\frac{1}{k+1}})$, where η possibly depends on ϵ .

4.4.2 Regularity of the eigenpairs along smooth control paths

The main goal of this section is to study the regularity of eigenpairs of H_f along smooth curves passing through a semi-conical intersection for f . Using the normal form obtained in Section 4.2.3, we can restrict our attention to the case where f has the form $f : (u, v) \mapsto \begin{pmatrix} u + v^2 \\ uh(u) \end{pmatrix}$, where $h \in C^\infty(\mathbb{R}, \mathbb{R})$ is such that $h(0) = 1$. Notice that for the simplicity of computations, we have inverted the two components f_1 and f_2 with respect to the normal form found in Section 4.2.3. However, (f_1, f_2) being left-equivalent to (f_2, f_1) , the same results hold for $f : (u, v) \mapsto \begin{pmatrix} uh(u) \\ u + v^2 \end{pmatrix}$.

Conical directions

We recall here the following regularity result which is a special case of [31, Proposition 3.1] and [10, Lemma 3.2].

Proposition 4.4.2 (Eigenpairs in the conical directions). *Consider a Hamiltonian H_f where $f : (u, v) \mapsto \begin{pmatrix} u + v^2 \\ uh(u) \end{pmatrix}$ and $h \in C^\infty(\mathbb{R}, \mathbb{R})$ is such that $h(0) = 1$. Let $\ell \in \mathbb{N}$, $t_0 \in (0, 1)$, and $(u(t), v(t))_{t \in [0, 1]}$ be a $C^{\ell+1}$ path such that $(u(t), v(t)) = 0$ if and only if $t = t_0$ and $\dot{u}(t_0) \neq 0$. Define $\lambda_0, \lambda_1 : [0, 1] \rightarrow \mathbb{R}$ by*

$$\begin{aligned} \lambda_0(t) &= \lambda_-(u(t), v(t)), \quad \lambda_1(t) = \lambda_+(u(t), v(t)), & \text{for } t < t_0, \\ \lambda_0(t) &= \lambda_+(u(t), v(t)), \quad \lambda_1(t) = \lambda_-(u(t), v(t)), & \text{for } t \geq t_0. \end{aligned}$$

Then λ_0 and λ_1 are $C^{\ell+1}$ on $[0, 1]$. Moreover, there exist $\Phi_0, \Phi_1 \in C^\ell([0, 1], \mathbb{R}^2)$ such that $\Phi_j(t)$ is a normalized eigenvector of $H_f(u(t), v(t))$ corresponding to the eigenvalue $\lambda_j(t)$ for $j \in \{0, 1\}$ and $t \in [0, 1]$.

The following proposition states that the limit eigenvectors along a C^2 curve crossing conically a semi-conical intersection do not depend on the choice of the curve.

Proposition 4.4.3 (Limit eigenvectors along a conical direction). *Consider $f, (u(t), v(t))_{t \in [0,1]}$, t_0 , and Φ_0, Φ_1 as in Proposition 4.4.2, which are uniquely defined up to multiplication to -1 . Then $\Phi_0(t_0)$ and $\Phi_1(t_0)$ depend only on the sign of $\dot{u}(t_0)$. More precisely, $\Phi_0(t_0) = \frac{1}{\sqrt{1+\bar{V}^2}} \begin{pmatrix} -1 \\ \bar{V} \end{pmatrix}$ and $\Phi_1(t_0) = \frac{1}{\sqrt{1+\bar{V}^2}} \begin{pmatrix} \bar{V} \\ 1 \end{pmatrix}$ with $\bar{V} = -(1 + \text{sign}(\dot{u}(t_0))\sqrt{2})$.*

Proof. By definition of Φ_0, Φ_1 , we have

$$\Phi_0(t) = \phi_-(u(t), v(t)), \quad \Phi_1(t) = \phi_+(u(t), v(t)), \quad \text{for } t < t_0.$$

Hence, up to multiplication by -1 ,

$$\Phi_0(t) = \frac{1}{\sqrt{1+V(t)^2}} \begin{pmatrix} -1 \\ V(t) \end{pmatrix}, \quad \Phi_1(t) = \frac{1}{\sqrt{1+V(t)^2}} \begin{pmatrix} V(t) \\ 1 \end{pmatrix}, \quad \text{for } t < t_0,$$

where $V(t) = 0$ if $u(t)h(u(t)) = 0$ and

$$V(t) = \frac{-u(t) - v(t)^2 + \sqrt{u(t)^2 h(u(t))^2 + (u(t) + v(t)^2)^2}}{u(t)h(u(t))}$$

otherwise. Then, as $t \rightarrow t_0^-$,

$$\begin{aligned} V(t) &= \frac{-\dot{u}(t_0)(t - t_0) + o(t - t_0) + \sqrt{\dot{u}(t_0)^2(t - t_0)^2(h(0)^2 + 1) + o((t - t_0)^2)}}{\dot{u}(t_0)h(0)(t - t_0)} \\ &= -\frac{\dot{u}(t_0)(t - t_0) + |t - t_0||\dot{u}(t_0)|\sqrt{2}}{\dot{u}(t_0)(t - t_0)} + o(1) \\ &= -(1 + \text{sign}(\dot{u}(t_0))\sqrt{2}) + o(1). \end{aligned}$$

Since Φ_0, Φ_1 are continuous on $[0, 1]$ by Proposition 4.4.2, the conclusion follows. \square

Non-conical direction

Proposition 4.4.4 (Continuity of the eigenstates in the non-conical direction). *Let f be as in Proposition 4.4.2. Let $\ell \in \mathbb{N}$, $t_0 \in (0, 1)$, and $(u(t), v(t))_{t \in [0,1]}$ be a $C^{\ell+2}$ path such that $(u(t), v(t)) = 0$ if and only if $t = t_0$ and $\dot{u}(t_0) = 0$ (i.e., $(u(t), v(t))$ passes through 0 in the non-conical direction at $t = t_0$ as on Figure 4.4). Then there exist $\lambda_0, \lambda_1 \in C^{\ell+2}([0, 1], \mathbb{R}^2)$, $\Phi_0, \Phi_1 \in C^\ell([0, 1], \mathbb{R}^2)$ such that $\lambda_0(t) = \lambda_-(t)$, $\lambda_1(t) = \lambda_+(t)$, $\Phi_0(t) = \phi_-(t)$ and $\Phi_1(t) = \phi_+(t)$ for every $t \in [0, t_0) \cup (t_0, 1]$. Moreover, $\Phi_0(t_0) = \frac{1}{\sqrt{1+\bar{V}^2}} \begin{pmatrix} -1 \\ \bar{V} \end{pmatrix}$*

and $\Phi_1(t_0) = \frac{1}{\sqrt{1+\bar{V}^2}} \begin{pmatrix} \bar{V} \\ 1 \end{pmatrix}$ where $\bar{V} = -\frac{\beta - \sqrt{\frac{\dot{u}(t_0)^2}{4} + \beta^2}}{\frac{\dot{u}(t_0)}{2}}$ where $\beta = \frac{\ddot{u}(t_0)}{2} + \dot{v}(t_0)^2$ if $\ddot{u}(t_0) \neq 0$.

If $\ddot{u}(t_0) = 0$, we have $\Phi_0(t_0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $\Phi_1(t_0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

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Proof. The condition $\dot{u}(t_0) = 0$ provides $u(t) + v(t)^2 = (t - t_0)^2 \left(\frac{\ddot{u}(t_0)}{2} + \dot{v}(t_0)^2 \right) + o((t - t_0)^2) = \beta(t - t_0)^2 + o((t - t_0)^2)$ when $t \rightarrow t_0$.

By direct computations, we show that $\frac{d^2 \lambda_{\pm}(t)}{dt^2} = \pm \sqrt{\beta^2 + \ddot{u}(t_0)^2} + o(1)$ when $t \rightarrow t_0$. Hence $t \mapsto \lambda_{\pm}(t)$ can be extended in a C^2 function at $t = t_0$ by fixing $\frac{d^2 \lambda_{\pm}(t_0)}{dt^2} = 2 \pm \sqrt{\beta^2 + \ddot{u}(t_0)^2}$. The $C^{\ell+2}$ regularity follows by higher order analog computations.

Define, for every $t \in [0, 1]$ such that $u(t)h(u(t)) \neq 0$,

$$V(t) = \frac{-(u(t) + v(t)^2) + \sqrt{u(t)^2 h(u(t))^2 + (u(t) + v(t)^2)^2}}{u(t)h(u(t))}.$$

Reasoning as in the proof of Proposition 6.2.2, we must prove that V can be extended as a C^{ℓ} function at t_0 by setting $V(t_0) = \bar{V}$.

First case: $\ddot{u}(t_0) \neq 0$. Assuming that $\ddot{u}(t_0) \neq 0$, we have, as $t \rightarrow t_0$,

$$V(t) = -\frac{\beta(t - t_0)^2 - \sqrt{\frac{(t-t_0)^4}{4} \ddot{u}(t_0)^2 + \beta^2(t - t_0)^4 + o((t - t_0)^4)}}{\frac{(t-t_0)^2}{2} \ddot{u}(t_0)} = -\frac{\beta - \sqrt{\frac{\ddot{u}(t_0)^2}{4} + \beta^2}}{\frac{\ddot{u}(t_0)}{2}} + o(1).$$

The continuity of V is proved in the case $\ddot{u}(t_0) \neq 0$. The same computations show that V is C^{ℓ} at t_0 if $(u(t), v(t))_{t \in [0,1]}$ is $C^{\ell+2}$.

Second case: $\ddot{u}(t_0) = 0$. In the case $\ddot{u}(t_0) = 0$, consider the left equivalence \tilde{f} of f associated with $\theta = \frac{\pi}{4}$ and $\zeta = -1$ as in Remark 4.2.16, so that, we have $H_{\tilde{f}} = P_{\theta, \zeta} H_f P_{\theta, \zeta}^{-1}$. If $f = (f_1, f_2) \in C^{\infty}(\mathbb{R}^2, \mathbb{R}^2)$, then we have $\tilde{f} = (f_2, f_1)$. Define, for every $t \in [0, 1]$ such that $u(t) + v(t)^2 \neq 0$, $\tilde{V}(t) = \frac{-u(t)h(u(t)) + \sqrt{u(t)^2 h(u(t))^2 + (u(t) + v(t)^2)^2}}{u(t) + v(t)^2}$. We have easily $\lim_{t \rightarrow t_0} \tilde{V}(t) = 1$. Hence we can define continuous eigenvectors $\tilde{\Phi}_0$ and $\tilde{\Phi}_1$ of $H_{\tilde{f}}$ along

$(u(t), v(t))_{t \in [0,1]}$, respectively equal, up to phases, to $\frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$ and $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ at $t = t_0$.

Knowing that the eigenvectors of H_f are equal, up to phases, to $P_{\theta, \zeta} \tilde{\Phi}_j$, for $j \in \{0, 1\}$, we can deduce the continuity of Φ_0 and Φ_1 at $t = t_0$, and that $\Phi_0(t_0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and

$\Phi_1(t_0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ in this case. □

4.4.3 Dynamical properties at semi-conical intersections of eigenvalues

By using the previous results, we get the following adiabatic approximations along curves going through a semi-conical intersection, either along conical directions (Proposition 4.4.5) or along the non-conical direction (Proposition 4.4.6).

Proposition 4.4.5. *Let f and $(u(t), v(t))_{t \in [0,1]}$ be as in Proposition 4.4.2. Consider a solution ψ_ϵ of Equation (5.3) such that $\tilde{\psi}_0 = \phi_-(u(0), v(0))$. Then $\langle \psi_\epsilon(\frac{1}{\epsilon}), \phi_-(u(1), v(1)) \rangle = O(\sqrt{\epsilon})$.*

Proof. First notice that λ_- and λ_+ are C^2 separately on $[0, t_0]$ and $[t_0, 1]$. Moreover, Corollary 4.7.7 proves that they satisfy (4.22) with $k = 1$ on $[0, t_0]$ and $[t_0, 1]$. By Proposition 6.2.2, moreover, there exists a C^2 basis of eigenvectors defined on $[0, 1]$ with $\lim_{t \rightarrow t_0^-} \phi_\pm(t) = \lim_{t \rightarrow t_0^+} \phi_\mp(t)$. By applying Theorem 4.4.1 on the interval $[0, t_0]$, then on the interval $[t_0, 1]$, we get the result. \square

Proposition 4.4.6. *Let f and $(u(t), v(t))_{t \in [0,1]}$ be as in Proposition 4.4.4 with $l \geq 2$ (see Figure 4.4). Consider a solution ψ_ϵ of Equation (4.13) such that $\psi_\epsilon(0) = \phi_-(u(0), v(0))$. Then $\langle \psi_\epsilon(\frac{1}{\epsilon}), \phi_+(u(1), v(1)) \rangle = O(\epsilon^{1/3})$.*

Proof. Let $\lambda(\tau) = \lambda_-(\tau)$ and $\phi(\tau) = \int_0^\tau \lambda_-(s) ds$ for $\tau \in [0, 1]$. Notice that λ is at least C^2 by Proposition 4.4.4 and that ϕ satisfies $\phi(t_0) = \phi'(t_0) = \phi''(t_0) = 0$ and $\phi^{(3)}(t_0) \neq 0$. Hence, by Lemma 4.7.4, λ satisfies the estimate (4.22) with $k = 2$. The result follows by applying Theorem 4.4.1 in combination with Proposition 4.4.4. \square

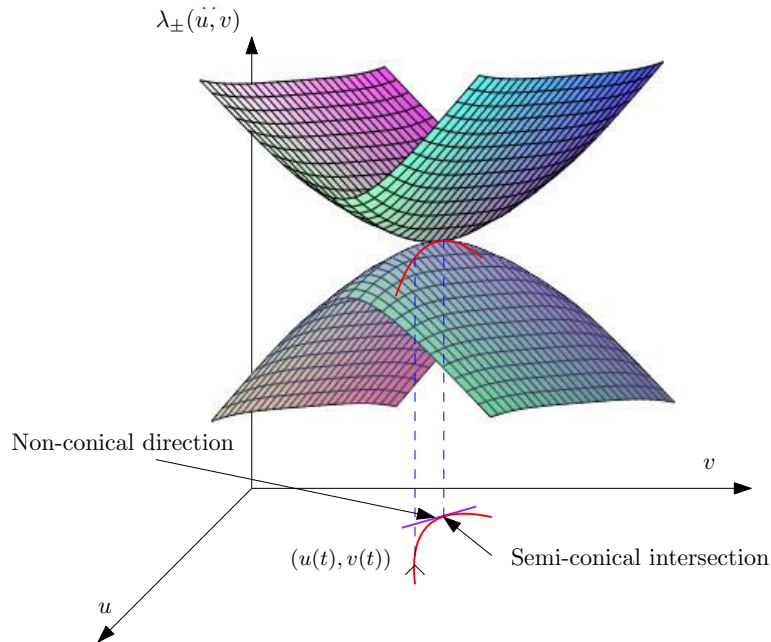


Figure 4.4 – A control path passing at a semi-conical intersection in the non-conical direction as a function of the controls $(u, v) \in \mathbb{R}^2$.

4.5 Control of a continuum of systems

4.5.1 Ensemble adiabatic dynamics

Let $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. Consider a smooth regular control path $(u(t), v(t))_{t \in [0,1]}$. In analogy with the previous sections, denote by

$$\lambda_z^\pm(u(t), v(t)) = \pm \sqrt{f_1(u(t), v(t), z)^2 + f_2(u(t), v(t), z)^2}$$

the eigenvalues of $H_f(u(t), v(t), z)$. Similarly, let $\phi_\pm^z(u(t), v(t))$ be two real normalized eigenvector of $H_f(u(t), v(t), z)$ at $(u(t), v(t))$ associated with $\lambda_z^\pm(u(t), v(t))$, uniquely defined up to a sign.

Let $V = [z_0, z_1]$ be a compact interval of \mathbb{R} . Assume that for every $z \in V$ there exist $P_z \in C^1([0, 1], \text{SO}_2(\mathbb{R}))$ and $\lambda_z \in C^1([0, 1], \mathbb{R})$ such that $\{\lambda_z(t), -\lambda_z(t)\}$ is the spectrum of $H_f(u(t), v(t), z)$ and the columns of P_z form a basis of eigenvectors of $H_f(u(t), v(t), z)$ for every $t \in [0, 1]$. We can write, for every $t \in [0, 1]$, $P_z(t) = \begin{pmatrix} \cos(\theta_z(t)) & -\sin(\theta_z(t)) \\ \sin(\theta_z(t)) & \cos(\theta_z(t)) \end{pmatrix}$ where $\theta_z \in C^1([0, 1], \mathbb{R})$.

Let us study the dynamics of

$$i \frac{d\psi_\epsilon^z(t)}{dt} = H_f(u(\epsilon t), v(\epsilon t), z) \psi_\epsilon^z(t), \quad \psi_\epsilon^z(0) = \tilde{\psi}_0^z, \quad (4.13)$$

where $t \in [0, \frac{1}{\epsilon}]$ and $\tilde{\psi}_0^z$ is independent of ϵ .

Defining $Y_\epsilon^z(\tau) = P_z(\tau) \psi_\epsilon^z(\frac{\tau}{\epsilon})$ for every $\tau \in [0, 1]$, we have

$$i \frac{dY_\epsilon^z(\tau)}{d\tau} = \left(\frac{1}{\epsilon} \begin{pmatrix} \lambda_z(\tau) & 0 \\ 0 & -\lambda_z(\tau) \end{pmatrix} + \begin{pmatrix} 0 & i\dot{\theta}_z(\tau) \\ -i\dot{\theta}_z(\tau) & 0 \end{pmatrix} \right) Y_\epsilon^z(\tau). \quad (4.14)$$

Thanks to the further change of variable $\tilde{Y}_\epsilon^z(\tau) = \begin{pmatrix} e^{\frac{i}{\epsilon} \int_0^\tau \lambda_z(s) ds} & 0 \\ 0 & e^{-\frac{i}{\epsilon} \int_0^\tau \lambda_z(s) ds} \end{pmatrix} Y_\epsilon^z(\tau)$, the dynamics is transformed into

$$\frac{d\tilde{Y}_\epsilon^z(\tau)}{d\tau} = \begin{pmatrix} 0 & i\dot{\theta}_z(\tau) e^{\frac{2i}{\epsilon} \int_0^\tau \lambda_z(s) ds} \\ -i\dot{\theta}_z(\tau) e^{-\frac{2i}{\epsilon} \int_0^\tau \lambda_z(s) ds} & 0 \end{pmatrix} \tilde{Y}_\epsilon^z(\tau). \quad (4.15)$$

Based on Corollary 4.7.8, one get the following result.

Theorem 4.5.1 (Parametric Adiabatic Theorem). *Let $k \in \mathbb{N}$. For every $z \in [z_0, z_1]$, assume that $\lambda_z : [0, 1] \rightarrow \mathbb{R}$ is C^k in $[0, 1]$ and θ_z is C^2 in $[0, 1]$. Let $\psi_\epsilon^z(t)$ be the solution of Equation (4.13). Assume that there exists $c > 0$ such that for every t in $[0, 1]$, and for every $z \in [z_0, z_1]$,*

$$\left| \int_0^t e^{\frac{2i}{\epsilon} \int_0^s \lambda_z(x) dx} ds \right| \leq c \epsilon^{\frac{1}{k+1}}, \quad \forall \epsilon > 0, \quad (4.16)$$

and that $(t, z) \mapsto \dot{\theta}_z(t)$ and $(t, z) \mapsto \ddot{\theta}_z(t)$ are uniformly bounded with respect to $(t, z) \in [0, 1] \times [z_0, z_1]$. Then we have $\tilde{Y}_\epsilon(\tau) = \tilde{Y}_\epsilon^z(0) + O(\epsilon^{\frac{1}{k+1}})$, uniformly w.r.t. $\tau \in [0, 1]$ and $z \in [z_0, z_1]$. In particular, if $\tilde{\psi}_0^z = \begin{pmatrix} \cos(\theta_z(0)) \\ \sin(\theta_z(0)) \end{pmatrix}$, then we have $\psi_\epsilon^z(\frac{1}{\epsilon}) = e^{i\eta} \begin{pmatrix} \cos(\theta_z(1)) \\ \sin(\theta_z(1)) \end{pmatrix} + O(\epsilon^{\frac{1}{k+1}})$, uniformly w.r.t. $z \in [z_0, z_1]$, where η is possibly depending on ϵ, z .

4.5.2 Controllability properties between the eigenstates for the normal forms

Let $f : (u, v, z) \mapsto \begin{pmatrix} h_1(u, v, z)(z - m(u)u) \\ h_2(u, v, z)(z + u + v^2) \end{pmatrix}$, where $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R})$ and $m \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfy $h_1(0) = h_2(0) \neq 0$ and $m(0) \notin \{-1, 0\}$. Recall that f has a F-semi-conical intersection at 0.

Consider a compact neighborhood \mathcal{S} of 0 in \mathbb{R}^3 on which the product $h_1 h_2$ does not vanish and m is different from 0 and -1 . Assume that \mathcal{S} writes $\mathcal{S} = U \times [z_0, z_1]$, where U is a compact neighborhood of 0 in \mathbb{R}^2 and $z_0 < 0 < z_1$. Define $\mathcal{C} = Z(f) \cap \mathcal{S}$ and, for every $(u, v, z) \in \mathcal{S}$, $h(u, v, z) = \frac{h_1(u, v, z)}{h_2(u, v, z)}$. Notice that $(u, v, z) \in \mathcal{S}$ is in \mathcal{C} if and only if $m(u)u = z = -u - v^2$. Up to restricting U , we can assume that $u \rightarrow (m(u) + 1)u$ is monotone, so that

$$(m(u) + 1)u = -v^2 \quad (4.17)$$

defines a smooth submanifold of U which contains the projection $\pi(\mathcal{C})$ of \mathcal{C} onto the plane of controls $(u, v) \in \mathbb{R}^2$.

Without loss of generality, assume that $m(0) > -1$ (the case $m(0) < -1$ being analogous). According to (4.17), this means that $\pi(\mathcal{C})$ lies in the intersection of U with the left half-plane. Notice that the sign of $z = m(u)u$ on \mathcal{C} is the opposite as the sign of $m(0)$.

Uniform adiabatic estimates when $(u(t), v(t))_{t \in [0, 1]} \subset \pi(\mathcal{C})$

Assume that $(u, v) : [0, 1] \rightarrow U$ is a regular C^∞ control path satisfying the following conditions, referred to as **(C)**:

- $(u, v) \subset \pi(\mathcal{C})$
- $(u, v)(0) = (u_0, v_0)$ where $(u_0, v_0, z_0) \in \mathcal{C}$ is a F-conical intersection for f ;
- $(u, v)(1) = (0, 0)$.

Under the previous assumptions, for every $z \in [z_0, 0]$, we can consider t_z as the unique element in $[0, 1]$ that satisfies $(u(t_z), v(t_z), z) \in \mathcal{C}$. On the other hand, for $z \in (0, z_1]$ there exist no $t \in [0, 1]$ such that $(u(t), v(t), z) \in \mathcal{C}$. By the regularity of (u, v) , the application $[z_0, 0] \ni z \mapsto t_z$ is C^∞ . Moreover, as a direct consequence of equation (4.17), which holds on \mathcal{C} , we have $f_1(u(t), v(t), z) = h(u(t), v(t), z)f_2(u(t), v(t), z)$ for every $t \in [0, 1]$ and $z \in [z_0, z_1]$.

4.5. Control of a continuum of systems

Definition 4.5.2. For any $z \in [z_0, z_1]$, define $V_z : [0, 1] \rightarrow \mathbb{R}$ as follows: if $z \in [z_0, 0)$, let

$$V_z(t) = -(h(u(t), v(t), z) - \sqrt{1 + h(u(t), v(t), z)^2})$$

for $t < t_z$ and $V_z(t) = -(h(u(t), v(t), z) + \sqrt{1 + h(u(t), v(t), z)^2})$ for $t \geq t_z$; if $z \in [0, z_1]$, let

$$V_z(t) = -(h(u(t), v(t), z) - \sqrt{1 + h(u(t), v(t), z)^2})$$

for every $t \in [0, 1]$.

By Propositions 4.4.2 and 4.4.4, we get the following result on the regularity of eigenpairs.

Proposition 4.5.3 (Regularity of eigenpairs for a control path $(u, v) \subset \pi(\mathcal{C})$). Let (u, v) satisfy **(C)**. For $z \in [0, z_1]$, define, for every $t \in [0, 1]$, $\Phi_0^z(t) = \phi_-(u(t), v(t))$, $\Phi_1^z(t) = \phi_+(u(t), v(t))$, $\lambda_0^z(t) = \lambda_-(u(t), v(t))$, and $\lambda_1^z(t) = \lambda_+(u(t), v(t))$. For $z \in [z_0, 0)$, define $\lambda_0^z, \lambda_1^z : [0, 1] \rightarrow \mathbb{R}$ by

$$\begin{aligned} \lambda_0^z(t) &= \lambda_-(u(t), v(t)), & \lambda_1^z(t) &= \lambda_+(u(t), v(t)), & \text{for } t < t_z, \\ \lambda_0^z(t) &= \lambda_+(u(t), v(t)), & \lambda_1^z(t) &= \lambda_-(u(t), v(t)), & \text{for } t \geq t_z, \end{aligned}$$

and $\Phi_0^z, \Phi_1^z : [0, 1] \rightarrow \mathbb{R}^2$ by

$$\begin{aligned} \Phi_0^z(t) &= \phi_-(u(t), v(t)), & \Phi_1^z(t) &= \phi_+(u(t), v(t)), & \text{for } t < t_z, \\ \Phi_0^z(t) &= \phi_+(u(t), v(t)), & \Phi_1^z(t) &= \phi_-(u(t), v(t)), & \text{for } t \geq t_z. \end{aligned}$$

Then, for every $z \in [z_0, z_1]$, λ_0^z, λ_1^z and Φ_0^z, Φ_1^z are C^∞ on $[0, 1]$. Moreover, Φ_0^z and Φ_1^z can be written as $\Phi_0^z = \frac{1}{\sqrt{1+V_z^2}} \begin{pmatrix} -1 \\ V_z \end{pmatrix}$ and $\Phi_1^z = \frac{1}{\sqrt{1+V_z^2}} \begin{pmatrix} V_z \\ 1 \end{pmatrix}$, where $V_z \in C^\infty([0, 1], \mathbb{R})$ is defined as in Definition 4.5.2.

A direct corollary of Proposition 4.5.3 is the following.

Proposition 4.5.4. For any $z \in [z_0, z_1]$, let $\theta_z = \arctan(V_z) \in C^\infty([0, 1], \mathbb{R})$, where V_z is defined as in Definition 4.5.2. Then $(t, z) \mapsto \dot{\theta}_z(t)$ and $(t, z) \mapsto \ddot{\theta}_z(t)$ are bounded w.r.t. $(t, z) \in [0, 1] \times [z_0, z_1]$.

Proof. By definition of V_z , for every $(t, z) \in [0, 1] \times [z_0, z_1]$, $\dot{\theta}_z(t)$ and $\ddot{\theta}_z(t)$ depend only on $\frac{d}{dt}h(u(t), v(t), z)$ and $\frac{d^2}{dt^2}h(u(t), v(t), z)$, which are uniformly bounded w.r.t. $(t, z) \in [0, 1] \times [z_0, z_1]$ because $h \in C^\infty(\mathcal{S}, \mathbb{R})$. \square

Remark 4.5.5. In the particular (non-generic) case in which h is constant, the curve (u, v) is non-mixing for all $z \in [z_0, z_1]$, in the sense developed in [22]. Non-mixing curves are characterized by an enhanced adiabatic approximation with respect to general curves passing through an eigenvalue intersection.

Proposition 4.5.6. *The functions λ_0^z, λ_1^z , defined as in Proposition 4.5.3, satisfy (4.16) with $k = 2$.*

Proof. As a first step of the proof, let us show the following local estimate: There exist $t_1 \in [0, 1)$, a nonempty compact neighborhood $W \subset [z_0, z_1]$ of 0, and $C_1 > 0$ independent of z such that for every $t \in [t_1, 1]$, $j \in \{0, 1\}$, and $z \in W$ we have

$$\left| \int_{t_1}^t e^{\frac{2i}{\epsilon} \int_0^s \lambda_j^z(r) dr} ds \right| \leq C_1 \epsilon^{\frac{1}{3}}, \quad \forall \epsilon > 0. \quad (4.18)$$

According to Corollary 4.7.8, it is enough to prove that there exist t_1 and W as above such that

$$|\ddot{\lambda}_z(t)| > c, \quad \forall z \in W, t \in [t_1, 1] \setminus \{t_z\}, \quad (4.19)$$

where $c > 0$ is independent of $z \in W$. Notice that

$$\lambda_z(t) = |z - m(u(t))u(t)| \sqrt{h_1(u(t), v(t), z)^2 + h_2(u(t), v(t), z)^2}.$$

By hypothesis **(C)**, $u(1) = \dot{u}(1) = 0$ and $\ddot{u}(1) = 0$. Hence,

$$\left. \frac{d}{dt} (z - m(u(t))u(t)) \right|_{t=1} = 0, \quad \left. \frac{d^2}{dt^2} (z - m(u(t))u(t)) \right|_{t=1} = (z - m(0))\ddot{u}(1),$$

and, in particular, for $z = 0$ we have

$$\lim_{z \rightarrow 0} \left| \frac{d^2}{dt^2} \lambda_z(t) \right|_{t=1} = |m(0)\ddot{u}(1)| > 0.$$

Inequality (4.19), and hence the required local estimate (4.18), follow by a continuity argument. Notice that, up to restricting W or increasing t_1 , we can assume that $\{t_z \mid z \in W \cap [z_0, 0]\} = [t_1, 1]$.

Let us now extend (4.18) to $z \in [z_0, z_1]$ and $t \in [0, 1]$. For $z \in [0, z_1] \setminus W$, there exists $c_1 > 0$ (independent of z) such that $|\lambda_0^z(t)| > c_1 > 0$ for every $t \in [0, 1]$. Hence, by applying Lemma 4.7.9, we have $|\int_0^t e^{\frac{2i}{\epsilon} \int_0^s \lambda_0^z(r) dr} ds| \leq C_1 \epsilon$, where $C_1 > 0$ is independent of $(t, z) \in [0, 1] \times ([0, z_1] \setminus W)$.

For every z in $[z_0, 0)$ we have $\dot{\lambda}_0^z(t_z) \neq 0$. By continuity of the applications $z \mapsto t_z$ and $(t, z) \mapsto \dot{\lambda}_0^z(t)$, there exist $\alpha, c_2 > 0$ such that $|\dot{\lambda}_0^z(t)| > c_2 > 0$ for every $z \in [z_0, 0]$ such that $t_z \leq (t_1 + 1)/2$ and every $t \in [t_z - \alpha, t_z + \alpha]$. By continuity of the application $(t, z) \mapsto \lambda_0^z(t)$, moreover, we get the existence of $c_3 > 0$ such that $|\lambda_0^z(t)| > c_3 > 0$ for every $z \in [z_0, 0] \setminus W$ and every $t \in [0, 1] \setminus [t_z - \alpha, t_z + \alpha]$, also for every $z \in [z_0, 0] \cap W$ and every $t \in [0, t_1] \setminus [t_z - \alpha, t_z + \alpha]$.

For $z \in [z_0, 0] \setminus W$ and $t \in [0, 1]$, we write

$$\begin{aligned} \int_0^t e^{\frac{2i}{\epsilon} \int_0^s \lambda_0^z(r) dr} ds &= \int_{[0, t] \cap [0, t_1 - \alpha]} e^{\frac{2i}{\epsilon} \int_0^s \lambda_0^z(r) dr} ds + \int_{[0, t] \cap [t_1 - \alpha, t_1 + \alpha]} e^{\frac{2i}{\epsilon} \int_0^s \lambda_0^z(r) dr} ds \\ &\quad + \int_{[0, t] \cap [t_1 + \alpha, 1]} e^{\frac{2i}{\epsilon} \int_0^s \lambda_0^z(r) dr} ds, \end{aligned}$$

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and we conclude, up a change of time variable, by applying Corollary 4.7.8 (on $[0, t] \cap [t_1 - \alpha, t_1 + \alpha]$, with $k = 2$) and Lemma 4.7.9 (on $[0, t] \cap [0, t_1 - \alpha]$ and $[0, t] \cap [t_1 + \alpha, 1]$).

We conclude similarly for $z \in W \cap [z_0, 0]$, by splitting $[0, 1]$ in the intervals $[0, \min(t_1, t_z - \alpha)]$, $[\min(t_1, t_z - \alpha), t_1]$, and $[t_1, 1]$ and by applying Corollary 4.7.8, Lemma 4.7.9, and (4.18). \square

Proposition 4.5.4 and 4.5.6 allow us to apply Theorem 4.5.1 and deduce the following ensemble adiabatic approximation result.

Theorem 4.5.7 (Semi-conical case). *Let (u, v) be a regular C^∞ control path satisfying condition (C). Let ψ_ϵ^z be the solution of Equation (4.13), where $\tilde{\psi}_0^z = \phi_-^z(u(0), v(0))$ for every $z \in (z_0, z_1]$ and $\tilde{\psi}_0^{z_0} = \lim_{t \rightarrow 0^+} \phi_-^{z_0}(u(t), v(t))$. Set $T_\epsilon(z) = |\langle \psi_\epsilon^z(\frac{1}{\epsilon}), \phi_+^z(u(1), v(1)) \rangle|$. Then*

$$\lim_{\epsilon \rightarrow 0} T_\epsilon(z) = \begin{cases} 0 & \text{if } z \in [0, z_1] \cup \{z_0\}, \\ 1 & \text{if } z \in (z_0, 0), \end{cases}$$

the convergence being uniform w.r.t. $z \in [z_0, z_1]$. More precisely, we have $T_\epsilon(z) = O(\epsilon^{1/3})$ for $z \in [0, z_1] \cup \{z_0\}$

4.5.3 The control path (u, v) exits from $\pi(f)$.

By similar arguments as those developed in [10], we get the following proposition.

Proposition 4.5.8 (Conical exit). *Let $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. Let (u_1, v_1, z_1) be a F -conical intersection for f . Let N be a neighborhood of (u_1, v_1, z_1) in \mathbb{R}^3 such that $Z(f) \cap N$ is made of F -conical intersections only and $\pi(Z(f) \cap N)$ is a C^∞ submanifold of \mathbb{R}^2 . Let $(u_0, v_0, z_0) \in Z(f) \cap N$ be such that $z_0 < z_1$. Consider a regular C^3 control path $(u(t), v(t))_{t \in [0, 1]}$ and a time $t_1 \in (0, 1)$ such that $(u(0), v(0)) = (u_0, v_0)$, $(u(t_1), v(t_1)) = (u_1, v_1)$, $(u(t), v(t)) \in \pi(Z(f) \cap N)$ for $t \in [0, t_1]$, and $(u(t), v(t)) \notin \pi(f)$ for $t > t_1$. For every $z \in \mathbb{R}$, consider $\theta_z \in C^2([0, 1], \mathbb{R})$ and $\lambda_z \in C^2([0, 1], \mathbb{R})$ as in Theorem 4.5.1. Then $(t, z) \mapsto \dot{\theta}_z(t)$ and $(t, z) \mapsto \ddot{\theta}_z(t)$ are uniformly bounded with respect to $(t, z) \in [0, 1] \times [z_0, z_1]$, and there exists $c > 0$ such that for every $z \in (z_0, z_1]$ and for every t in $[0, 1]$,*

$$\left| \int_0^t e^{\frac{2i}{\epsilon} \int_0^s \lambda_z(x) dx} ds \right| \leq c\epsilon^{\frac{1}{2}}, \quad \forall \epsilon > 0.$$

Corollary 4.5.9. *Let $f, (u, v)$ as in Proposition 4.5.8. Define ψ_ϵ^z as the solution of (4.13) with $\tilde{\psi}_0^z = \phi_-^z(u(0), v(0))$ for $z \neq 0$ and $\tilde{\psi}_0^{z_0} = \lim_{t \rightarrow 0} \phi_-^{z_0}(u(t), v(t))$. Then for every $z \in (z_0, z_1]$ and for every t in $[0, 1]$,*

$$|\langle \psi_\epsilon^z(1/\epsilon), \phi_+^z(u(1), v(1)) \rangle| = 1 + O(\epsilon^{1/2}).$$

Moreover, for every $\bar{z} \leq z_0$, we have, uniformly w.r.t. $z \in [\bar{z}, z_0]$,

$$|\langle \psi_\epsilon^z(1/\epsilon), \phi_+^z(u(1), v(1)) \rangle| = O(\epsilon^{1/2}).$$

Remark 4.5.10. For such a control path, we can notice that the adiabatic approximation is not uniform for every $z \in (z_1, z_1 + \alpha]$ for $\alpha > 0$.

4.5.4 Proof of Theorem 4.1.3

Proof of Theorem 4.1.3. Consider a regular C^4 control path $(\eta(t))_{t \in [0,1]} = (u(t), v(t))_{t \in [0,1]}$ such that $\eta(0) = \eta(1)$, $\eta(t_0) = (u_0, v_0)$, $\eta(t_1) = (u_1, v_1)$, $\eta(t) \in \pi(\gamma)$ for $t \in [t_0, t_1]$, and $\eta(t) \notin \pi(f)$ for $t \notin [t_0, t_1]$. Under these hypotheses, we can define, for every $z \in \mathbb{R}$, $\theta_z \in C^2([0, 1], \mathbb{R})$ and $\lambda_z \in C^2([0, 1], \mathbb{R})$ along the path η , as required in Theorem 4.5.1.

For $t \in [t_0, t_1]$, the hypothesis of non-existence of self-intersections for $\pi(\gamma)$ guarantees that we can apply the same arguments as those used in the proof of Proposition 4.5.6 for the normal form in order to get

$$\left| \int_{t_0}^t e^{\frac{2i}{\epsilon} \int_0^s \lambda_z(r) dr} ds \right| \leq C \epsilon^{\frac{1}{3}}, \quad \forall \epsilon > 0$$

where $C > 0$ is independent of $(t, z) \in [t_0, t_1] \times [z_0, z_1]$. Moreover by Proposition 4.5.4, $(t, z) \mapsto \dot{\theta}_z(t)$ and $(t, z) \mapsto \ddot{\theta}_z(t)$ are bounded on $[t_0, t_1] \times [z_0, z_1]$.

Under the assumptions that $z \in [z_0, z_1]$ for every z and t such that $(u(t), v(t), z) \in \gamma$ and that (u_1, v_1, z_1) is a F-conical intersection, we can apply Proposition 4.5.8 and get that $(t, z) \mapsto \dot{\theta}_z(t)$ and $(t, z) \mapsto \ddot{\theta}_z(t)$ are uniformly bounded with respect to $(t, z) \in [t_1, 1] \times [z_0, z_1]$, and there exists $c > 0$ such that for every $z \in [z_0, z_1]$ and for every t in $[t_1, 1]$,

$$\left| \int_{t_1}^t e^{\frac{2i}{\epsilon} \int_0^s \lambda_z(x) dx} ds \right| \leq c \epsilon^{\frac{1}{2}}, \quad \forall \epsilon > 0.$$

By similar arguments for $t \in [0, t_0]$, we obtain that on the whole interval $t \in [0, 1]$, $(t, z) \mapsto \dot{\theta}_z(t)$ and $(t, z) \mapsto \ddot{\theta}_z(t)$ are uniformly bounded with respect to $(t, z) \in [0, 1] \times [z_0, z_1]$, and by triangular inequality, there exists $\tilde{C} > 0$ such that for every $z \in [z_0, z_1]$ and for every t in $[0, 1]$,

$$\left| \int_0^t e^{\frac{2i}{\epsilon} \int_0^s \lambda_z(x) dx} ds \right| \leq \tilde{C} \epsilon^{\frac{1}{3}}, \quad \forall \epsilon > 0.$$

We get the expected result by applying Theorem 4.5.1. □

4.6 Extension to n -level systems

4.6.1 Generic assumptions on n -level Hamiltonians and adiabatic decoupling

In this section, we show that the study of a n -level real Hamiltonian can be reduced locally to the study of a 2-level Hamiltonian in the adiabatic regime and that such a

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transformation preserves the codimension of the generic conditions expressed in Section 4.2.1. Such a reduction allows us to define a semi-conical intersection model for a n -level real Hamiltonian.

For every $H \in S_n(\mathbb{R})$ denote by $(\lambda_j(H))_{j=1}^n$ the spectrum of H , where $j \mapsto \lambda_j(H)$ is the nondecreasing sequence of eigenvalues of H repeated according to their multiplicities. We write $(\phi_1(H), \dots, \phi_n(H))$ to denote an orthonormal basis of associated eigenvectors.

Next lemma is a classical result of continuity of the spectrum (see, for instance [68]).

Lemma 4.6.1. *Let $H_0 \in S_n(\mathbb{R})$ and $j \in \{1, \dots, n-1\}$ be such that $\lambda_j(H_0), \lambda_{j+1}(H_0)$ are separated from the rest of the spectrum of H_0 . Then, there exists a neighborhood V of H_0 in $S_n(\mathbb{R})$ and a Jordan curve c in \mathbb{C} separating $\{\lambda_q(H) \mid q \in \{j, j+1\}, H \in V\}$ from $\cup_{H \in V} (\text{Spectrum}(H) \setminus \{\lambda_j(H), \lambda_{j+1}(H)\})$.*

From now on, we consider H_0, j, c, V verifying Lemma 4.6.1. For all $H \in V$, we consider $P_{j,j+1}(H) = \frac{1}{2i\pi} \int_c (H - \xi)^{-1} d\xi$. Notice that, $P_{j,j+1}(H)$ is a real matrix because H is real. By construction of c , $V \ni H \mapsto P_H$ is smooth. Up to reducing V , for every H we can consider an orthogonal mapping $I(H) : \mathbb{R}^2 \rightarrow \text{Im}(P_{j,j+1}(H))$ such that $V \ni H \mapsto I(H)$ is smooth. For every $H \in V$ define $\pi_{j,j+1}(H) = \text{Im}(P_{j,j+1}(H))$, $I^{-1}(H)$ as the inverse of $I(H)$ on $\pi_{j,j+1}(H)$ and

$$F(H) = I^{-1}(H)HI(H) \in S_2(\mathbb{R}).$$

Notice that $I^{-1}(H) = {}^tI(H)$.

Consider $H \in C^\infty(\mathbb{R}^k, S_n(\mathbb{R}))$ such that $H(0) = H_0$, and denote by W a neighborhood of 0 in \mathbb{R}^k such that $H(u) \in V$ for every $u \in W$. Define $h \in C^\infty(\mathbb{R}^k, S_2(\mathbb{R}))$ such that for every $u \in W$, $h(u) = (F \circ H)(u)$. We say that h is a *reduced Hamiltonian* for H . Notice that if $\phi \in \mathbb{C}^2$ is an eigenvector of $h(u)$ associated with the eigenvalue $\lambda \in \mathbb{R}$ then $I(H(u))\phi$ is an eigenvector of $H(u)$ associated with the same eigenvalue λ . We deduce from this, as it has been already used in [10], that the regularity of the eigenpairs of H with respect to $u \in W$ can be deduced from the regularity of those of h .

Proposition 4.6.2. *F is a submersion from V to $S_2(\mathbb{R})$.*

Proof. Consider $A \in V$. Define $\psi_1 = I(A)e_1, \psi_2 = I(A)e_2$ where (e_1, e_2) is the canonical basis of \mathbb{C}^2 .

— Define $H = h_{11}\psi_1 {}^t\psi_1 + h_{22}\psi_2 {}^t\psi_2 + h_{12}\psi_1 {}^t\psi_2 + h_{12}\psi_2 {}^t\psi_1$ with $h_{11}, h_{22}, h_{12} \in \mathbb{R}$. By direct computations, we get

$${}^tI(A)HI(A) = \begin{pmatrix} h_{11} & h_{12} \\ h_{12} & h_{22} \end{pmatrix}.$$

Hence, the application $S_n(\mathbb{R}) \ni H \mapsto {}^tI(A)HI(A) \in S_2(\mathbb{R})$ is surjective.

— For $H \in S_n(\mathbb{R})$ such that $A + H \in V$,

$$\begin{aligned} F(A + H) &= {}^tI(A + H)(A + H)I(A + H) \\ &= F(A) + {}^tI(A)HI(A) + {}^tDI_A(H)AI(A) + {}^tI(A)ADI_A(H) + o(H). \end{aligned}$$

Hence, $\forall H \in S_n(\mathbb{R})$, $DF_A(H) = {}^tI(A)HI(A) + {}^tDI_A(H)AI(A) + {}^tI(A)ADI_A(H)$. Let us consider $H = h_{11}\psi_1{}^t\psi_1 + h_{22}\psi_2{}^t\psi_2 + h_{12}\psi_1{}^t\psi_2 + h_{12}\psi_2{}^t\psi_1$. Then, we have $DF_A(H) = {}^tI(A)HI(A)$. Hence, F is a submersion. □

Using classical facts on the composition of k -jets (see [65]), we obtain the following result.

Proposition 4.6.3. *Consider $\mathcal{F} : J^2(W, S_n(\mathbb{R})) \rightarrow J^2(W, S_2(\mathbb{R}))$ such that for every $u \in W$, $j^2(h)(u) = \mathcal{F}(j^2(H)(u))$. Then \mathcal{F} is a submersion.*

It follows that if S is a codimension q smooth submanifold of $J^2(W, S_2(\mathbb{R}))$, then $\mathcal{F}^{-1}(S)$ is a codimension q smooth submanifold of $J^2(W, S_n(\mathbb{R}))$. This can be used to deduce generic properties for $H \in C^\infty(W, S_n(\mathbb{R}))$ from generic properties for $h \in C^\infty(W, S_2(\mathbb{R}))$.

4.6.2 Adiabatic decoupling

We present here some results of adiabatic decoupling. They are adapted from [78], and are interesting because the adiabatic structure is preserved for the local two-levels dynamics.

Theorem 4.6.4 (Adiabatic decoupling). *Let $H \in C^\infty(\mathbb{R}^k, S_n(\mathbb{R}))$ and $j \in \{1, \dots, n-1\}$ be such that $\{\lambda_q(H(u)) \mid q \in \{j, j+1\}\}$ is separated from*

$$\text{Spectrum}(H(u)) \setminus \{\lambda_q(H(u)) \mid q \in \{j, j+1\}\}$$

for u in a neighborhood W of 0 in \mathbb{R}^k . Define, for every $u \in W$, $I(H(u))$ and $h(u)$ as in Section 4.6.1. Consider a C^2 regular path $u : [0, 1] \rightarrow W$ such that there exist $\ell \in \mathbb{N}$ and C^ℓ functions $\Lambda_j, \Lambda_{j+1} : [0, 1] \rightarrow \mathbb{R}$ such that for every $t \in [0, 1]$, $\{\Lambda_j(t), \Lambda_{j+1}(t)\} = \{\lambda_j(H(u(t))), \lambda_{j+1}(H(u(t)))\}$ and that h admits C^2 eigenvectors along u .

Assume that there exists $c > 0$ such that

$$\left| \int_0^t e^{\frac{i}{\epsilon} \int_0^s (\Lambda_{j+1}(x) - \Lambda_j(x)) dx} ds \right| \leq c\epsilon^{1/(\ell+1)}, \quad \forall t \in [0, 1]. \quad (4.20)$$

Let $\tilde{\psi}_0 \in \mathbb{C}^2$. Then the solutions ψ_ϵ and $\tilde{\psi}_\epsilon$ of, respectively,

$$i \frac{d\psi}{dt} = H(u(\epsilon t))\psi, \quad \psi(0) = I(H(u(0)))\tilde{\psi}_0, \quad \text{and} \quad i \frac{d\tilde{\psi}}{dt} = h(u(\epsilon t))\tilde{\psi}, \quad \tilde{\psi}(0) = \tilde{\psi}_0,$$

are such that $\psi_\epsilon(1/\epsilon)$ is $O(\epsilon^{\frac{1}{\ell+1}})$ -close to $I(H(u(1)))\tilde{\psi}_\epsilon(1/\epsilon)$.

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Proof. Define for $q \in \{1, 2\}$, and for every $u \in W$, $\psi_q(u) = I(H(u))e_q$, where (e_1, e_2) is the canonical basis of \mathbb{C}^2 . Define $\psi_\epsilon^{\text{eff}}(t)$ as the solution for $t \in [0, \frac{1}{\epsilon}]$, of

$$i \frac{d\psi_\epsilon^{\text{eff}}(t)}{dt} = \left(h(u(\epsilon t)) - i\epsilon \begin{pmatrix} 0 & \langle \dot{\psi}_j(u(\epsilon t)), \psi_{j+1}(u(\epsilon t)) \rangle \\ \langle \dot{\psi}_{j+1}(u(\epsilon t)), \psi_j(u(\epsilon t)) \rangle & 0 \end{pmatrix} \right) \psi_\epsilon^{\text{eff}}(t), \quad (4.21)$$

with $\psi_\epsilon^{\text{eff}}(0) = \tilde{\psi}_0$.

By [78, Theorem 1.4], there exists $C > 0$, such that, for every $t \in [0, \frac{1}{\epsilon}]$,

$$\|\psi_\epsilon(t) - I(h(u(\epsilon t)))\psi_\epsilon^{\text{eff}}(t)\| \leq C\epsilon, \quad \forall \epsilon > 0.$$

Under the assumptions of the theorem, we can consider a C^2 basis of eigenvectors of h along u . Hence, by the same arguments as those used in Section 4.4.1 in order to prove Theorem 4.4.1, there exists $c > 0$ such that, for every $t \in [0, \frac{1}{\epsilon}]$,

$$\|\tilde{\psi}_\epsilon(t) - \psi_\epsilon^{\text{eff}}(t)\| \leq c\epsilon^{\frac{1}{\ell+1}}, \quad \forall \epsilon > 0.$$

We get the expected result by triangular inequality. □

In the parametric case, using estimates that are uniform with respect to the parameter z , we get the following extension of Theorem 4.6.4.

Theorem 4.6.5 (Adiabatic decoupling for parametric systems). *Let $H \in C^\infty(\mathbb{R}^{k+1}, S_n(\mathbb{R}))$ and $j \in \{1, \dots, n-1\}$ be such that $\{\lambda_q(H(u, z)) \mid q \in \{j, j+1\}\}$ is separated from*

$$\text{Spectrum}(H(u, z)) \setminus \{\lambda_q(H(u, z)) \mid q \in \{j, j+1\}\}$$

for u in a neighborhood W of 0 in \mathbb{R}^k and $z \in [z_0, z_1]$. Define, for every $(u, z) \in W \times [z_0, z_1]$, $I(H(u, z))$ and $h(u, z)$ as in Section 4.6.1. Consider a C^2 regular path $u : [0, 1] \rightarrow W$ and $\tilde{\psi}_0^z \in \mathbb{C}^2$, for every $z \in [z_0, z_1]$. Let $\ell \in \mathbb{N}$ and assume that for every $z \in [z_0, z_1]$, there exist C^ℓ functions $\Lambda_j^z, \Lambda_{j+1}^z : [0, 1] \rightarrow \mathbb{R}$ such that for every $t \in [0, 1]$, $\{\Lambda_j^z(t), \Lambda_{j+1}^z(t)\} = \{\lambda_j^z(u(t)), \lambda_{j+1}^z(u(t))\}$ and that, for every $z \in [z_0, z_1]$, $h(u(\cdot), z)$ admits C^2 eigenvectors Φ_j^z, Φ_{j+1}^z such that $(t, z) \mapsto \frac{d\Phi_j^z(t)}{dt}$ and $(t, z) \mapsto \frac{d^2\Phi_j^z(t)}{dt^2}$ are bounded uniformly with respect to $(t, z) \in [0, 1] \times [z_0, z_1]$, for every $q \in \{j, j+1\}$. Assume that there exists $c > 0$ such that

$$\left| \int_0^t e^{\frac{i}{\epsilon} \int_0^s (\Lambda_{j+1}^z(x) - \Lambda_j^z(x)) dx} ds \right| \leq c\epsilon^{1/(\ell+1)}, \quad \forall t \in [0, 1], \quad \forall z \in [z_0, z_1]. \quad (4.22)$$

Then the solutions ψ_ϵ^z and $\tilde{\psi}_\epsilon^z$ of, respectively,

$$i \frac{d\psi^z}{dt} = H(u(\epsilon t))\psi^z, \quad \psi^z(0) = I(H(u(0), z))\tilde{\psi}_0^z, \quad \text{and} \quad i \frac{d\tilde{\psi}^z}{dt} = h(u(\epsilon t), z)\tilde{\psi}^z, \quad \tilde{\psi}^z(0) = \tilde{\psi}_0^z,$$

are such that $\psi^z(1/\epsilon)$ is $O(\epsilon^{\frac{1}{\ell+1}})$ -close to $I(H(u(1), z))\tilde{\psi}^z(1/\epsilon)$, uniformly w.r.t. $z \in [z_0, z_1]$.

4.6.3 Semi-conical intersections for n -level quantum systems

Let $H \in C^\infty(\mathbb{R}^k, S_n(\mathbb{R}))$ and $j \in \{1, \dots, n-1\}$ be such that $\{\lambda_q(H(u)) \mid q \in \{j, j+1\}\}$ is separated from $\text{Spectrum}(H(u)) \setminus \{\lambda_q(H(u)) \mid q \in \{j, j+1\}\}$ for u in a neighborhood W of 0 in \mathbb{R}^k . Define, for every $u \in W$, $I(H(u))$ and $h(u)$ as in Section 4.6.1. Define for $q \in \{1, 2\}$, and for every $u \in W$, $\psi_q(u) = I(H(u))e_q$, where (e_1, e_2) is the canonical basis of \mathbb{C}^2 . Then we have the identity

$$h(u) = \begin{pmatrix} \langle \psi_1(u), H(u)\psi_1(u) \rangle & \langle \psi_1(u), H(u)\psi_2(u) \rangle \\ \langle \psi_1(u), H(u)\psi_2(u) \rangle & \langle \psi_2(u), H(u)\psi_2(u) \rangle \end{pmatrix}.$$

Definition 4.6.6. *By removing the trace of $H(u)$, that is equivalent to changing a global phase in the dynamics, define the reduced zero-trace Hamiltonian of H as, for every $u \in W$,*

$$h_{\text{red}}(u) = \begin{pmatrix} f_1(u) & f_2(u) \\ f_2(u) & -f_1(u) \end{pmatrix},$$

with $f_1(u) = \frac{1}{2}(\langle \psi_1(u), H(u)\psi_1(u) \rangle - \langle \psi_2(u), H(u)\psi_2(u) \rangle)$ and $f_2(u) = \langle \psi_1(u), H(u)\psi_2(u) \rangle$.

Assume $k = 2$. By a slight abuse of notations, write $u := (u, v) \in U$, where U is a connected open neighborhood of the origin in \mathbb{R}^2 . In the next proposition, we prove that conicity properties do not depend on the choice of the unitary transformation $I(H(u, v)) : \mathbb{C}^2 \rightarrow \text{Im}(P_{j,j+1}(H(u, v)))$.

Proposition 4.6.7. *Let $f \in C^\infty(U, \mathbb{R}^2)$ and define*

$$R_\theta(u, v) = \begin{pmatrix} \cos(\theta(u, v)) & -\sin(\theta(u, v)) \\ \sin(\theta(u, v)) & \cos(\theta(u, v)) \end{pmatrix} \in \text{SO}_2(\mathbb{R}),$$

with $\theta \in C^\infty(U, \mathbb{R})$. Define $\tilde{f} \in C^\infty(U, \mathbb{R}^2)$ such that $H_{\tilde{f}}(u, v) = R_\theta(u, v)H_f(u, v)^t R_\theta(u, v)$ for every (u, v) in U . Then

- 0 is conical for f if and only if 0 is conical for \tilde{f} ;
- 0 is semi-conical for f if and only if 0 is semi-conical for \tilde{f} . Moreover, their non-conical directions are the same.

Proof. Using the fact that $f_1(0) = f_2(0) = 0$, we get

$$\chi(\tilde{f})(0) = \chi(f)(0).$$

Hence we get the first claim.

Assume that 0 is semi-conical for f . With no loss of generality, assume that the non-conical direction for f is e_2 , where (e_1, e_2) is the canonical basis of \mathbb{R}^2 . By direct computations, we have that $\nabla \tilde{f}_1(0)$ and $\nabla \tilde{f}_2(0)$ are not both equal to zero. Moreover, we get

4.6. Extension to n -level systems

$\partial_2 H_{\tilde{f}}(0) = R_\theta(0) \partial_2 H_f(0) {}^t R_\theta(0) = 0$. Hence e_2 is a non-conical direction for \tilde{f} . Differentiating at the second order, we get

$$\begin{aligned} \partial_2 \chi(\tilde{f})(0) &= \text{Det} \left(R_{2\theta}(0) \begin{pmatrix} \partial_1 f_1(0) & \partial_{22} f_1(0) \\ \partial_1 f_2(0) & \partial_{22} f_2(0) \end{pmatrix} {}^t R_{2\theta}(0) \right) \\ &= \partial_2 \chi(f)(0) \neq 0. \end{aligned}$$

Hence 0 is semi-conical for \tilde{f} . □

The same result holds when for every $(u, v) \in U$, $S_\theta(u, v) \in \text{O}_2^-(\mathbb{R})$, and

$$H_{\tilde{f}}(u, v) = S_\theta(u, v) H_f(u, v) {}^t S_\theta(u, v).$$

By similar computations, we show that in the parametric case, F -conical intersections and F -semi-conical intersections are invariant under such a orthogonal mapping, possibly depending on the parameter z . We define semi-conical intersections of eigenvalues for $H(\cdot) \in C^\infty(U, S_n(\mathbb{R}))$ and F -conical (respectively F -semi-conical intersections) for $H(\cdot) \in C^\infty(U \times \mathbb{R}, S_n(\mathbb{R}))$ (see Section 4.2.26 for precise definitions of these notions for two level systems) as follows.

Definition 4.6.8. *Let $j \in \{1, \dots, n-1\}$.*

- *We say that $(\bar{u}, \bar{v}) \in U$ is a semi-conical intersection for $H \in C^\infty(U, S_n(\mathbb{R}))$ between the levels j and $j+1$ if and only if there exists a unitary mapping $I(H(u, v)) : \mathbb{C}^2 \rightarrow \text{Im}(P_{j,j+1}(H(u, v)))$, C^∞ with respect to $(u, v) \in U$, such that (\bar{u}, \bar{v}) is a semi-conical intersection for the associated reduced Hamiltonian $h_{\text{red}} \in C^\infty(U, S_2(\mathbb{R}))$.*
- *We say that $(\bar{u}, \bar{v}, \bar{z}) \in U \times \mathbb{R}$ is a F -conical (respectively F -semi-conical) intersection for $H \in C^\infty(U \times \mathbb{R}, S_n(\mathbb{R}))$ between the levels j and $j+1$ if and only if there exists a unitary mapping $I(H(u, v, z)) : \mathbb{C}^2 \rightarrow \text{Im}(P_{j,j+1}(H(u, v, z)))$, C^∞ with respect to $(u, v, z) \in U \times \mathbb{R}$, such that $(\bar{u}, \bar{v}, \bar{z})$ is a F -conical (respectively F -semi-conical) intersection for the associated reduced Hamiltonian $h_{\text{red}} \in C^\infty(U \times \mathbb{R}, S_2(\mathbb{R}))$.*

By Proposition 4.6.3, we get that F -conical intersections and F -semi-conical intersections as defined in Definition 4.6.8 are generic for $H \in C^\infty(\mathbb{R}^3, S_n(\mathbb{R}))$ endowed with the Whitney topology.

Remark 4.6.9. *For $j \in \{1, \dots, n-1\}$ set $Z_j = \{(u, v, z) \in U \times \mathbb{R} \mid \lambda_j(u, v, z) = \lambda_{j+1}(u, v, z)\}$. By Definition 4.6.8, we have the expected result (see Proposition 4.2.9 for the same property for two-level systems) that if $(\bar{u}, \bar{v}, \bar{z})$ is a F -semi-conical intersection between the levels j and $j+1$, then Z_j is tangent to the plane $z = \bar{z}$ at the point $(\bar{u}, \bar{v}, \bar{z})$ and, considering a local smooth and regular parametrization $(u(t), v(t), z(t))_{t \in [0,1]}$ of Z_j and $\bar{t} \in [0, 1]$ such that $(u(\bar{t}), v(\bar{t}), z(\bar{t})) = (\bar{u}, \bar{v}, \bar{z})$, we have $\dot{z}(\bar{t}) = 0$ and $\ddot{z}(\bar{t}) \neq 0$.*

4.6.4 Controllability result

We consider the controlled Schrödinger equation in \mathbb{C}^n , $n \in \mathbb{N}$,

$$i \frac{d\psi(t)}{dt} = H(u(t), v(t), z)\psi(t). \quad (4.23)$$

Definition 4.6.10. *Let $z_0, z_1 \in \mathbb{R}$. We say that system (4.23) is ensemble approximately controllable between eigenstates if for every $\epsilon > 0$, $j, k \in \{1, \dots, n\}$, and $(u_0, v_0), (u_1, v_1) \in U$ such that $\lambda_j(u_0, v_0, z)$ and $\lambda_k(u_0, v_0, z)$ are simple for every $z \in [z_0, z_1]$, there exists a control $(u(\cdot), v(\cdot)) \in L^\infty([0, T], U)$ such that for every $z \in [z_0, z_1]$ the solution of (4.23) with initial condition $\psi^z(0) = \phi_j^z(u_0, v_0)$ satisfies $\|\psi^z(T) - e^{i\theta} \phi_k^z(u_1, v_1)\| < \epsilon$ for some $\theta \in \mathbb{R}$ (possibly depending on z and ϵ).*

For $j \in \{1, \dots, n-1\}$, let us denote by γ_j the set $\{(u, v, z) \in U \times [z_0, z_1] \mid \lambda_j(u, v, z) = \lambda_{j+1}(u, v, z)\}$. Let, moreover, $\gamma_0 = \gamma_n = \emptyset$. Denote by π the projection $\pi : (u, v, z) \mapsto (u, v)$.

ASSUMPTION A_j . There exists a connected component $\hat{\gamma}_j$ of γ_j such that

- $\hat{\gamma}_j$ is a one-dimensional submanifold of \mathbb{R}^3 made of F-conical intersections and F-semi-conical intersections only;
- There exist $(u_0, v_0) \in U$ and $(u_1, v_1) \in U$ such that $(u_0, v_0, z_0), (u_1, v_1, z_1) \in \hat{\gamma}_j$ are F-conical intersections for H ;
- $\pi(\hat{\gamma}_j)$ is a C^∞ embedded curve of \mathbb{R}^2 without self-intersections, which is contained in $U \setminus (\pi(\gamma_{j-1}) \cup \pi(\gamma_{j+1}))$.

Using the control strategy proposed in Theorem 4.1.3 and the result of adiabatic decoupling proposed in Theorem 4.6.5, we get the following result.

Theorem 4.6.11. *Consider a C^∞ map $U \times [z_0, z_1] \ni (u, v, z) \mapsto H(u, v, z) \in S_n(\mathbb{R})$. Let assumption A_j be satisfied for every $j \in \{1, \dots, n-1\}$. Then system (4.23) is ensemble approximately controllable between eigenstates.*

Remark 4.6.12. *If the map $U \times [z_0, z_1] \ni (u, v, z) \mapsto H(u, v, z) \in S_n(\mathbb{R})$ is C^4 then the same result holds.*

4.7 Appendix

4.7.1 Averaging theorems and estimates of oscillatory integrals

The following theorem is a quantitative version in $u(n)$ of a more general averaging result stated in [5, Lemma 8.2]. Its proof is similar to the proof of [5, Lemma 8.2] using an explicit inequality that yields the speed of convergence of order $O(\epsilon)$.

4.7. Appendix

Theorem 4.7.1. Consider A and $(A_\epsilon)_{\epsilon>0}$ in $C^\infty([0, 1], u(n))$ and assume that $A_\epsilon(\tau)$ is uniformly bounded w.r.t. (τ, ϵ) . Denote the flow of the equation $\frac{dx(\tau)}{d\tau} = A(\tau)x(\tau)$ at time τ by $P_\tau \in U(n)$ and the flow of the equation $\frac{dx(\tau)}{d\tau} = A_\epsilon(\tau)x(\tau)$ at time τ by $P_\tau^\epsilon \in U(n)$. If

$$\int_0^\tau A_\epsilon(s)ds = \int_0^\tau A(s)ds + O(\epsilon)$$

then

$$P_\tau^\epsilon = P_\tau + O(\epsilon),$$

both estimates being uniform w.r.t. $\tau \in [0, 1]$.

Remark 4.7.2. Notice that the hypothesis that $\|A_\epsilon\|_\infty$ is bounded w.r.t. ϵ is not explicitly mentioned in [5, Lemma 8.2], but is necessary also for the qualitative version (i.e., for concluding that $P_\tau^\epsilon \rightarrow P_\tau$ as $\epsilon \rightarrow 0$).

A direct consequence of Theorem 6.2.3 is the following.

Corollary 4.7.3 (Quantum 2-level systems averaging). Let $v, \phi : [0, 1] \rightarrow \mathbb{R}$ be two smooth functions and, for every $\epsilon > 0$, denote by P_τ^ϵ the flow at time $\tau \in [0, 1]$ of

$$i \frac{dX}{d\tau} = \begin{pmatrix} 0 & v(\tau)e^{i\phi(\tau)} \\ v(\tau)e^{-i\phi(\tau)} & 0 \end{pmatrix} X(\tau).$$

If $|\int_0^\tau v(s)e^{i\phi(s)}ds| \leq c\epsilon^q$, where q is a positive real number and $c > 0$ is independent of ϵ, τ , then P_τ^ϵ satisfies $P_\tau^\epsilon = \text{Id} + O(\epsilon^q)$.

We recall a classical result (see [76]) which is useful to estimate oscillatory integrals.

Lemma 4.7.4 (Van Der Corput). Let $k \in \mathbb{N}$ and $\phi : [a, b] \rightarrow \mathbb{R}$ be smooth and such that $|\phi^{(k)}(x)| \geq 1$ for all $x \in [a, b]$. Assume either that $k \geq 2$ or that $k = 1$ and ϕ' is monotone. Then

$$\left| \int_a^b e^{i\phi(x)/\epsilon} dx \right| \leq c_k \epsilon^{1/k},$$

where c_k is independent of ϕ and ϵ .

In the case $k = 1$, if ϕ' is not monotone we may lose the uniformity of the estimate with respect to the phase ϕ . However, we can recover by a direct integration by parts the following estimate.

Lemma 4.7.5 (The case $k = 1$). Let $\phi : [a, b] \rightarrow \mathbb{R}$ be smooth and such that $|\phi'(x)| \geq 1$ for all $x \in [a, b]$. Then

$$\left| \int_a^b e^{i\phi(x)/\epsilon} dx \right| \leq 2\epsilon + \epsilon \int_a^b \left| \frac{d}{dx} \frac{1}{\phi'(x)} \right| dx.$$

By integration by parts we also get the following results.

Corollary 4.7.6. *Let ϕ and k be as in Lemma 4.7.4. Let, moreover, $v : [a, b] \rightarrow \mathbb{R}$ be smooth. Then*

$$\left| \int_a^b v(x) e^{i\phi(x)/\epsilon} dx \right| \leq c_k \epsilon^{1/k} \left[|v(b)| + \int_a^b |v'(x)| dx \right]$$

where c_k is the constant obtained in Lemma 4.7.4.

Corollary 4.7.7. *Let ϕ be as in Lemma 4.7.5 and consider a smooth function $v : [a, b] \rightarrow \mathbb{R}$. Then*

$$\left| \int_a^b v(x) e^{i\phi(x)/\epsilon} dx \right| \leq c\epsilon$$

where c is independent of ϵ .

Corollary 4.7.8. *Consider an open subset V of \mathbb{R} . Assume that $\phi : [a, b] \times V \rightarrow \mathbb{R}$ and $v : [a, b] \times V \rightarrow \mathbb{R}$ are real-valued and smooth with respect to the first variable $x \in [a, b]$. Assume that there exists $k > 1$ such that $|\frac{\partial^k \phi}{\partial x^k}(x, y)| \geq 1$ for all $x \in [a, b]$ and $y \in V$. Then*

$$\left| \int_a^b v(x, y) e^{i\phi(x, y)/\epsilon} dx \right| \leq c_k \epsilon^{1/k} \left[|v(b, y)| + \int_a^b \left| \frac{\partial v}{\partial x}(x, y) \right| dx \right]$$

where c_k is the constant obtained in the Lemma 4.7.4 (independent of ϕ , y and ϵ). If we assume that v and $\frac{\partial v}{\partial x}$ are uniformly bounded on $[a, b] \times V$, then

$$\left| \int_a^b v(x, y) e^{i\phi(x, y)/\epsilon} dx \right| \leq d_k \epsilon^{1/k}$$

where d_k depends on v and is independent of ϕ , $y \in V$ and ϵ .

Next lemma is a direct consequence of Lemma 4.7.5.

Lemma 4.7.9. *Consider a compact subset V of \mathbb{R} . Consider two real-valued and smooth functions $\phi : [a, b] \times V \rightarrow \mathbb{R}$ and $v : [a, b] \times V \rightarrow \mathbb{R}$. Assume that $|\frac{\partial \phi}{\partial x}(x, y)| \geq 1$ for all $x \in [a, b]$ and $y \in V$. Then*

$$\left| \int_a^b v(x, y) e^{i\phi(x, y)/\epsilon} dx \right| \leq d\epsilon$$

where d depends on v and ϕ and is independent of $y \in V$ and ϵ .

4.7.2 Two useful lemmas

We recall some classical results that are derived from [3, §9]

4.7. Appendix

Lemma 4.7.10. *Let $n \in \mathbb{N}$ and let $\mathbb{R}^n \times \mathbb{R} \ni (x, y) \mapsto F(x, y) \in \mathbb{R}$ be a smooth function vanishing on the graph $y = \eta(x)$, where $\eta : \mathbb{R}^n \rightarrow \mathbb{R}$ is a smooth function. Then for every point $x_0 \in \mathbb{R}^n$ there exist a neighborhood W of $(x_0, \eta(x_0))$ and a smooth function $\phi : W \rightarrow \mathbb{R}$ such that*

$$\forall (x, y) \in W, \quad F(x, y) = (y - \eta(x))\phi(x, y).$$

Lemma 4.7.11. *Let $n \in \mathbb{N}$ and let $F : \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}$ be a smooth function such that $(x, y) \mapsto F(x, y)$ is vanishing on the smooth hypersurface $y = \eta(x)$. Then for every point $x_0 \in \mathbb{R}^n$ there exist a neighborhood W of $(x_0, \eta(x_0))$ that can be written as $W = W_1 \times W_2$ where W_1 is an open subset of \mathbb{R}^n and W_2 is an open subset of \mathbb{R} , and smooth functions $\phi : W \rightarrow \mathbb{R}$ and $f_0 : W_1 \rightarrow \mathbb{R}$ such that*

$$\forall (x, y) \in W, F(x, y) = (y - \eta(x))^2\phi(x, y) + f_0(x).$$

Chapter 5

Classification of the singularities of the non-mixing field

In this chapter, we classify completely the singularities of the non-mixing field for two-level systems and for generic one-parameter families of two-level systems, and we propose a new model for the avoided crossing problem. Then we continue the analysis of the singularities of the non-mixing field started in [22] for general quantum systems and we prove that it has interesting topological properties. In particular it can exhibit both singularities having a half-integer index, which are usually generic for proto line fields on \mathbb{R}^2 (see Section 5.3.1), and singularities having an integer index, usually generic for C^∞ vector fields on \mathbb{R}^2 . It opens new prospects for the construction of a topology on line-fields which allows such properties.

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5.1 General definition of the non-mixing field

Let \mathcal{H} be a separable Hilbert space, and $\mathcal{L}_{sa}(\mathcal{H})$ be the set of essentially self-adjoint operators on \mathcal{H} . Denote the scalar product on \mathcal{H} by $\langle \cdot, \cdot \rangle$. Let V be an open set of \mathbb{R}^k and $\gamma : [0, 1] \rightarrow V$ be a regular smooth control path. Let $H(\cdot) \in C_b^2(V, \mathcal{L}_{sa}(\mathcal{H}))$ such that the operators $H(u)$ have a common dense domain $D \subset \mathcal{H}$ for every $u \in V$, and are bounded from below, uniformly with respect to $u \in V$. For every $u \in V$, denote the spectrum of $H(u)$ by $\sigma(u)$. Let $j \in \mathbb{N}$. Assume that $\sigma_*(u) = \{\lambda_{j-1}(u), \lambda_j(u)\} \subset \sigma(u)$ is a locally discrete separated part of σ , for $u \in V$, and let $P_{j-1,j}(u)$ be the spectral projection of $H(u)$ onto the eigenspace associated with $\sigma_*(u)$. Let $\gamma = (\gamma(\tau))_{\tau \in [0,1]}$ a smooth regular curve of \mathbb{R}^2 along which the eigenvectors ϕ_{j-1} and ϕ_j associated with λ_{j-1} and λ_j are smooth. For every $\tau \in [0, 1]$, consider a unitary mapping $\mathcal{U}(\tau)$ from \mathbb{C}^2 to $\text{Im}P_{j-1,j}(\gamma(\tau))$, which is C^2 with respect to $\tau \in [0, 1]$, such that $\mathcal{U}(\tau)(e_1) = \phi_{j-1}(\gamma(\tau))$ and $\mathcal{U}(\tau)(e_2) = \phi_j(\gamma(\tau))$, where (e_1, e_2) is the canonical basis of \mathbb{C}^2 . Then the Effective Hamiltonian associated with H and the transformation \mathcal{U} reads

$$H_{\text{eff}}(\gamma(\tau)) = \begin{pmatrix} \lambda_{j-1}(\gamma(\tau)) & 0 \\ 0 & \lambda_j(\gamma(\tau)) \end{pmatrix} - i\epsilon \begin{pmatrix} 0 & \langle \dot{\phi}_{j-1}(\gamma(\tau)), \phi_j(\gamma(\tau)) \rangle \\ \langle \dot{\phi}_j(\gamma(\tau)), \phi_{j-1}(\gamma(\tau)) \rangle & 0 \end{pmatrix}, \quad (5.1)$$

where $\dot{\phi}_q(\gamma(\tau))$, $q \in \{j-1, j\}$ is the derivative of ϕ_q along the path γ . Denoting the propagator of Equation

$$i\epsilon \frac{d\psi(\tau)}{d\tau} = H(\gamma(\tau))\psi(\tau)$$

by $U^\epsilon(\tau)$ and the propagator of Equation

$$i\epsilon \frac{d\psi(\tau)}{d\tau} = H_{\text{eff}}(\gamma(\tau))\psi(\tau)$$

by $U_{\text{eff}}^\epsilon(\tau)$, Theorem 2.1.1 yields

$$\| (U^\epsilon(\tau) - \mathcal{U}(\gamma(\tau))U_{\text{eff}}^\epsilon(\tau)\mathcal{U}^{-1}(\gamma(0))) P_{j-1,j}(0) \| \leq C\epsilon, \quad (5.2)$$

for every $\tau \in [0, 1]$.

For a general Hamiltonian H depending on two real controls, the non-mixing curves between λ_{j-1} and λ_j for $j \geq 2$ have been defined in [22] as the curves $\gamma = (\gamma(\tau))_{t \in [0,1]}$ of \mathbb{R}^2 along which $\dot{\phi}_{j-1}(\gamma(\tau))$ is orthogonal to $\phi_j(\gamma(\tau))$ for the scalar product $\langle \cdot, \cdot \rangle$, for every $\tau \in [0, 1]$. Let $\psi_0 = \phi_j(\gamma(0))$ and for every $\tau \in [0, 1]$, $\psi_\epsilon(\tau) = U^\epsilon(\tau)\psi_0$. By the inequality (5.2), when γ is a non-mixing curve, we have, $\|\psi_\epsilon(\tau) - e^{i\theta}\phi_j(\gamma(\tau))\| \leq C\epsilon$, for $\tau \in [0, 1]$, where θ is possibly depending on ϵ .

The precision of the adiabatic approximation along such a curve is improved. Qualitatively speaking, the error made in the adiabatic regime along a non-mixing curve does not depend on the gap between λ_{j-1} and λ_j and on the variations of their associated eigenvectors but on the gap between $\{\lambda_{j-1}(\cdot), \lambda_j(\cdot)\}$ and the rest of the spectrum of $H(\cdot)$ and the

variations of the eigenvectors associated with $\text{Spectrum}(H(\cdot)) \setminus \{\lambda_{j-1}(\cdot), \lambda_j(\cdot)\}$. In particular, the error of order $\sqrt{\epsilon}$ for a control path ending a conical intersection between λ_{j-1} and λ_j is transformed into $O(\epsilon)$ along a control path which follows a non-mixing curve. This property has been used in [22] for a precise control of the Schrödinger Equation with real Hamiltonians and an extension has been presented in [31] for complex Hamiltonians with three real controls. In this section, we study the singularities of the non-mixing curves for two level systems, then for more general quantum systems.

5.2 The non-mixing field for two level systems

Let $f = (f_1, f_2) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ and $k \in \mathbb{N}$. Consider a smooth regular control path $\gamma(t) = (u(t), v(t))_{t \in [0,1]}$ such that there exist $P \in C^2([0, 1], \text{SO}_2(\mathbb{R}))$ and $\lambda \in C^k([0, 1], \mathbb{R})$ such that $\{\lambda(t), -\lambda(t)\}$ is the spectrum of $H_f(u, v) = \begin{pmatrix} f_1(u, v) & f_2(u, v) \\ f_2(u, v) & -f_1(u, v) \end{pmatrix}$, and the columns of P form a basis of eigenvectors of $H_f(\gamma(t))$ for every $t \in [0, 1]$. We can write, for every $t \in [0, 1]$, $P(t) = \begin{pmatrix} \cos(\theta(t)) & -\sin(\theta(t)) \\ \sin(\theta(t)) & \cos(\theta(t)) \end{pmatrix}$ where $\theta \in C^2([0, 1], \mathbb{R})$.

Let us study the dynamics of

$$i \frac{d\psi_\epsilon(t)}{dt} = H_f(u(\epsilon t), v(\epsilon t))\psi_\epsilon(t), \quad \psi_\epsilon(0) = \tilde{\psi}_0, \quad (5.3)$$

where $t \in [0, \frac{1}{\epsilon}]$ and $\tilde{\psi}_0$ is independent of ϵ .

Defining $Y_\epsilon(\tau) = P(\tau)\psi_\epsilon(\frac{\tau}{\epsilon})$ for every $\tau \in [0, 1]$, we have

$$i \frac{dY_\epsilon(\tau)}{d\tau} = \left(\frac{1}{\epsilon} \begin{pmatrix} \lambda(\tau) & 0 \\ 0 & -\lambda(\tau) \end{pmatrix} + \begin{pmatrix} 0 & i\dot{\theta}(\tau) \\ -i\dot{\theta}(\tau) & 0 \end{pmatrix} \right) Y_\epsilon(\tau). \quad (5.4)$$

Using the previous notations, we have that γ is a non-mixing curve if it satisfies $\dot{\theta}(t) = 0$, for every $t \in [0, 1]$. Along a non-mixing curve γ , the error occurring in the adiabatic theorem (see Theorem 4.4.1) is equal to 0, that is, the non-mixing curves can be followed at an arbitrary speed.

By a direct computation of the eigenvectors of H_f , we show the following

Proposition 5.2.1. *γ is a non-mixing curve of H_f if and only if there exists $(c_1, c_2) \in \mathbb{R}^2 \setminus \{(0, 0)\}$ such that*

$$c_1 f_1(\gamma(t)) + c_2 f_2(\gamma(t)) = 0, \quad (*)$$

for every $t \in [0, 1]$.

Proposition 5.2.2. *The non-mixing curves of H_f are the integral curves of the C^∞ vector field $\chi(f) = \begin{pmatrix} f_1 \partial_2 f_2 - f_2 \partial_2 f_1 \\ f_2 \partial_1 f_1 - f_1 \partial_1 f_2 \end{pmatrix}$, called the non-mixing field.*

5.2. The non-mixing field for two level systems

Proof. Let $(\gamma(t))_{t \in [0,1]}$ be a regular smooth curve of \mathbb{R}^2 and let $t_0 \in [0, 1]$. Assume that $f_2(\gamma(t)) \neq 0$, for every t in a neighborhood V of t_0 . Then γ satisfies Equation (*) for every $t \in V$ if and only if $\frac{f_1(\gamma(\cdot))}{f_2(\gamma(\cdot))}$ is constant on V . Provided that $\frac{f_1}{f_2}$ is C^∞ in a neighborhood of $\gamma(t_0)$, we deduce that the previous condition is satisfied if and only if, for every $t \in V$, $\gamma'(t)$ is orthogonal to $\nabla \frac{f_1}{f_2}(\gamma(t))$. Hence, γ is an integral curve of $\chi(f)$, up to a time reparametrization. The same holds if $f_1(\gamma(t)) \neq 0$, for every t in a neighborhood of t_0 . □

5.2.1 Classification of the singularities of the non-mixing field of a generic two-level system

The zeros of $\chi(f)$ are defined by

$$\begin{aligned} f_1(u, v)\partial_2 f_2(u, v) - f_2(u, v)\partial_2 f_1(u, v) &= 0 \\ f_2(u, v)\partial_1 f_1(u, v) - f_1(u, v)\partial_1 f_2(u, v) &= 0. \end{aligned}$$

First we study zeros of $\chi(f)$ in the set $\Sigma = \{(u, v) \in \mathbb{R}^2 \mid f_1(u, v) = f_2(u, v) = 0\}$. We recall that generically w.r.t. $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ an intersection of eigenvalues is conical.

Proposition 5.2.3. *Assume that H_f admits a conical intersection of eigenvalues at $(0, 0)$. Then the non-mixing curves of H_f are locally diffeomorphic to a critical node, that is, to the integral curves of the smooth vector field $\mathbb{R}^2 \ni (u, v) \mapsto \begin{pmatrix} u \\ v \end{pmatrix}$ (see Figure 5.1).*

Proof. Under the assumption that $(0, 0)$ is a conical intersection for H_f , the results of Section 4.2.3 ensure that there exists a diffeomorphism $\phi \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ such that $(f \circ \phi)(u, v) = (u, v)$ in a neighborhood of $(0, 0)$. The proposition follows. □

Then we study zeros of $\chi(f)$ in the set $\mathbb{R}^2 \setminus \Sigma$.

Proposition 5.2.4. *Generically with respect to $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, critical points of $\chi(f)$ belonging to $\mathbb{R}^2 \setminus \Sigma$ are saddles or centers, that is, the non-mixing curves are locally diffeomorphic to the integral curves of, respectively, $(u, v) \mapsto \begin{pmatrix} u \\ -v \end{pmatrix}$, or $(u, v) \mapsto \begin{pmatrix} -v \\ u \end{pmatrix}$.*

Proof. Assume that $(0, 0)$ is a zero of $\chi(f)$ such that $f_2(0) \neq 0$. Then $(0, 0)$ is a critical point of $g = \frac{f_1}{f_2}$, which is C^∞ in a neighborhood of $(0, 0)$. Using the fact that the application $\mathcal{F} : J^2(\mathbb{R}^2, \mathbb{R}^2) \rightarrow J^2(\mathbb{R}^2, \mathbb{R})$ such that $\mathcal{F}(j^2(f)(0)) = j^2(g)(0)$ is a submersion and that Morse functions are open and dense in $C^\infty(\mathbb{R}^2, \mathbb{R})$ (see [41, Theorem 6.2]), we deduce the result. □

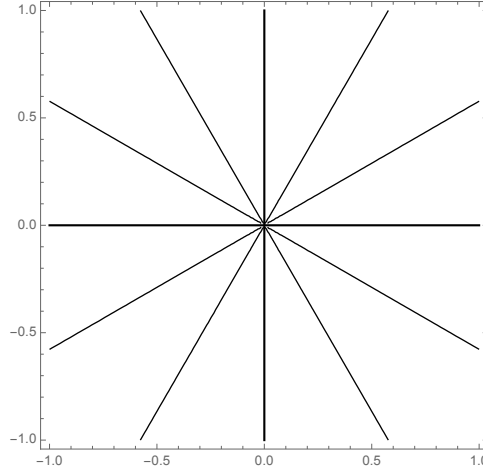


Figure 5.1 – Non-mixing curves at a conical intersection.

5.2.2 Bifurcations of the non-mixing field for two-level systems and the avoided crossing problem

Non-mixing curves for semi-conical intersections

Let $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ having a semi-conical intersection (see Section 4.2.2 for a precise definition) at $(0, 0)$. The non-mixing curves defined for a general function $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ having a semi-conical intersection at $(0, 0)$ are diffeomorphic to those of the normal form defined in Section 4.2.3 in a neighborhood of $(0, 0)$. More precisely, up to an admissible transformation (as defined in Section 4.2.2), it is sufficient to study the non-mixing curves of the normal form, that is, for every $(u, v) \in \mathbb{R}^2$,

$$H(u, v) = \begin{pmatrix} h(u)u & u + v^2 \\ u + v^2 & -h(u)u \end{pmatrix},$$

where $h \in C^\infty(\mathbb{R}, \mathbb{R})$ is a smooth function such that $h(0) = 1$. We introduce the following condition:

$$h'(0) \neq 0. \quad (\mathbf{L})$$

Assume in this section that the condition (\mathbf{L}) holds.

The non-mixing field is defined (see Proposition 5.2.2) as

$$\chi(u, v) = \begin{pmatrix} 2vuh(u) \\ u^2h'(u) + v^2uh'(u) + v^2h(u) \end{pmatrix}.$$

From Proposition 5.2.1, for $f \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, γ is a non-mixing curve of H_f if and only if there exists $(c_1, c_2) \in \mathbb{R}^2 \setminus \{(0, 0)\}$ such that

$$0 = c_1 f_1(\gamma(t)) + c_2 f_2(\gamma(t)) = c_1 u(t)h(u(t)) + c_2 (u(t) + v(t)^2), \quad (*)$$

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for every $t \in [0, 1]$.

Hence we can define $\forall (u, v) \in U, F_c(u, v) = uh(u) - cu - cv^2$. The set of the non mixing curves is the union of the curves along which F_c is equal to zero for some $c \in \mathbb{R}$ with the parabola of equation $u + v^2 = 0$.

Proposition 5.2.5. *For $c \neq 1$, $F_c(u, v) = 0 \iff u = \phi_c(v)$, where $\phi_c \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfies $\phi'_c(0) = 0$ and $\phi''_c(0) = \frac{2c}{1-c}$.*

Proof. Assume $c \neq 1$. By direct computations, we have $\frac{\partial F_c}{\partial u} = h(u) + uh'(u) - c$. Evaluating at $u = 0$ and using the condition $h(0) = 1$, we get $\frac{\partial F_c}{\partial u} \Big|_{(0,0)} = 1 - c \neq 0$. The Implicit Function Theorem ensures the existence of $\phi_c \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfying $\phi_c(0) = 0$ such that $F_c(u, v) = 0 \iff u = \phi_c(v)$, for every (u, v) in a neighborhood of $(0, 0)$. Differentiating twice the relation $F_c(\phi_c(v), v) = 0$ w.r.t. v , we get $\phi'_c(0) = 0$ and $\phi''_c(0) = \frac{2c}{1-c}$. \square

Remark 5.2.6. *Notice that for every $\alpha \in \mathbb{R}$, there exists a non-mixing curve that can be parametrized as $u = \phi_\alpha(v)$ with a smooth function ϕ_α such that $\phi_\alpha(0) = \phi'_\alpha(0) = 0$ and $\phi''_\alpha(0) = \alpha$. This property can be used to get precise superpositions of states by using control paths passing at the singularity in the non-conical direction whose second order derivatives change (see [22] for a similar first order technique at conical intersections), such developments will be exposed in future works.*

Theorem 5.2.7. *The set $\{(u, v) \in U \mid F_1(u, v) = 0\}$ is diffeomorphic to $\{(0, 0)\}$ or $\{(u, v) \in U, |u| = |v|\}$.*

Proof. Consider the function g defined by $g(u) = h(u) - 1$. Under assumption **(L)**, we have $g(0) = 0$ and $g'(0) = h'(0) \neq 0$. Then we get the equivalence

$$F_1(u, v) = 0 \iff v^2 = ug(u),$$

for every $(u, v) \in \mathbb{R}^2$. If $g'(0) < 0$, the previous equation has no solution but $u = v = 0$. If $g'(0) > 0$, we can write $g(u) = u(g'(0) + u\tilde{g}(u))$, where $\tilde{g} \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfies $\tilde{g}(0) \neq 0$. Then we have $F_1(u, v) = 0 \iff v^2 = u^2\tilde{g}(u) = u^2(g'(0) + ug_1(u))$. Applying the the right transformation $(u, v) \mapsto \begin{pmatrix} u\sqrt{g'(0) + ug_1(u)} \\ v \end{pmatrix}$, we have in new coordinates $F_1(u, v) = 0 \iff v^2 = u^2$. \square

We have shown that the non-mixing curves can have two different behaviours depending on the sign of $h'(0)$:

- The case where $h'(0) < 0$ that we refer as the *Elliptic semi-conical singularity* (see Figure 5.2). 0 is an index 2 singularity for the vector field χ . Every non-mixing curve passes through 0 and is tangent to the non-conical direction at 0.

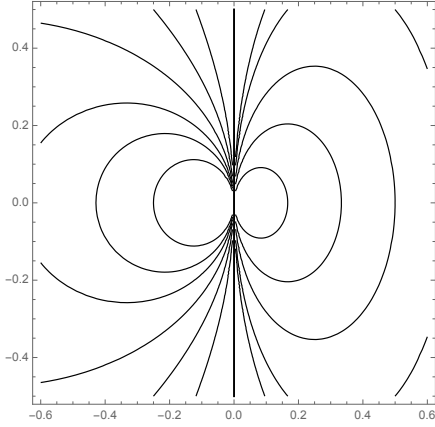


Figure 5.2 – An example of *elliptic semi-conical singularity* with $h(u) = 1 - u$ for every u . The non-conical direction is $(0, 1)$. Every non-mixing curve passes through the singularity in the non-conical direction. The index is 2.

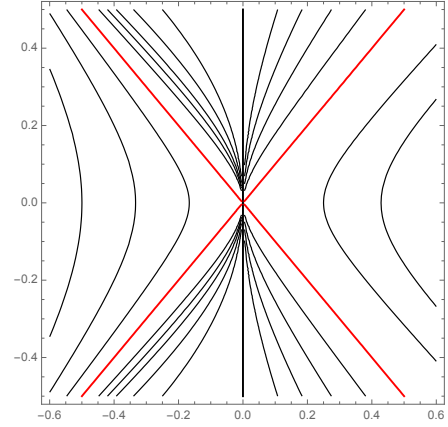


Figure 5.3 – A example of *hyperbolic semi-conical singularity* with $h(u) = 1 + u$ for every u . The non-conical direction is $(0, 1)$. The red curves are the only non-mixing curves passing through the singularity in conical directions. The index is 0.

- The case where $h'(0) > 0$ that we refer as the *Hyperbolic semi-conical singularity* (see Figure 5.3). 0 is an index zero singularity for the vector field χ . Every non-mixing curve passing at the origin is tangent to the non-conical direction except the level $c = 1$ which passes through the origin in a conical direction (see the red curves on Figure 5.3). There exist also some non-mixing curves which do not pass through the origin. Notice that even the index of the singularity is equal to zero, the non-mixing curves are not homeomorphic to the integral curves of a non-singular vector field at 0.

We can achieve an homogeneous blow-up in the polar coordinates $(r, \theta) \in \mathbb{R} \times \mathbb{S}^1$. Then the origin is blown up to \mathbb{S}^1 . In polar coordinates, the non-mixing field field χ is transformed into

$$\tilde{\chi}(r, \theta) = \eta_1(r, \theta) \frac{\partial}{\partial \theta} + \eta_2(r, \theta) r \frac{\partial}{\partial r},$$

where

$$\eta_1(r, \theta) = \cos^3(\theta)h'(r \cos(\theta)) - \cos(\theta) \sin^2(\theta)h(r \cos(\theta)) + r \cos^2(\theta) \sin^2(\theta)h'(r \cos(\theta)),$$

and

$$\begin{aligned} \eta_2(r, \theta) = & \cos(\theta) \sin(2\theta)h(r \cos(\theta)) + \sin(\theta) \cos^2(\theta)h(r \cos(\theta)) \\ & + \sin^3(\theta)h(r \cos(\theta)) + r \sin^3(\theta) \cos(\theta)h'(r \cos(\theta)). \end{aligned}$$

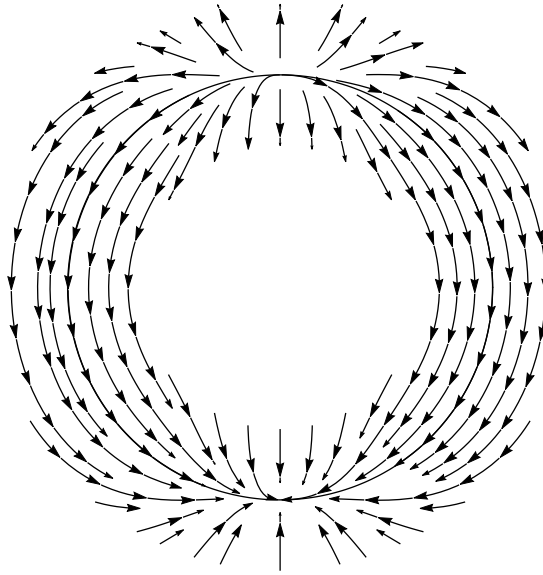


Figure 5.4 – Elliptic semi-conical singularity in the coordinates $(r, \theta) \in \mathbb{R} \times \mathbb{S}^1$ after desingularization with $h(u) = 1 - u$ for every u .

By direct computations, we prove that the singularities of $\tilde{\chi}$ on $\{0\} \times \mathbb{S}^1$ are hyperbolic. More precisely, we can show that an elliptic semi-conical singularity can be desingularized into two nodes (one attractive and one repulsive) for a value of the angle $\theta = \pm\frac{\pi}{2}$ (see Figure 5.4). By classical results on hyperbolic singularities of vector fields (see [36]), we deduce that the non-mixing curves are in this case homeomorphic to those obtained with $h(u) = 1 - u$ for every u in the original coordinates $(u, v) \in \mathbb{R}^2$. On the other hand, an hyperbolic semi-conical singularity can be desingularized into two nodes for a value of the angle $\theta = \pm\frac{\pi}{2}$ and four saddles for the angles θ such that $(\tan(\theta))^2 = h'(0)$ (see Figure 5.5). We can deduce that the non-mixing curves are in this case homeomorphic to those obtained with $h(u) = 1 + u$ for every u , in the original coordinates $(u, v) \in \mathbb{R}^2$.

5.2.3 Parametric families of real Hamiltonians

Avoided crossing model

Consider $(H_z(u, v))_{z \in \mathbb{R}}$ a family of real symmetric matrices such that $(u, v, z) \mapsto H_z(u, v)$ is C^∞ , such that, for $z > 0$, H_z has simple eigenvalues and H_0 has an isolated double eigenvalue at $(u, v) = (\bar{u}, \bar{v})$, that is, the family $(H_z(\cdot))_{z \in \mathbb{R}}$ has an *avoided crossing* at $(0, 0)$ (see [49, 48] for results about the use of avoided crossings in semi-classical analysis). It results from the structural stability of conical intersections for a real Hamiltonian with two controls (see [22]) that (\bar{u}, \bar{v}) is a non-conical intersection for $H_0(\bar{u}, \bar{v})$.

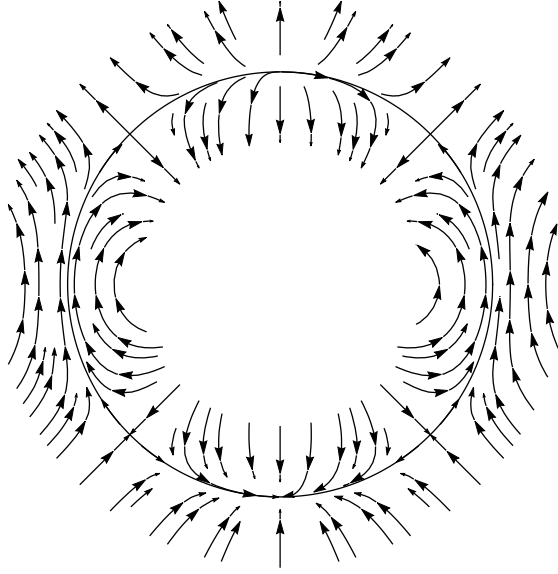


Figure 5.5 – Hyperbolic semi-conical singularity in the coordinates $(r, \theta) \in \mathbb{R} \times \mathbb{S}^1$ after desingularization with $h(u) = 1 + u$ for every u .

In Section 4.2.4, we have proved that the least degenerate local two level model is the model of F-semi-conical intersections, that is, for every $(u, v, z) \in \mathbb{R}^3$ in a neighborhood of 0,

$$\tilde{H}_z(u, v) = \begin{pmatrix} h_1(u, v, z)(z - m(u)u) & h_2(u, v, z)(z + u + v^2) \\ h_2(u, v, z)(z + u + v^2) & -h_1(u, v, z)(z - m(u)u) \end{pmatrix},$$

where $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ satisfy $h_1(0) = h_2(0) = 1$ and $m \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfies $m(0) \notin \{-1, 0\}$, where $m(0) > -1$, the case $m(0) < -1$ being similar (see Section 4.5.2).

This model has not been classified yet (see [48] for a classification of the normal forms occurring in avoided crossings) because \tilde{H}_0 is not generic as a Hamiltonian depending on the two parameters $(u, v) \in \mathbb{R}^2$. However, $(u, v, z) \mapsto \tilde{H}_z(u, v)$ is generic as a Hamiltonian depending on $(u, v, z) \in \mathbb{R}^3$.

- For $z < 0$, the energy levels have two conical intersections, as illustrated on Figure 5.6.
- For $z \rightarrow 0$, these two singular points join in the non-conical direction, their common point is a semi-conical intersection, as illustrated on Figure 5.7.
- For $z > 0$, the energy levels are then separated, as illustrated on Figure 5.8

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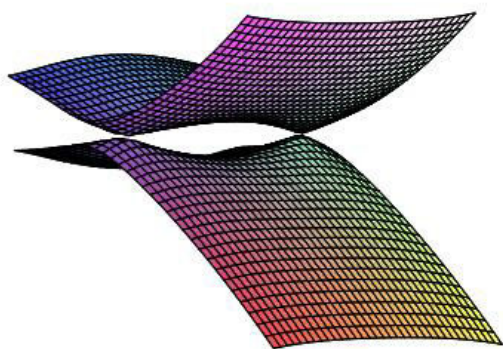


Figure 5.6 – Energy levels of $\tilde{H}_z(u, v)$ with $z < 0$, as a function of (u, v) .

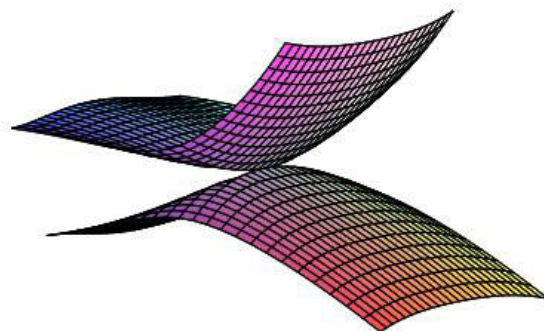


Figure 5.7 – Energy levels of $\tilde{H}_0(u, v)$, as a function of (u, v) .

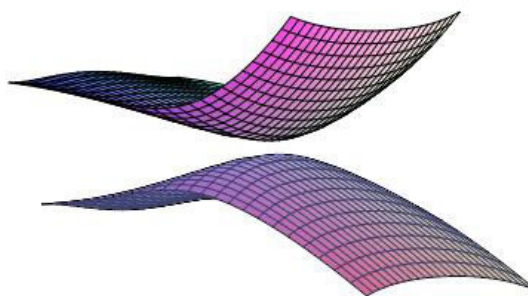


Figure 5.8 – Energy levels of $\tilde{H}_z(u, v)$ with $z > 0$, as a function of (u, v) .

Bifurcations of the non-mixing field for two-level systems

Let $f = (f_1, f_2) \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ and for every $(u, v, z) \in \mathbb{R}^3$,

$$H_f(u, v, z) = \begin{pmatrix} f_1(u, v, z) & f_2(u, v, z) \\ f_2(u, v, z) & -f_1(u, v, z) \end{pmatrix}.$$

For every z in \mathbb{R} , let $\chi_z(f)$ be the non-mixing field associated with $f(\cdot, \cdot, z) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$. According to Chapter 4, there are two typical cases for f at intersections of eigenvalues.

FIRST CASE: If f has a F-conical intersection at $(0, 0, 0)$, then H_f is equivalent in the sense defined in Section 4.2.2 to $\begin{pmatrix} h_1(u, v, z)(z - u) & h_2(u, v, z)(z - v) \\ h_2(u, v, z)(z - v) & -h_1(u, v, z)(z - u) \end{pmatrix}$ for every (u, v, z) in a neighborhood of $(0, 0, 0)$, where $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ satisfy $h_1(0) = h_2(0) = 1$. By Section 5.2, for every z the non-mixing field $\chi_z(f)$ has a critical node singularity at the conical intersection $(u, v) = (z, z)$.

SECOND CASE: If f has a F-semi-conical intersection at $(0, 0, 0)$, then H_f is equivalent to $\begin{pmatrix} h_1(u, v, z)(z - m(u)u) & h_2(u, v, z)(z + u + v^2) \\ h_2(u, v, z)(z + u + v^2) & -h_1(u, v, z)(z - m(u)u) \end{pmatrix}$ for every (u, v, z) in a neighborhood of $(0, 0, 0)$, where $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ satisfy $h_1(0) = h_2(0) = 1$ and $m \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfies $m(0) \notin \{-1, 0\}$. Using the results of Section 4.2.3, up to reducing the open and dense subset G of $C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ defined in Section 4.2.1, we can assume that generically w.r.t. $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$, $H_f(\cdot, \cdot, 0)$ is locally equivalent to

$$H(u, v) = \begin{pmatrix} uh(u) & u + v^2 \\ u + v^2 & -uh(u) \end{pmatrix} \quad (5.5)$$

where $h : \mathbb{R} \rightarrow \mathbb{R}$ is a smooth function such that $h(0) = 1$ and $h'(0) \neq 0$. The case where $h'(0) > 0$ is referred as the *Hyperbolic bifurcation*, and the case where $h'(0) < 0$ is referred as the *Elliptic bifurcation*. We can show that the condition $h'(0) \neq 0$ is satisfied when f is such that the normal form algorithm in the parametric case (see Section 4.2.4) provides three functions (h_1, h_2, m) such that $-4\partial_1 \tilde{h}(0, 0, 0)\tilde{h}(0, 0, 0) \neq \partial_2 \tilde{h}(0, 0, 0)^2$, where for every (u, v, z) in a neighborhood of 0 in \mathbb{R}^3 , $\tilde{h}(u, v, z) = -\frac{h_1(u, v, z)m(u)}{h_2(u, v, z)}$.

Under these assumptions, by Section 5.2, the non-mixing field $\chi_0(f)$ has an elliptic or hyperbolic semi-conical singularity at $(0, 0)$. Assume $m(0) > -1$ (respectively $m(0) < -1$). Then for $z > 0$ (respectively, $z < 0$), $f(\cdot, \cdot, z)$ has no intersection of eigenvalues. For $z < 0$ (respectively $z > 0$), $f(\cdot, \cdot, z)$ has two conical intersections of eigenvalues, and by Section 5.2, $\chi_z(f)$ has critical nodes at these points.

We present the next lemma, which is classical and can be deduced from [60, §4.3].

Lemma 5.2.8. *For $g \in C^\infty(\mathbb{R}^3, \mathbb{R})$, we define, for every $(u, v) \in \mathbb{R}^2$, $g_z(u, v) = g(u, v, z)$. Generically with respect to $g \in C^\infty(\mathbb{R}^3, \mathbb{R})$, for every $z \in \mathbb{R}$, the critical points of g_z are such that the level-lines of g_z are locally diffeomorphic to a saddle, a center as in Proposition 5.2.4, or a cusp, that is the level lines of $(u, v) \mapsto v^3 - u^2$.*

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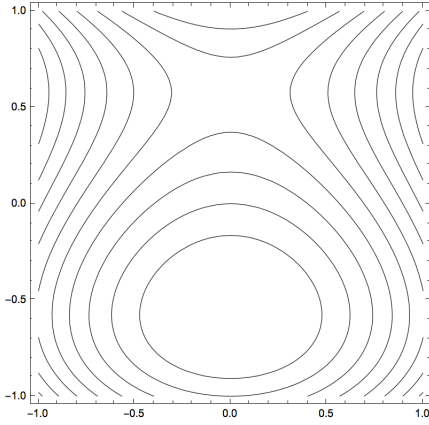


Figure 5.9 – Saddle-center bifurcation for $z < \bar{z}$, \bar{z} being the value of z for which the bifurcation occurs.

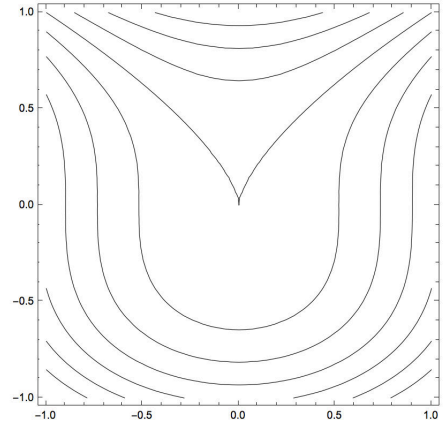


Figure 5.10 – Saddle-center bifurcation for $z = \bar{z}$.

More precisely, the cusp singularity is obtained by a *saddle-center bifurcation*, that is $g_z(u, v) = v^3 \pm (z - \bar{z})v - u^2$, the bifurcation occurs for a value of the parameter $z = \bar{z}$ (see [60, §4.3]), and it is illustrated on the Figures 5.9 and 5.10.

Now we can classify the bifurcations of singularities occurring in Theorem 2.2.7 when the parameter z varies.

Theorem 5.2.9. *Generically with respect to $f \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$, for every $z \in \mathbb{R}$, $\chi_z(f)$ has the following singularities, up to a C^∞ -diffeomorphic coordinate change:*

- *Critical nodes at conical intersections of eigenvalues,*
- *Hyperbolic or elliptic semi-conical singularities at semi-conical intersections of eigenvalues,*
- *Saddles, centers or cusps at points that are not intersections of eigenvalues.*

Remark 5.2.10. *Semi-conical singularities and cusps are singularities of maximal codimension. Hence, generically, we cannot find them simultaneously for the same value of the parameter z .*

Description of the bifurcation of the non-mixing field for F -semi-conical intersections We describe the non-mixing curves for the normal form

$$\tilde{H}_z(u, v) = \begin{pmatrix} h_1(u, v, z)(z - m(u)u) & h_2(u, v, z)(z + u + v^2) \\ h_2(u, v, z)(z + u + v^2) & -h_1(u, v, z)(z - m(u)u) \end{pmatrix}$$

for every (u, v, z) in a neighborhood of $(0, 0, 0)$, where $h_1, h_2 \in C^\infty(\mathbb{R}^3, \mathbb{R}^2)$ satisfy $h_1(0) = h_2(0) = 1$ and $m \in C^\infty(\mathbb{R}, \mathbb{R})$ satisfies $m(0) \notin \{-1, 0\}$, $m(0) > -1$, in the generic case where $-4\partial_1 \tilde{h}(0, 0, 0) \tilde{h}(0, 0, 0) \neq \partial_2 \tilde{h}(0, 0, 0)^2$, where for every (u, v, z) in a neighborhood of 0 in \mathbb{R}^3 , $\tilde{h}(u, v, z) = -\frac{h_1(u, v, z)m(u)}{h_2(u, v, z)}$.

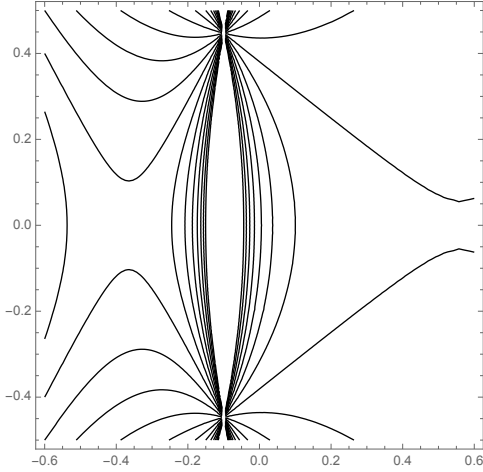


Figure 5.11 – Hyperbolic non-mixing curves for $z < 0$.

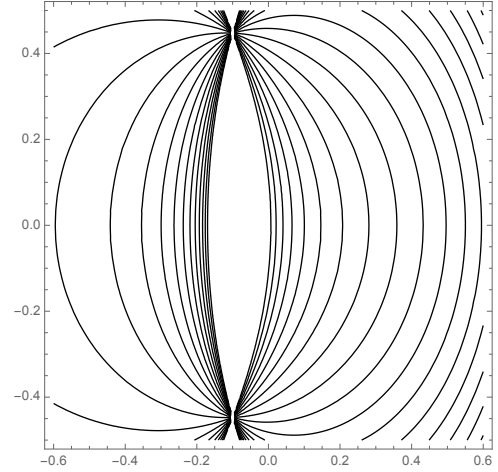


Figure 5.12 – Elliptic non-mixing curves for $z < 0$.

For $z < 0$ (see Figures 5.11 and 5.12), the non-mixing curves are the integral curves of a smooth vector field vanishing at each conical intersections which has an index equal to 1 at conical intersections. In the hyperbolic case, the two critical nodes (of index +1) are combined with two saddles (of index -1). By continuity with respect to the parameter z , it is coherent with the fact that the index of the hyperbolic semi-conical singularity vanishes. In the elliptic case, the two critical nodes join in the non-conical direction and there is no other singularity in a neighborhood of 0.

For $z = 0$ (see Figures 5.2 and 5.3 the singularity that we obtain has an index either equal to 2 in the elliptic case or 0 in the hyperbolic case.

For $z > 0$ (see Figures 5.13 and 5.14), the energy levels are separated. The non-mixing curves are the integral curves of a smooth vector field which is non-singular at 0. For $z \rightarrow 0$, the direction of the non-mixing curves at 0 converges to the non-conical direction for H_0 . In the elliptic case, however, there are two center singularities in a neighborhood of the origin. By a continuity argument w.r.t. z , this is coherent with the fact that the index of the elliptic semi-conical singularity is equal to 2.

Remark 5.2.11. *For a very small $z > 0$, one could be interested in ensuring that the system remains on the lower energy level. Following the non-mixing curves reduces the possible loss to the higher energy level, which are normally inverse proportionnal to the gap between the two levels. For two-level systems, this loss is reduced to 0.*

5.3. The non-mixing field for general quantum systems

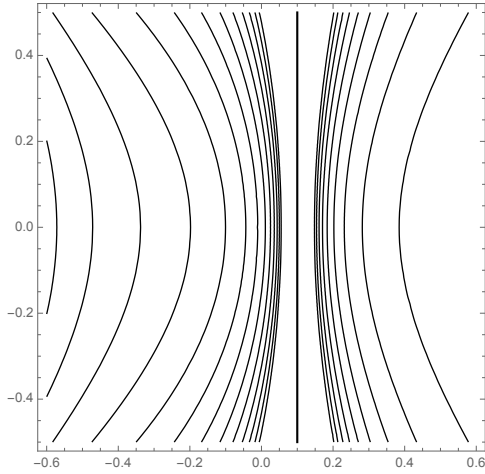


Figure 5.13 – Hyperbolic non-mixing curves for $z > 0$.

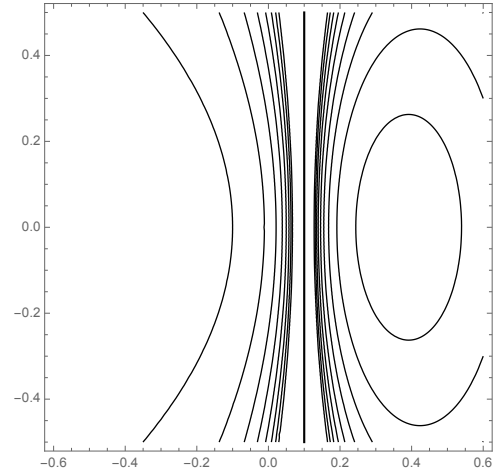


Figure 5.14 – Elliptic non-mixing curves for $z > 0$.

5.3 The non-mixing field for general quantum systems

5.3.1 Useful results about line fields

We start this section by stating some results on line fields. We refer to [21] for a precise definition and classification of the singularities of line fields on two-dimensional Riemannian manifolds. Let (M, g) be a 2-dimensional Riemannian manifold. A *line field* on M is a section of $PT(M \setminus K)$, where K is a closed subset of M .

The next propositions (until Theorem 5.3.6) are directly taken from [21].

Definition 5.3.1. *Let (M, g) be a 2-dimensional Riemannian manifold. A proto-line-field is a pair (X, Y) of vector fields on M . Denote by z_X and z_Y the sets of zeros of X and Y . The line field associated with (X, Y) , denoted by $B(X, Y)$, is the section of $PT(M \setminus (z_X \cup z_Y))$ defined at a point $p \in M \setminus (z_X \cup z_Y)$ as the line $B(X(p), Y(p))$ of $T_p M$ bisecting $(X(p), Y(p))$ for the metric $g(p)$.*

Proposition 5.3.2. *Let (M, g) be a 2-dimensional Riemannian manifold, K be a closed subset of M and L be a section of $PT(M \setminus K)$. There exist two vector fields X and Y such that $L = B(X, Y)$.*

With this definition, the Whitney topology on pairs of vector fields on M defines a topology on line fields on M , the zeros of X and Y become singularities of the associated line-field.

Definition 5.3.3. *A one-dimensional connected immersed submanifold N of $M \setminus (z_X \cup z_Y)$ is said to be an integral manifold of the proto-line-field (X, Y) if for any point p of N , the tangent line to N at p is given by $B(X, Y)$.*

We say that a proto-line-field L has a *Darbouxian singularity* if its integral manifolds are locally homeomorphic to those of the proto-line-fields defined by (X_L, Y_L) , (X_M, Y_M) and (X_S, Y_S) defined as follows:

- The *Lemon proto-line-field* (see Figure 5.15) is the pair of vector fields on $(\mathbb{R}^2, Eucl)$ defined by

$$X_L(x, y) = \begin{pmatrix} x + y \\ y - x \end{pmatrix}, \quad Y_L(x, y) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

- The *Monstar proto-line-field* (see Figure 5.16) is the pair of vector fields on $(\mathbb{R}^2, Eucl)$ defined by

$$X_M(x, y) = \begin{pmatrix} x \\ 3y \end{pmatrix}, \quad Y_M(x, y) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

- The *Star proto-line-field* (see Figure 5.17) is the pair of vector fields on $(\mathbb{R}^2, Eucl)$ defined by

$$X_S(x, y) = \begin{pmatrix} x \\ -y \end{pmatrix}, \quad Y_S(x, y) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Darbouxian singularities have an index equal to $\pm\frac{1}{2}$.

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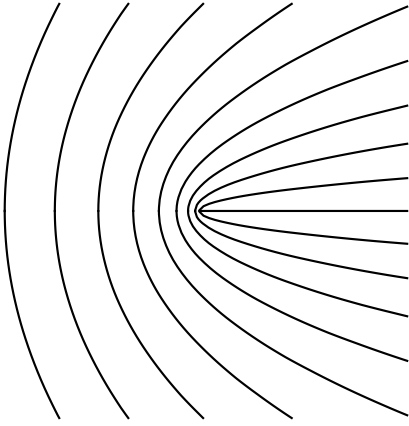


Figure 5.15 – The Lemon singularity, of index $\frac{1}{2}$.

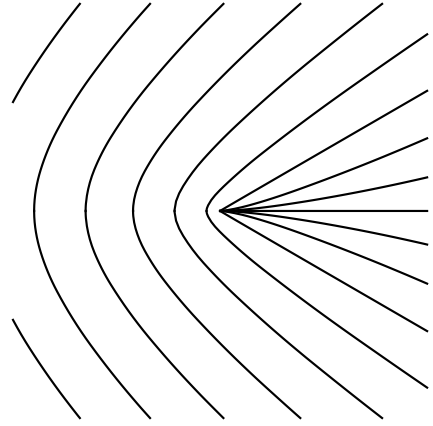


Figure 5.16 – The Monstar singularity, of index $\frac{1}{2}$.

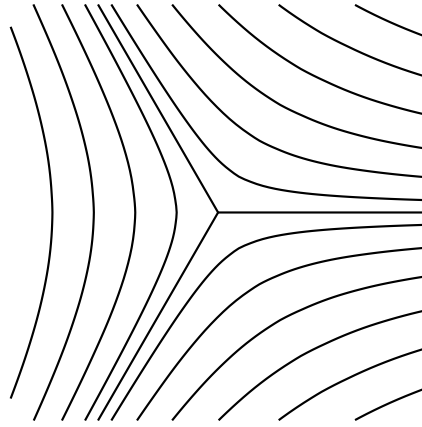


Figure 5.17 – The Star singularity, of index $-\frac{1}{2}$.

Definition 5.3.4. Let (X, Y) be a proto-line field on (M, g) , and (X', Y') be a proto-line-field on (M', g') . Fix $p \in M$ and $p' \in M'$. Then (X, Y) and (X', Y') are said to be topologically equivalent at p and p' if there exist two neighborhoods V_p and $W_{p'}$ of p and p' respectively and a homeomorphism $h : V_p \rightarrow W_{p'}$, with $h(p) = p'$, which takes the integral manifolds of (X, Y) onto those of (X', Y') .

Definition 5.3.5. We say that a proto-line-field (X, Y) has a non-degenerate singularity (respectively, a hyperbolic singularity) at a point $p \in M$ if one of the two vector fields has a non-degenerate singularity (respectively, a hyperbolic singularity) and the other is non-vanishing at p .

Theorem 5.3.6 (Hyperbolic singularities of line fields). Let (M, g) be a two-dimensional Riemannian manifold. Hyperbolic singularities of proto line fields on M are Darbouxian.

Now we prove two technical results that will be useful for the proof of Theorem 5.3.12.

Proposition 5.3.7 (Non-degenerate singularities of line fields). *Let (M, g) be a two-dimensional Riemannian manifold. Non-degenerate singularities of proto-line-fields on M are Darbouxian. Moreover, consider a proto line field (X, Y) on M such that \bar{p} is a non-degenerate singularity of (X, Y) . Then there exists two sequences $(X_n)_{n \in \mathbb{N}}$ and $(Y_n)_{n \in \mathbb{N}}$ of smooth vector fields on M converging respectively to X and Y for the C^∞ -Whitney topology, such that for every $n \in \mathbb{N}$, \bar{p} is an hyperbolic singularity of (X_n, Y_n) and $B_g(X(p), Y(p)) = B_g(X_n(p), Y_n(p))$ for p in a punctured neighborhood of \bar{p} .*

Proof. Consider a proto line field (X, Y) such that X has a non-degenerate zero at $\bar{p} \in M$ and $Y(\bar{p}) \neq 0$. If \bar{p} is hyperbolic, then Theorem 5.3.6 proves the result.

Assume now that X is non-degenerate and not hyperbolic at \bar{p} . Define \tilde{X} and \tilde{Y} as the smooth vector fields which are the image of respectively, X and Y by the rotation of angle $\frac{\pi}{2}$ for the metric g . This construction is always possible, at least locally around \bar{p} . By using local charts, one can easily show that \tilde{X} is hyperbolic at \bar{p} . Define a neighborhood V of \bar{p} such that \tilde{X} and \tilde{Y} are well defined on V and \bar{p} is the only zero of X in V , Y is non-zero on V , and set $W = V \setminus \{\bar{p}\}$. We can notice that for every $p \in W$, $\frac{\tilde{X}(p)}{\|\tilde{X}(p)\|} - \frac{\tilde{Y}(p)}{\|\tilde{Y}(p)\|}$ is colinear to $B_g(X(p), Y(p))$, hence we can deduce the equality $B_g(X(p), Y(p)) = B_g(\tilde{X}(p), -\tilde{Y}(p))$. By construction, \bar{p} is hyperbolic for (\tilde{X}, \tilde{Y}) , hence Theorem 5.3.6 proves that \bar{p} is Darbouxian. The first claim is proved. In order to prove the second claim, define, for p in W and $\epsilon > 0$, $X_\epsilon(p) = X(p) + \epsilon\tilde{X}(p)$ and $Y_\epsilon(p) = Y(p) - \epsilon\tilde{Y}(p)$. By construction of \tilde{X} and \tilde{Y} , we have, for every p in W , $\|X_\epsilon(p)\| = \sqrt{1 + \epsilon^2}\|X(p)\|$ and $\|Y_\epsilon(p)\| = \sqrt{1 + \epsilon^2}\|Y(p)\|$. It follows that, for p in W , $\frac{X_\epsilon(p)}{\|X_\epsilon(p)\|} + \frac{Y_\epsilon(p)}{\|Y_\epsilon(p)\|} = \frac{1}{\sqrt{1 + \epsilon^2}} \left(\left(\frac{X(p)}{\|X(p)\|} + \frac{Y(p)}{\|Y(p)\|} \right) + \epsilon \left(\frac{\tilde{X}(p)}{\|\tilde{X}(p)\|} - \frac{\tilde{Y}(p)}{\|\tilde{Y}(p)\|} \right) \right)$. Noticing that for p in W , $\frac{\tilde{X}(p)}{\|\tilde{X}(p)\|} - \frac{\tilde{Y}(p)}{\|\tilde{Y}(p)\|}$ and $\frac{X(p)}{\|X(p)\|} + \frac{Y(p)}{\|Y(p)\|}$ are colinear to $B_g(X(p), Y(p))$, we can deduce that $\frac{X_\epsilon(p)}{\|X_\epsilon(p)\|} + \frac{Y_\epsilon(p)}{\|Y_\epsilon(p)\|}$ is colinear to $B_g(X(p), Y(p))$. Hence $B_g(X(p), Y(p)) = B_g(X_\epsilon(p), Y_\epsilon(p))$, for every $p \in W$. The hyperbolicity of \tilde{X} at \bar{p} implies that X_ϵ is hyperbolic at \bar{p} . Moreover, for $\epsilon > 0$, we have $Y_\epsilon(\bar{p}) \neq 0$. For such ϵ , \bar{p} is a hyperbolic singularity for the proto-line-field (X_ϵ, Y_ϵ) . Setting for $n \geq 1$, $\epsilon_n = \frac{1}{n}$ and $X_n = X_{\epsilon_n}, Y_n = Y_{\epsilon_n}$, we have clearly that $(X_n)_n$ and $(Y_n)_n$ converge respectively to X and Y for the C^∞ -Whitney topology. The result is proved. □

Theorem 5.3.8. *Consider a two dimensional Riemannian manifold (M, g) . Let L be a line field on M and A a smooth section of $GL(TM) = \cup_{p \in M} GL(T_p M)$. Denote by $K \subset M$ the closed set of singular points of L . Let \tilde{L} be the line field defined on M by $\tilde{L}(p) = A(p)(L(p))$ (where the equality is defined as the equality of the associated directions in $T_p M$) for every $p \in M \setminus K$. Let $\bar{p} \in K$. Consider two vector fields X and Y on M such that, for every $p \in M \setminus K$, $L(p) = B_g(X(p), Y(p))$, and satisfying the conditions $X(\bar{p}) = 0$, $DX(\bar{p})$ is non-degenerate, and $Y(\bar{p}) \neq 0$. Then there exists a metric \tilde{g} on M such that,*

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for every $p \in M \setminus K$, $\tilde{L}(p) = B_{\tilde{g}}(A(p)X(p), A(p)Y(p))$. Moreover p is non-degenerate for (AX, AY) if and only if p is non-degenerate for (X, Y) .

Proof. Define the metric \tilde{g} by $\tilde{g}(p)(x, y) = g(p)(A^{-1}(p)x, A^{-1}(p)y)$ for every $p \in M$ and $(x, y) \in T_pM \times T_pM$. Then we get easily that, for every $p \in M \setminus K$, $\tilde{L}(p) = B_{\tilde{g}}(A(p)X(p), A(p)Y(p))$. Let $\bar{p} \in K$. Using the conditions $A(\bar{p}) \in GL(T_{\bar{p}}M)$, we have $A(\bar{p})Y(\bar{p}) \neq 0$, $A(\bar{p})X(\bar{p}) = 0$, and that $D(AX)(\bar{p})$ is non-degenerate. The theorem is proved. \square

5.3.2 Non-mixing field

Let \mathcal{H} be a separable Hilbert space. Let U be a connected open set of \mathbb{R}^2 . Assume that for every $(u, v) \in U$, $H(u, v) = H_0 + uH_1 + vH_2$ where H_0, H_1, H_2 are essentially self-adjoint operators on \mathcal{H} having a common dense domain $\mathcal{D} \subset \mathcal{H}$ such that:

- H_0 has a discrete spectrum;
- H_1, H_2 are bounded;
- There exists an orthonormal basis $(b_j)_j$ of the Hilbert space \mathcal{H} such that $\langle b_j, H_0 b_q \rangle$, $\langle b_j, H_1 b_q \rangle$, $\langle b_j, H_2 b_q \rangle$ are real for every j, q .

It has been proven in [22] that the non-mixing curves between two eigenvalues $\lambda_{j-1}(\cdot)$ and $\lambda_j(\cdot)$ of $H(\cdot)$ are the integral curves of a line field on \mathbb{R}^2 , defined up to a sign, for $(u, v) \in \mathbb{R}^2$, by $\chi_{j-1,j}(u, v) = \begin{pmatrix} -\langle H_2 \phi_{j-1}(u, v), \phi_j(u, v) \rangle \\ \langle H_1 \phi_{j-1}(u, v), \phi_j(u, v) \rangle \end{pmatrix}$ where $\langle \cdot, \cdot \rangle$ is the natural scalar product on \mathcal{H} .

Remark 5.3.9. *The non-mixing curves of H between the levels $\lambda_{j-1}(\cdot)$ and $\lambda_j(\cdot)$ are not those of a zero trace two-level reduced Hamiltonian $h_{red}(u, v)$, that can be defined by removing the trace of $I_{j-1,j}^{-1}(u, v)H(u, v)I_{j-1,j}(u, v)$ as in Section 4.6.3, where $I_{j-1,j}(u, v)$ is a smooth orthogonal mapping between \mathbb{R}^2 and the real span of $(\phi_{j-1}(u, v), \phi_j(u, v))$ and can be defined locally for (u, v) in a neighborhood of points where $\sigma(u, v) = \{\lambda_{j-1}(u, v), \lambda_j(u, v)\}$ is separated from the rest of the spectrum of $H(u, v)$. Indeed, the non-mixing curves of $h_{red}(u, v)$ depend on the choice of the mapping $I_{j-1,j}$, while it is not the case for those of $H(u, v)$.*

Proposition 5.3.10. — Let $f = (f_1, f_2) \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$, $H_f = \begin{pmatrix} f_1 & f_2 \\ f_2 & -f_1 \end{pmatrix}$, and g be the Euclidean metric on \mathbb{R}^2 . Then the real eigendirections of h_f associated with the eigenvalues $\lambda_\pm = \pm\sqrt{f_1^2 + f_2^2}$ can be written as the line-fields $L_- = B_g\left(\begin{pmatrix} -f_2 \\ f_1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)$, and $L_+ = B_g\left(\begin{pmatrix} -f_2 \\ f_1 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \end{pmatrix}\right)$. Assume moreover that f has a conical intersection at 0, that is, $f(0) = 0$ and $Df(0) \in GL_2(\mathbb{R})$. Then the proto-

line-fields $\left(\begin{pmatrix} -f_2 \\ f_1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)$ and $\left(\begin{pmatrix} -f_2 \\ f_1 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \end{pmatrix}\right)$ have non-degenerate singularities at 0.

- Let $f = (f_1, f_2, f_3) \in C^\infty(\mathbb{R}^2, \mathbb{R}^3)$ and $M_f = \begin{pmatrix} f_1 & f_2 \\ f_2 & f_3 \end{pmatrix}$. Define $\tilde{f} \in C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ as $\tilde{f} = \left(\frac{f_1 - f_3}{2}, f_2\right)$. Then the real eigendirections of M_f are those of $H_{\tilde{f}}$. Moreover M_f has a conical intersection at 0 if and only if $H_{\tilde{f}}$ has a conical intersection at 0.

Proof. Let $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ be such that $f(\bar{u}, \bar{v}) \neq 0$. By direct computations, $\begin{pmatrix} x \\ y \end{pmatrix} \in \mathbb{R}^2$ is an eigenvector of $H_f(u, v)$ associated with $\lambda_\pm(u, v)$ if and only if $x(f_1(u, v) - \lambda_\pm(u, v)) + yf_2(u, v) = 0$, that is, $\begin{pmatrix} x \\ y \end{pmatrix}$ is colinear to $\frac{1}{\lambda_\pm(u, v)} \begin{pmatrix} -f_2(u, v) \\ f_1(u, v) \end{pmatrix} + \begin{pmatrix} 0 \\ -1 \end{pmatrix}$. We can deduce the first claim. Define the vector field X , for every $(u, v) \in \mathbb{R}^2$, by $X(u, v) = \begin{pmatrix} -f_2(u, v) \\ f_1(u, v) \end{pmatrix}$. The hypothesis that 0 is a conical intersection for f yields that $X(0) = 0$ and $DX(0)$ is non-degenerate. The first claim is proved. The second claim is obtained by similar computations. \square

We recall here some results from [22]. In a neighborhood of a conical intersection $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ between the levels $j - 1$ and j ,

- For every $(u, v) \neq (\bar{u}, \bar{v})$, there exists a smooth choice of the sign of the eigenvectors $\phi_{j-1}(u, v)$ and $\phi_j(u, v)$ such that $\chi_{j-1, j}$ defines a C^∞ vector field in a punctured neighborhood of (\bar{u}, \bar{v}) ,
- The integral curves of $\chi_{j-1, j}$ are C^∞ and the eigenvectors ϕ_{j-1} and ϕ_j are C^∞ along them,
- For every direction η of \mathbb{R}^2 , there exists an integral curve $\gamma : [0, 1) \rightarrow \mathbb{R}^2$ of $\chi_{j-1, j}$ such that $\lim_{t \rightarrow 1^-} \gamma(t) = (\bar{u}, \bar{v})$, $\lim_{t \rightarrow 1^-} \frac{\dot{\gamma}(t)}{\|\dot{\gamma}(t)\|} = \eta$.

We say that the singularity of $\chi_{j-1, j}$ has type **(N)**, for node. In particular the third condition implies that the non-mixing curves are homeomorphic to the integral curves of the vector field $(u, v) \mapsto \begin{pmatrix} u \\ v \end{pmatrix}$ locally around (\bar{u}, \bar{v}) and the index of $\chi_{j-1, j}$ at (\bar{u}, \bar{v}) is equal to 1.

5.3.3 Singularities of $\chi_{j-1, j}$ at intersections $(j, j + 1)$.

Let $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ be such that $\lambda_j(\bar{u}, \bar{v}) = \lambda_{j+1}(\bar{u}, \bar{v})$. Define a neighborhood U of (\bar{u}, \bar{v}) in \mathbb{R}^2 such that, for every $(u, v) \in U \setminus \{(\bar{u}, \bar{v})\}$, $\lambda_j(u, v) \notin \{\lambda_{j+1}(u, v), \lambda_{j-1}(u, v)\}$. For every $(u, v) \in U$, let $P_{j, j+1}(u, v) : \mathbb{R}^n \rightarrow \mathbb{R}^n$ be the orthogonal projection of H onto the eigenspace associated with $\lambda_j(u, v)$ and $\lambda_{j+1}(u, v)$, which is smooth with respect to

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$(u, v) \in U$. As in Section 4.6.3, for every $(u, v) \in U$, define an orthogonal map $I_{j,j+1}(u, v) : \mathbb{R}^2 \rightarrow \text{Im}P_{j,j+1}(u, v)$, smoothly depending on (u, v) . Consider a normalized real eigenvector $\phi_j(u, v)$ (respectively, $\phi_{j+1}(u, v)$) of $H(u, v)$ associated with $\lambda_j(u, v)$ (respectively, $\lambda_{j+1}(u, v)$) and a normalized real eigenvector $\tilde{\phi}_j(u, v)$ (respectively, $\tilde{\phi}_{j+1}(u, v)$) of $h_{\text{red}}(u, v)$ as defined in Section 4.6.3 associated with $\lambda_j(u, v)$ (respectively, $\lambda_{j+1}(u, v)$). Then we have $I_{j,j+1}(u, v)(\tilde{\phi}_j(u, v)) = \eta\phi_j(u, v)$, where $\eta = \pm 1$. Consider a smooth vector field X on \mathbb{R}^2 such that, for every $(u, v) \in U$, $I_{j,j+1}(u, v)(X(u, v)) = P_{j,j+1}(u, v)(H_2\phi_{j-1}(u, v))$, and a smooth vector field Y on \mathbb{R}^2 such that, for every $(u, v) \in U$, $I_{j,j+1}(u, v)(Y(u, v)) = -P_{j,j+1}(u, v)(H_1\phi_{j-1}(u, v))$. Notice that the smoothness of X and Y rely on the fact that $\phi_{j-1}(u, v)$ can be chosen smooth with respect to $(u, v) \in U$. Denote by g the Euclidean scalar product on \mathbb{R}^2 .

Proposition 5.3.11. *There exists $A \in C^\infty(\mathbb{R}^2, M_2(\mathbb{R}))$ such that, for every $(u, v) \in U \setminus \{(\bar{u}, \bar{v})\}$, $\chi_{j-1,j}(u, v)$ defines the same direction as $A(u, v)\tilde{\phi}_j(u, v)$.*

Proof. We can write

$$\begin{aligned} \langle H_2\phi_{j-1}(u, v), \phi_j(u, v) \rangle &= \langle H_2\phi_{j-1}(u, v), \eta I_{j,j+1}(u, v)(\tilde{\phi}_j(u, v)) \rangle \\ &= \eta \langle P_{j,j+1}(u, v)(H_2\phi_{j-1}(u, v)), I_{j,j+1}(u, v)(\tilde{\phi}_j(u, v)) \rangle \\ &= \eta \langle I_{j,j+1}(u, v)(X(u, v)), I_{j,j+1}(u, v)(\tilde{\phi}_j(u, v)) \rangle \\ &= \eta g(X(u, v), \tilde{\phi}_j(u, v)), \end{aligned}$$

where the last equality is obtained using that $I_{j,j+1}(u, v)$ is an orthogonal map between \mathbb{R}^2 and $\text{Im}P_{j,j+1}(u, v)$, for every $(u, v) \in U$. By the same computations as previously, we have $-\langle H_1\phi_{j-1}(u, v), \phi_j(u, v) \rangle = \eta g(Y(u, v), \tilde{\phi}_j(u, v))$. Denoting the coordinates of X and Y in the canonical basis of \mathbb{R}^2 by $X(u, v) = \begin{pmatrix} x_1(u, v) \\ x_2(u, v) \end{pmatrix}$ and $Y(u, v) = \begin{pmatrix} y_1(u, v) \\ y_2(u, v) \end{pmatrix}$, we have, for every $(u, v) \in U \setminus \{(\bar{u}, \bar{v})\}$, $\chi_{j-1,j}(u, v) = \eta A(u, v)\tilde{\phi}_j(u, v)$, where, for every $(u, v) \in U$, $A(u, v) = \begin{pmatrix} x_1(u, v) & x_2(u, v) \\ y_1(u, v) & y_2(u, v) \end{pmatrix}$, and $\eta = \pm 1$. We deduce the result. \square

Let $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ be a conical intersection between λ_j and λ_{j+1} . We introduce the following condition:

Condition (C): The vectors $P_{j,j+1}H_1\phi_{j-1}(\bar{u}, \bar{v})$ and $P_{j,j+1}H_2\phi_{j-1}(\bar{u}, \bar{v})$ are not colinear.

We prove the following theorem.

Theorem 5.3.12. *Let $(\bar{u}, \bar{v}) \in \mathbb{R}^2$ be such that $\lambda_j(\bar{u}, \bar{v}) = \lambda_{j+1}(\bar{u}, \bar{v})$ is a conical intersection. Assume that Condition (C) is satisfied at (\bar{u}, \bar{v}) . Then $\chi_{j-1,j}$ has a Darbouxian singularity at (\bar{u}, \bar{v}) .*

Proof. By definition $\tilde{\phi}_j$ is the eigendirection associated with the eigenvalue λ_j of the two-level Hamiltonian h_{red} having a conical intersection at (\bar{u}, \bar{v}) . Hence Proposition 5.3.10 proves that the line field $\tilde{\phi}_j$ has a non-degenerate singularity at (\bar{u}, \bar{v}) . Under assumption **(C)**, the matrix $A \in C^\infty(\mathbb{R}^2, M_2(\mathbb{R}))$ defined in Proposition 5.3.11 is invertible. By Proposition 5.3.8, we deduce that $\chi_{j-1,j} = A\tilde{\phi}_j$ (where the equality is defined as the equality of the associated directions in \mathbb{R}^2) has a non-degenerate singularity at (\bar{u}, \bar{v}) . We deduce the theorem by using Proposition 5.3.7. \square

We show without difficulty that Condition **(C)** is satisfied in the following case.

Corollary 5.3.13. *Let $E_1, E_2, E_3 \in \mathbb{R}$ such that $E_1 < E_2 < E_3$ and $H(u, v) = \begin{pmatrix} E_1 & u & 0 \\ u & E_2 & v \\ 0 & v & E_3 \end{pmatrix}$.*

Then $\chi_{1,2}$ (respectively $\chi_{2,3}$) has Darbouxian singularities at the points $(u, v) \in \mathbb{R}^2$ such that $\lambda_2(u, v) = \lambda_3(u, v)$ (respectively, $\lambda_1(u, v) = \lambda_2(u, v)$) that are

$$(u, v) = (\pm\sqrt{(E_1 - E_3)(E_2 - E_3)}, 0) \text{ (respectively } (0, \pm\sqrt{(E_1 - E_3)(E_1 - E_2)})).$$

Let $E_1, E_2, E_3 \in \mathbb{R}$ and $H(u, v) = \begin{pmatrix} E_1 & u & 0 \\ u & E_2 & v \\ 0 & v & E_3 \end{pmatrix}$. On Figure 5.18, we have plotted

the non-mixing curves between the levels λ_1 and λ_2 when $E_1 < E_2 < E_3$. Along these curves the precision of the adiabatic approximation for a regular control path at speed ϵ has an order equal to $O(\epsilon)$ on a time interval of length $\frac{1}{\epsilon}$.

When considering the case where $E_1 = E_2 < E_3$, we can prove that the system admits two conical intersections between the levels λ_2 and λ_3 at the points

$$(u, v) = (\pm\sqrt{(E_1 - E_3)(E_2 - E_3)}, 0) = (\pm|E_1 - E_3|, 0),$$

and a semi-conical intersection between the levels λ_1 and λ_2 at $(0, 0)$. On Figure 5.20, we have plotted the non-mixing curves between the levels λ_1 and λ_2 in this case. By direct computations, we can show that Condition **(C)** is not satisfied at the points

$$(u, v) = (\pm\sqrt{(E_1 - E_3)(E_2 - E_3)}, 0) = (\pm|E_1 - E_3|, 0),$$

and we observe that the non-mixing field χ_{12} between the levels λ_1 and λ_2 is non-singular at these points. We observe a node at the semi-conical intersection $(0, 0)$ between the levels λ_1 and λ_2 . In further studies, it would be interesting to prove that the singularity at the origin is a node, by studying the non-mixing field at a semi-conical intersection for n -level systems.

When considering the case where $E_2 < E_1 < E_3$, we can prove that the system admits two conical intersections between the levels λ_2 and λ_3 at the points

$$(u, v) = (\pm\sqrt{(E_1 - E_3)(E_2 - E_3)}, 0),$$

5.3. The non-mixing field for general quantum systems

and admits no intersection between the levels λ_1 and λ_2 at $(0, 0)$. By direct computations, we can show that Condition **(C)** is satisfied at the points

$$(u, v) = (\pm\sqrt{(E_1 - E_3)(E_2 - E_3)}, 0).$$

As a consequence, the non-mixing field χ_{12} between the levels λ_1 and λ_2 has Darbouxian singularities at these points. On Figure 5.22, we have plotted the non-mixing curves between the levels λ_1 and λ_2 in this case. We notice the presence of Lemon singularities at the points

$$(u, v) = (\pm\sqrt{(E_1 - E_3)(E_2 - E_3)}, 0).$$

Then we have plotted the non-mixing field between λ_1 and λ_2 in the three remaining cases, that require to be studied more precisely:

- The case where $E_1 < E_2 = E_3$ on Figure 5.24. In this case, there is a semi-conical intersection between the levels $\lambda_2 = \lambda_3$ and two conical intersections between the levels λ_1 and λ_2 . The non-mixing field between the levels λ_1 and λ_2 has two singularities of type **(N)** at the conical intersections between the levels λ_1 and λ_2 . Moreover, the two Star singularities that occurred in the case $E_1 < E_2 < E_3$ join at the origin $(0, 0)$ into a singularity that is a bifurcation of singularities of line-fields. Bifurcations for one-parameter families of line-fields is a future topic of study.
- The case where $E_1 < E_3, E_2 > E_3$, on Figure 5.26. In this case, there is no intersection of eigenvalue between λ_2 and λ_3 , and two conical intersections of eigenvalues between λ_1 and λ_2 . Hence there are two singularities of type **(N)** at the conical intersections between λ_1 and λ_2 , and we notice graphically that there is a saddle at $(0, 0)$.
- The case where $E_1 = E_2 = E_3$ on Figure 5.28. Up to a change of global phase in the dynamics, we can assume $E_1 = E_2 = E_3 = 0$. In this case, the eigenvectors of $H(u, v)$ are constant functions along every half-straight line with $(0, 0)$ as the origin of the half-straight lines.

Remark 5.3.14. *Notice that the construction of the non-mixing field could be a first step to build a topology on line fields on dimension 2 manifolds that allows both generic singularities of integer and half-integer index.*

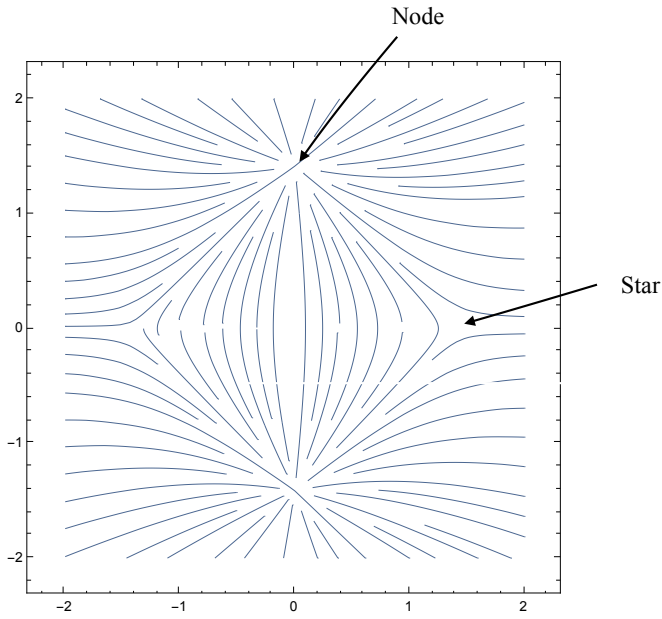


Figure 5.18 – Non-mixing field between λ_1 and λ_2 for the STIRAP of Corollary 5.3.13.

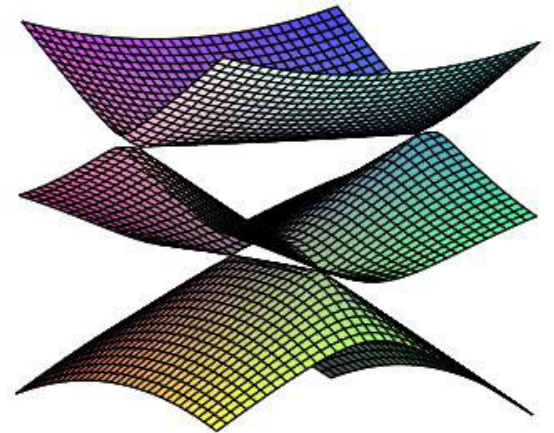


Figure 5.19 – Spectrum as a function of (u, v) for the STIRAP, where $E_1 < E_2 < E_3$.

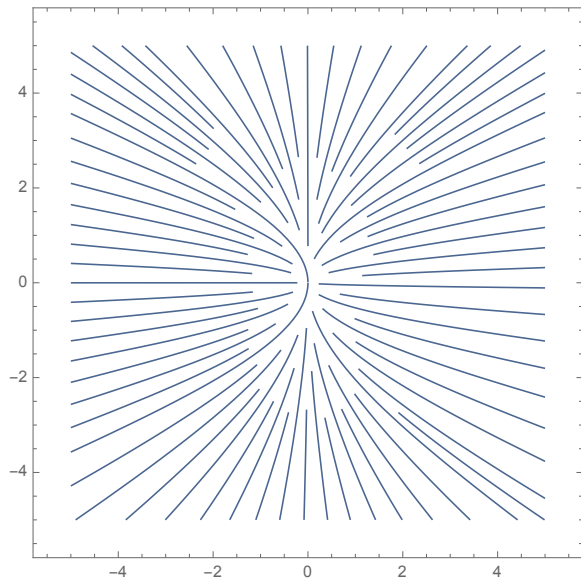


Figure 5.20 – Non-mixing field between λ_1 and λ_2 for the degenerate STIRAP, where $E_1 = E_2 < E_3$.

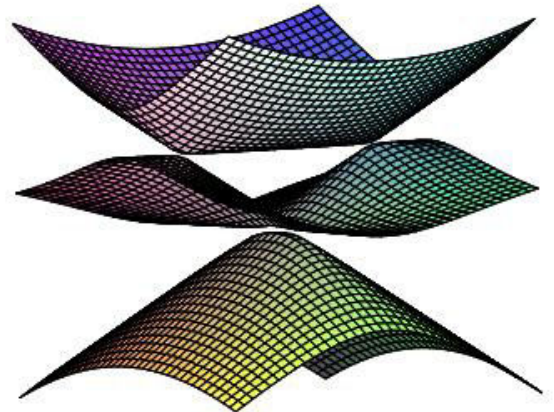


Figure 5.21 – Spectrum as a function of (u, v) for the degenerate STIRAP, where $E_1 = E_2 < E_3$.

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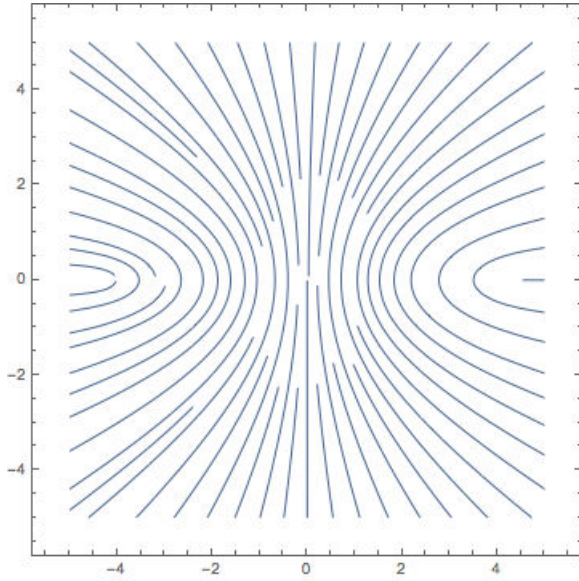


Figure 5.22 – Non-mixing field between λ_1 and λ_2 for the STIRAP, where $E_2 < E_1 < E_3$.

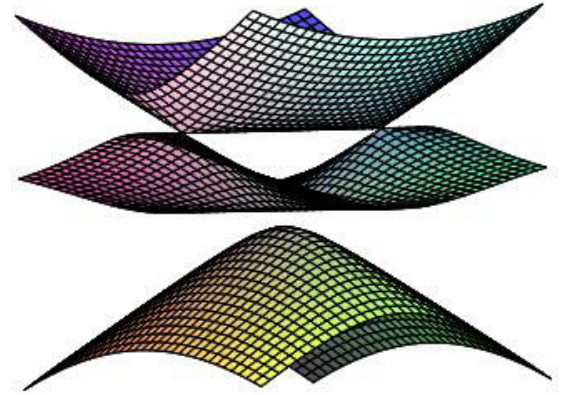


Figure 5.23 – Spectrum as a function of (u, v) for the STIRAP, where $E_2 < E_1 < E_3$.

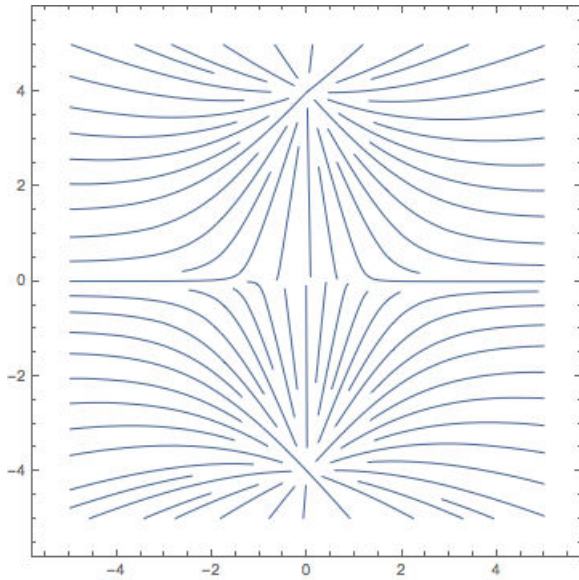


Figure 5.24 – Non-mixing field between λ_1 and λ_2 for the STIRAP, where $E_1 < E_2 = E_3$.

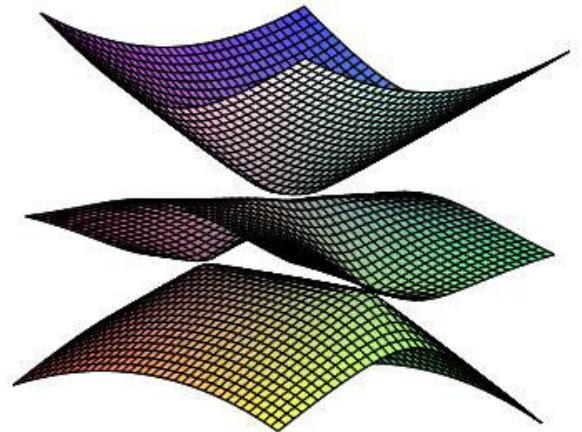


Figure 5.25 – Spectrum as a function of (u, v) for the STIRAP, where $E_1 < E_2 = E_3$.

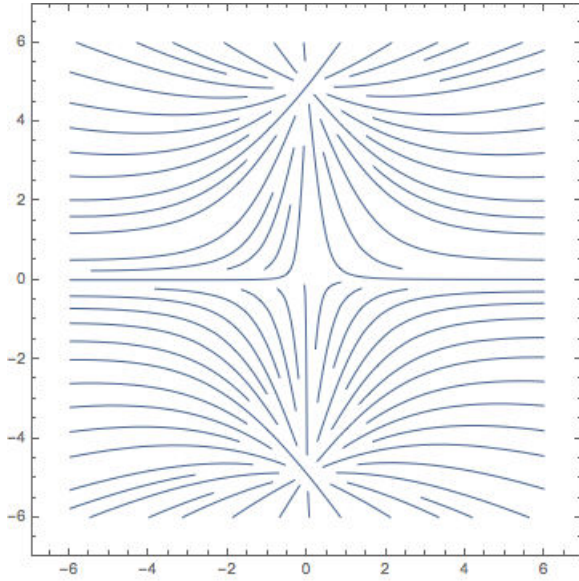


Figure 5.26 – Non-mixing field between λ_1 and λ_2 for the STIRAP, where $E_1 < E_3$, $E_2 > E_3$.

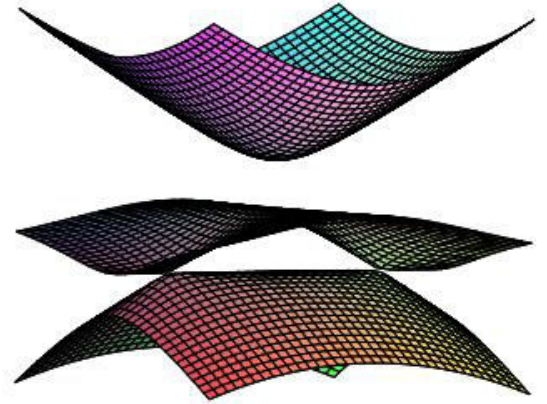


Figure 5.27 – Spectrum as a function of (u, v) for the STIRAP, where $E_1 < E_3$ and $E_2 > E_3$.

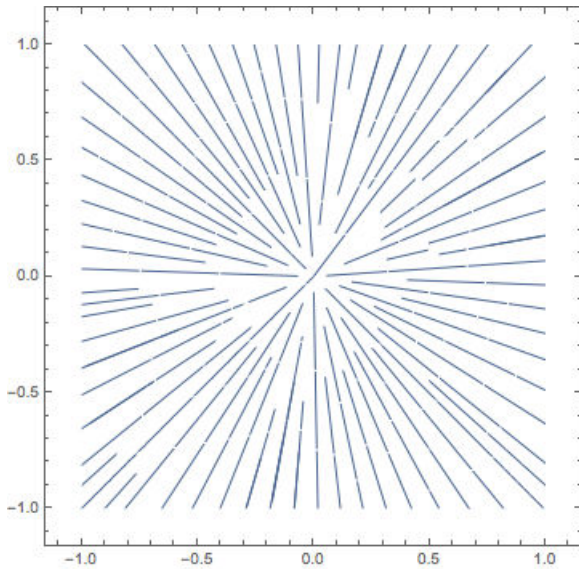


Figure 5.28 – Non-mixing field between λ_1 and λ_2 for the STIRAP, where $E_1 = E_2 = E_3$.

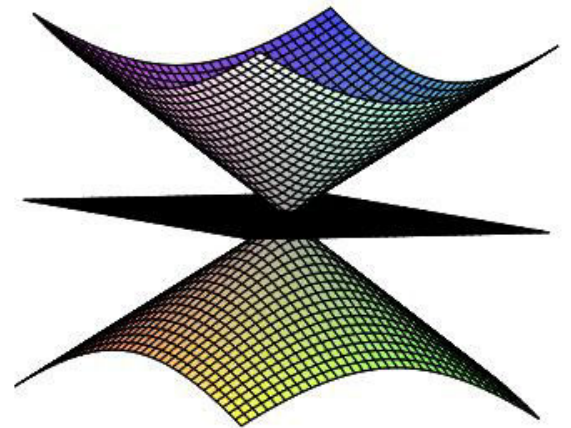


Figure 5.29 – Spectrum as a function of (u, v) for the STIRAP, where $E_1 = E_2 = E_3$.

5.3. *The non-mixing field for general quantum systems*

Chapter 6

Control of quantum systems with a single input

In this chapter, we discuss the compatibility between the *rotating-wave* and the *adiabatic* approximations for controlled quantum systems. We introduce the problem on two-level quantum systems, then we prove results which are valid in higher dimension. Under some suitable hypotheses on the time scales, the two approximations can be combined. As a natural consequence of this, it is possible to design control laws achieving transitions of states between two energy levels of the Hamiltonian that are robust with respect to inhomogeneities of the amplitude of the control input.

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6.1 General framework and main results

6.1.1 Problem formulation

Rotating frame

Consider $v, \varphi \in C^\infty([0, 1], \mathbb{R})$ such that $\varphi(0) = 0$, $E > 0$, and $\psi_0 \in \mathbb{C}^2$. Denote by $\psi : [0, 1] \rightarrow \mathbb{C}^2$ the solution of the equation

$$i \frac{d\psi(t)}{dt} = \begin{pmatrix} E & w(t) \\ \bar{w}(t) & -E \end{pmatrix} \psi(t), \quad \psi(0) = \psi_0, \quad (6.1)$$

where $w(t) = v(t)e^{i(2Et+\varphi(t))}$. Define $\eta(t) = \mathbf{U}(t)\psi(t)$ where

$$\mathbf{U}(t) = \begin{pmatrix} e^{-i(Et+\frac{\varphi(t)}{2})} & 0 \\ 0 & e^{i(Et+\frac{\varphi(t)}{2})} \end{pmatrix}.$$

Then $\eta(t)$ satisfies

$$i \frac{d\eta(t)}{dt} = \begin{pmatrix} -\frac{\varphi'(t)}{2} & v(t) \\ v(t) & \frac{\varphi'(t)}{2} \end{pmatrix} \eta(t), \quad \eta(0) = \psi_0. \quad (6.2)$$

We say that the dynamics are expressed in the *rotating frame* of speed $E + \frac{\varphi'(t)}{2}$. Such an equation can be controlled using several approaches, namely via the well-known Rabi oscillations and the adiabatic approach presented below (see [80] for a comparison between the two approaches).

Adiabatic control in the rotating frame

In order to design an adiabatic control strategy for Equation (6.2), let us add a parameter ϵ in the control w and introduce $w_\epsilon(t) = v(\epsilon t)e^{i(2Et+\frac{\varphi(\epsilon t)}{\epsilon})}$. Consider the solution of (6.2) with initial condition ψ_0 corresponding to such (v, φ) , that is,

$$i \frac{d\eta_\epsilon(t)}{dt} = \begin{pmatrix} -\frac{\varphi'(\epsilon t)}{2} & v(\epsilon t) \\ v(\epsilon t) & \frac{\varphi'(\epsilon t)}{2} \end{pmatrix} \eta_\epsilon(t), \quad \eta_\epsilon(0) = \psi_0.$$

In the variable $\tau = \epsilon t \in [0, 1]$, the reparameterized trajectory $\tilde{\eta}_\epsilon(\tau) = \eta_\epsilon(\tau/\epsilon)$ satisfies

$$i \frac{d\tilde{\eta}_\epsilon(\tau)}{d\tau} = \frac{1}{\epsilon} \begin{pmatrix} -\frac{\varphi'(\tau)}{2} & v(\tau) \\ v(\tau) & \frac{\varphi'(\tau)}{2} \end{pmatrix} \tilde{\eta}_\epsilon(\tau), \quad \tilde{\eta}_\epsilon(0) = \psi_0. \quad (6.3)$$

Let v and φ be chosen so that the curve $(v, \varphi') : [0, 1] \rightarrow \mathbb{R}^2$ connects $(0, -1)$ to $(0, 1)$ intersecting the vertical axis only at its endpoints. Then, by standard adiabatic approximation (see Theorem 2.1.1), if $\psi_0 = (1, 0)$, then $\tilde{\eta}_\epsilon(1)$ converges, up to phases, to $(0, 1)$ as $\epsilon \rightarrow 0$. In the literature, this control strategy is now very classical and is called *chirped adiabatic pulse*. Its robustness properties have been studied within a mathematical framework in Chapter 3.

Rotating wave approximation

In many applications only one real control is available. A classical strategy to duplicate the control input is the so-called *rotating wave approximation* (RWA) that works as follows. Let $\varphi_{\tilde{\epsilon}} : [0, 1/\tilde{\epsilon}] \rightarrow \mathbb{C}^2$ be the solution of (6.1) where w is replaced by the control $u_{\tilde{\epsilon}}(t) = 2\tilde{\epsilon}v(\tilde{\epsilon}t) \cos(2Et + \varphi(\tilde{\epsilon}t))$. Let

$$\mathbf{U}_{\tilde{\epsilon}}(t) = \begin{pmatrix} e^{-i(Et + \frac{\varphi(\tilde{\epsilon}t)}{2})} & 0 \\ 0 & e^{+i(Et + \frac{\varphi(\tilde{\epsilon}t)}{2})} \end{pmatrix}.$$

The RWA then states (see [70]) that $\tau \mapsto \mathbf{U}_{\tilde{\epsilon}}(\tau/\tilde{\epsilon})\varphi_{\tilde{\epsilon}}(\tau/\tilde{\epsilon})$ converges uniformly, as $\tilde{\epsilon} \rightarrow 0$, to the solution of

$$i \frac{d\eta(t)}{dt} = \begin{pmatrix} -\frac{\varphi'(t)}{2} & v(t) \\ v(t) & \frac{\varphi'(t)}{2} \end{pmatrix} \eta(t), \quad \eta(0) = \psi_0. \quad (6.4)$$

Notice that the limit equation (6.4) coincides with (6.2), which is the original equation (6.1) with complex controls in the rotating frame. We have already described how to control (6.2) via adiabatic theory. It is not clear, however, if the RWA and the adiabatic approximations can be combined.

For this purpose, we introduce $u_{\epsilon_1, \epsilon_2}(t) = 2\epsilon_1 v(\epsilon_1 \epsilon_2 t) \cos(2Et + \frac{1}{\epsilon_2} \varphi(\epsilon_1 \epsilon_2 t))$, where ϵ_1 and ϵ_2 play the role of $\tilde{\epsilon}$ and ϵ , respectively. In order to establish in which regime the two approximations can be combined, we set $\epsilon_1 = \epsilon^\alpha$, $\epsilon_2 = \epsilon$ where $\alpha \in \mathbb{R}$ and $u_\epsilon = u_{\epsilon^\alpha, \epsilon}$. Consider the Cauchy problem

$$i \frac{d\psi_\epsilon(t)}{dt} = \begin{pmatrix} E & u_\epsilon(t) \\ u_\epsilon(t) & -E \end{pmatrix} \psi_\epsilon(t), \quad \psi_\epsilon(0) = \psi_0. \quad (6.5)$$

Define $\Psi_\epsilon(t) = U_\epsilon(t)\psi_\epsilon(t)$ where $U_\epsilon(t) = \begin{pmatrix} e^{-i(Et + \frac{\varphi(\epsilon^{\alpha+1}t)}{2\epsilon})} & 0 \\ 0 & e^{+i(Et + \frac{\varphi(\epsilon^{\alpha+1}t)}{2\epsilon})} \end{pmatrix}$. In the variable $\tau = \epsilon^{\alpha+1}t \in [0, 1]$, the reparameterized trajectory $\tilde{\Psi}_\epsilon(\tau) = \Psi_\epsilon(\tau/\epsilon)$ satisfies,

$$\frac{d\tilde{\Psi}_\epsilon(\tau)}{d\tau} = \left(\frac{1}{\epsilon} A(\tau) + B_\epsilon(\tau) \right) \tilde{\Psi}_\epsilon(\tau), \quad \tilde{\Psi}_\epsilon(0) = \psi_0, \quad (6.6)$$

where

$$A(\tau) = -i \begin{pmatrix} -\varphi'(\tau)/2 & v(\tau) \\ v(\tau) & \varphi'(\tau)/2 \end{pmatrix}, \quad \text{and } B_\epsilon(\tau) = \frac{-i}{\epsilon} \begin{pmatrix} 0 & v(\tau) e^{i(\frac{4E\tau}{\epsilon^{\alpha+1}} + \frac{2\varphi(\tau)}{\epsilon})} \\ v(\tau) e^{-i(\frac{4E\tau}{\epsilon^{\alpha+1}} + \frac{2\varphi(\tau)}{\epsilon})} & 0 \end{pmatrix}.$$

The dynamics of $\tilde{\Psi}$ are characterized by the sum of the term that we had in Equation (6.3), that corresponds to the dynamics for the complex control case in the rotating frame, and of an oscillating term $B_\epsilon(\tau)$. The RWA consists in neglecting the term B_ϵ . We are going to show that this can be mathematically justified if $\alpha > 1$.

6.1.2 Main results

In order to obtain the asymptotic analysis announced in the previous section, we show a result of approximation of adiabatic trajectories for general n -level systems under the form of Equation (6.6). Then we deduce results in the particular case of two-level systems with a drift term.

Adiabatic approximation result

Definition 6.1.1. For $A \in C^\infty([0, 1], u(n))$, denote by $j \mapsto \lambda_j(\tau)$ the nondecreasing sequence of eigenvalues of $iA(\tau)$. We say that A satisfies a gap condition if and only if there exists $C > 0$ such that

$$\forall j \neq k, \forall \tau \in [0, 1], |\lambda_j(\tau) - \lambda_k(\tau)| > C. \quad (\text{GAP})$$

We say that A has a k -th order intersection of eigenvalues if and only if there exist $\tau_0 \in [0, 1]$ and $j \in \{1, \dots, n\}$ such that λ_j, λ_{j+1} is separated from the rest of the spectrum and for every $\tau \in [0, 1]$ and $l \neq j$, $\lambda_l(\tau) \neq \lambda_{l+1}(\tau)$, and

$$\lambda_j(\tau_0) = \lambda_{j+1}(\tau_0), \quad \forall \tau \neq \tau_0, \lambda_j(\tau) \neq \lambda_{j+1}(\tau), \quad \text{and} \quad \frac{d^k(\lambda_{j+1} - \lambda_j)}{d\tau^k}(\tau_0) \neq 0. \quad (\text{k-GAP})$$

Definition 6.1.2. Let α be a nonzero real number. Define by $S(\alpha)$ the set of families $(B_\epsilon)_{\epsilon > 0}$ of functions in $C^\infty([0, 1], u(n))$ such that

- $(B_\epsilon(\tau))_{jj} = 0$ for every $j \in \{1, \dots, n\}$ and every $\tau \in [0, 1]$ and
- for every $k > j$ there exist $\beta_{jk} \in \mathbb{R} \setminus \{0\}$ and $v_{jk}, h_{jk} \in C^\infty([0, 1], \mathbb{R})$ such that $(B_\epsilon(\tau))_{jk} = -\frac{i}{\epsilon} v_{jk}(\tau) e^{i(\frac{\beta_{jk}\tau}{\epsilon^{\alpha+1}} + \frac{h_{jk}(\tau)}{\epsilon})}$ for every $\tau \in [0, 1]$.

Theorem 6.1.3. Consider $A \in C^\infty([0, 1], u(n))$ and a finite sum $(B_\epsilon)_{\epsilon > 0}$ of elements belonging to $S(\alpha)$ with $\alpha > 1$. Assume that $A(\cdot)$ satisfies (GAP). Set $X_0 \in \mathbb{C}^n$ independent of ϵ . Let X_ϵ be the solution of $\frac{dX_\epsilon(\tau)}{d\tau} = (\frac{1}{\epsilon}A(\tau) + B_\epsilon(\tau))X_\epsilon(\tau)$ such that $X_\epsilon(0) = X_0$ and \hat{X}_ϵ be the solution of $\frac{d\hat{X}_\epsilon(\tau)}{d\tau} = \frac{1}{\epsilon}A(\tau)\hat{X}_\epsilon(\tau)$ such that $\hat{X}_\epsilon(0) = X_0$. Then there exists $c > 0$ independent of τ, ϵ such that for every $\tau \in [0, 1]$,

$$\|X_\epsilon(\tau) - \hat{X}_\epsilon(\tau)\| \leq c\epsilon^{\min(1, \alpha-1)}.$$

Remark 6.1.4. If A satisfies (k-GAP), then Theorem 6.1.3 remains true, replacing the error of order $\epsilon^{\min(1, \alpha-1)}$ by $\epsilon^{\min(\frac{1}{k+1}, \alpha-1)}$.

Application to two-level systems

We consider $v, \varphi \in C^\infty([0, 1], \mathbb{R})$ such that $\varphi(0) = 0$ and $E > 0$. We consider now Equation (6.5) where $u_\epsilon(t) = 2\epsilon^\alpha v(\epsilon^{\alpha+1}t) \cos(2Et + \frac{1}{\epsilon}\varphi(\epsilon^{\alpha+1}t))$. In the fast time scale

$\tau = \epsilon^{\alpha+1}t \in [0, 1]$, Equation (6.5) can be rewritten as

$$i \frac{d\psi_\epsilon(\tau)}{d\tau} = \begin{pmatrix} \frac{E}{\epsilon^{\alpha+1}} & u_\epsilon(\tau) \\ u_\epsilon(\tau) & -\frac{E}{\epsilon^{\alpha+1}} \end{pmatrix} \psi_\epsilon(\tau) \quad (6.7)$$

for $\tau \in [0, 1]$ where by a slight abuse of notation, we write $u_\epsilon(\tau) = \frac{2}{\epsilon}v(\tau) \cos(\frac{2E\tau}{\epsilon^{\alpha+1}} + \frac{1}{\epsilon}\varphi(\tau))$. Set $\psi_0 \in \mathbb{C}^2$ independent of ϵ . Let $\psi_\epsilon(\cdot)$ be the solution of Equation (6.7) such that $\psi_\epsilon(0) = \psi_0$. Similarly, let $\hat{\psi}_\epsilon$ be the solution of

$$i \frac{d\hat{\psi}_\epsilon(\tau)}{d\tau} = \begin{pmatrix} \frac{E}{\epsilon^{\alpha+1}} & w_\epsilon(\tau) \\ \bar{w}_\epsilon(\tau) & -\frac{E}{\epsilon^{\alpha+1}} \end{pmatrix} \hat{\psi}_\epsilon(\tau), \quad \hat{\psi}_\epsilon(0) = \psi_0 \quad (6.8)$$

for $\tau \in [0, 1]$ and $w_\epsilon(\tau) = \frac{1}{\epsilon}v(\tau)e^{i(\frac{2E\tau}{\epsilon^{\alpha+1}} + \frac{1}{\epsilon}\varphi(\tau))}$.

Theorem 6.1.5. *Assume that $\alpha > 1$. Consider v, φ in $C^\infty([0, 1], \mathbb{R})$ such that $\varphi(0) = 0$ and $v^2 + \frac{\varphi'^2}{4}$ is bounded from below by $C > 0$. Then the solution ψ_ϵ of Equation (6.7) satisfies*

$$\|\psi_\epsilon(\tau) - \hat{\psi}_\epsilon(\tau)\| < c\epsilon^{\min(1, \alpha-1)}$$

where $c > 0$ is independent of (τ, ϵ) .

Proof. Apply the unitary transformation $X_\epsilon(\tau) = U_\epsilon(\tau)\psi_\epsilon(\tau)$ where

$$U_\epsilon(\tau) = \begin{pmatrix} e^{-i(\frac{E\tau}{\epsilon^{\alpha+1}} + \frac{\varphi(\tau)}{2\epsilon})} & 0 \\ 0 & e^{i(\frac{E\tau}{\epsilon^{\alpha+1}} + \frac{\varphi(\tau)}{2\epsilon})} \end{pmatrix}.$$

Then X_ϵ satisfies the equation

$$\frac{dX_\epsilon(\tau)}{d\tau} = \left(\frac{1}{\epsilon}A(\tau) + B_\epsilon(\tau) \right) X_\epsilon(\tau), \quad X_\epsilon(0) = \psi_0,$$

where $A(\tau) = -i \begin{pmatrix} -\varphi'(\tau)/2 & v(\tau) \\ v(\tau) & \varphi'(\tau)/2 \end{pmatrix}$, and

$$B_\epsilon(\tau) = \frac{-i}{\epsilon} \begin{pmatrix} 0 & v(\tau)e^{i(\frac{4E\tau}{\epsilon^{\alpha+1}} + \frac{2\varphi(\tau)}{\epsilon})} \\ v(\tau)e^{-i(\frac{4E\tau}{\epsilon^{\alpha+1}} + \frac{2\varphi(\tau)}{\epsilon})} & 0 \end{pmatrix}.$$

The condition $v(\tau)^2 + \frac{\varphi'(\tau)^2}{4} > C$ for every $\tau \in [0, 1]$ implies that A satisfies Condition (GAP). Let $\hat{X}_\epsilon : [0, 1] \rightarrow \mathbb{C}^2$ be the solution of

$$\frac{d\hat{X}_\epsilon(\tau)}{d\tau} = \frac{1}{\epsilon}A(\tau)\hat{X}_\epsilon(\tau), \quad \hat{X}_\epsilon(0) = \psi_0.$$

Theorem 6.1.3 then implies that $\|X_\epsilon(\tau) - \hat{X}_\epsilon(\tau)\| \leq c\epsilon^{\min(1, \alpha-1)}$. Noticing that $\tilde{\psi}_\epsilon(\tau) = U_\epsilon^*(\tau)\hat{X}_\epsilon(\tau)$, we get the result. \square

Theorem 6.1.5 will be used in Section 6.3 to design control laws for two-level systems using the key fact that $\hat{\psi}_\epsilon(\tau)$ follows an adiabatic evolution up to a change of frame.

Application to n -level quantum systems

Let $E_1, \dots, E_n \in \mathbb{R}$ such that $|E_k - E_q| \neq |E_j - E_l|$, for every $k, q, j, l \in \{1, \dots, n\}$ such that $l \neq j$ and $(k, q) \notin \{(j, l), (l, j)\}$. Let $H_0 = \text{diag}(E_j)_{j=1}^n$ and let H_1 be a real symmetric matrix such that, for every $j, k \in \{1 \dots n\}$, $(H_1)_{jj} = 0$. Define

$$u_\epsilon(t) = 2\epsilon^\alpha \sum_{k < q} v_{kq}(\epsilon^{\alpha+1}t) \cos((E_k - E_q)t + \frac{1}{\epsilon} (\varphi_k(\epsilon^{\alpha+1}t) - \varphi_q(\epsilon^{\alpha+1}t))),$$

where, for every $k, q \in \{1 \dots n\}$, φ_k, φ_q are smooth real functions such that $\varphi_k(0) = \varphi_q(0) = 0$, and for every $k < q$, v_{kq} is a smooth real function. For every $\tau \in [0, 1]$, define $A(\tau) \in u(n)$ such that, for every $j, k \in \{1, \dots, n\}$, $(A(\tau))_{jj} = -i\varphi'_j(\tau)$ and for $j \neq k$, $(A(\tau))_{jk} = -iv_{jk}(\tau)(H_1)_{jk}$.

Theorem 6.1.6. *Set $\psi_0 \in \mathbb{C}^n$. Let $\psi_\epsilon(\cdot)$ be the solution of*

$$i \frac{d\psi_\epsilon(\tau)}{d\tau} = \left(\frac{1}{\epsilon^{\alpha+1}} H_0 + u_\epsilon(\tau) H_1 \right) \psi_\epsilon(\tau) \quad (6.9)$$

for $\tau \in [0, 1]$, with $\psi_\epsilon(0) = \psi_0$, where by a slight abuse of notation, we write

$$u_\epsilon(\tau) = \frac{2}{\epsilon} \sum_{k < q} v_{kq}(\tau) \cos\left(\frac{(E_k - E_q)\tau}{\epsilon^{\alpha+1}} + \frac{1}{\epsilon} (\varphi_k(\tau) - \varphi_q(\tau))\right).$$

Similarly, let $\hat{\psi}_\epsilon(\cdot)$ be the solution of

$$i \frac{d\hat{\psi}_\epsilon(\tau)}{d\tau} = \left(\frac{1}{\epsilon^{\alpha+1}} H_0 + \Omega_\epsilon(\tau) \right) \hat{\psi}_\epsilon(\tau), \quad \hat{\psi}_\epsilon(0) = \psi_0, \quad (6.10)$$

for $\tau \in [0, 1]$ and, for every $\tau \in [0, 1]$ and $\epsilon > 0$, $\Omega_\epsilon(\tau)$ is a $n \times n$ Hermitian matrix such that $(\Omega_\epsilon(\tau))_{kq} = \frac{1}{\epsilon} v_{kq}(\tau) e^{i\left(\frac{(E_k - E_q)\tau}{\epsilon^{\alpha+1}} + \frac{1}{\epsilon} (\varphi_k(\tau) - \varphi_q(\tau))\right)} (H_1)_{kq}$. Assume moreover that A satisfies Condition (GAP). Then

$$\|\psi_\epsilon(\tau) - \hat{\psi}_\epsilon(\tau)\| < c\epsilon^{\min(1, \alpha-1)}$$

where $c > 0$ is independent of (τ, ϵ) .

Proof. We proceed in the same way as in the proof of Theorem 6.1.5. Define $\Psi_\epsilon(\tau) = U_\epsilon(\tau)\psi_\epsilon(\tau)$ and $\hat{\Psi}_\epsilon(\tau) = U_\epsilon(\tau)\hat{\psi}_\epsilon(\tau)$ where $U_\epsilon(\tau) = \text{diag}(e^{i\left(\frac{E_k\tau}{\epsilon^{\alpha+1}} + \frac{\varphi_k(\tau)}{\epsilon}\right)})_{k \in \{1 \dots n\}}$. By direct computations, $\hat{\Psi}_\epsilon$ satisfies

$$\frac{d\hat{\Psi}_\epsilon(\tau)}{d\tau} = \frac{1}{\epsilon} A(\tau) \hat{\Psi}_\epsilon(\tau), \quad \hat{\Psi}_\epsilon(0) = \psi_0, \quad (6.11)$$

and Ψ_ϵ satisfies

$$\frac{d\Psi_\epsilon(\tau)}{d\tau} = \left(\frac{1}{\epsilon} A(\tau) + B_\epsilon(\tau) \right) \Psi_\epsilon(\tau), \quad \Psi_\epsilon(0) = \psi_0, \quad (6.12)$$

where, for $j < l$,

$$\begin{aligned} (B_\epsilon(\tau))_{jl} &= -\frac{i}{\epsilon}(H_1)_{jl}v_{jl}(\tau)e^{i\left(\frac{2(E_l-E_j)\tau}{\epsilon^{\alpha+1}}+\frac{2(\varphi_l(\tau)-\varphi_j(\tau))}{\epsilon}\right)} \\ &\quad -\frac{i}{\epsilon}(H_1)_{jl}\sum_{(k,q)|(k,q)\neq(j,l)}v_{kq}(\tau)e^{i\left(\frac{(E_j-E_l-E_k+E_q)\tau}{\epsilon^{\alpha+1}}+\frac{\varphi_j(\tau)-\varphi_l(\tau)-\varphi_k(\tau)+\varphi_q(\tau)}{\epsilon}\right)} \\ &\quad -\frac{i}{\epsilon}(H_1)_{jl}\sum_{(k,q)|(k,q)\neq(j,l)}v_{kq}(\tau)e^{i\left(\frac{(E_l-E_j-E_k+E_q)\tau}{\epsilon^{\alpha+1}}+\frac{\varphi_l(\tau)-\varphi_j(\tau)-\varphi_k(\tau)+\varphi_q(\tau)}{\epsilon}\right)}, \end{aligned}$$

$(B_\epsilon(\tau))_{jj} = 0$, and $(B_\epsilon(\tau))_{lj} = -(B_\epsilon(\tau))_{lj}^*$. Recall that $|E_k - E_q| \neq |E_j - E_l|$, for every $k, q, j, l \in \{1 \dots n\}$ such that $(k, q) \notin \{(j, l), (l, j)\}$. Hence we deduce that $(B_\epsilon)_{\epsilon>0}$ is a finite sum of elements of $S(\alpha)$. By applying Theorem 6.1.3, we get for every $\tau \in [0, 1]$,

$$\|\Psi_\epsilon(\tau) - \hat{\Psi}_\epsilon(\tau)\| < c\epsilon^{\min(1, \alpha-1)}$$

where $c > 0$ is independent of (τ, ϵ) . □

6.2 Approximation results

6.2.1 Variation formula

We recall here without proof a classical formula which will be useful to neglect highly oscillating parts of the dynamics.

Proposition 6.2.1 (Variation formula). *Let A, B be in $C^\infty([0, 1], u(n))$. Consider the equation*

$$\frac{dx(\tau)}{d\tau} = (A(\tau) + B(\tau))x(\tau), \quad x(\tau) \in \mathbb{C}^n. \quad (6.13)$$

Denote the flow of the equation $\frac{dx(\tau)}{d\tau} = A(\tau)x(\tau)$ at time τ by $P_\tau \in U(n)$ and the flow of the equation $\frac{dx(\tau)}{d\tau} = P_\tau^{-1}B(\tau)P_\tau x(\tau)$ at time τ by $W_\tau \in U(n)$. Then the flow of Equation (6.13) at time τ is equal to $Q_\tau = P_\tau W_\tau$.

6.2.2 Regularity of the eigenstates

We recall here a well-known regularity result.

Lemma 6.2.2. — *Let $A \in C^\infty([0, 1], u(n))$ satisfy (GAP). Then the eigenvectors and the eigenvalues of $iA(\tau)$ can be chosen C^∞ with respect to τ .*

— *Let $A \in C^\infty([0, 1], u(n))$ have a k -th order intersection of eigenvalues at τ_0 . Then the eigenvectors and the eigenvalues of $iA(\tau)$ can be chosen C^∞ with respect to τ .*

6.2.3 Averaging of quantum systems

Theorem 6.2.3. Consider A and $(A_\epsilon)_{\epsilon>0}$ in $C^\infty([0, 1], u(n))$ and assume that $A_\epsilon(\tau)$ is uniformly bounded w.r.t. (τ, ϵ) . Denote the flow of the equation $\frac{dx(\tau)}{d\tau} = A(\tau)x(\tau)$ at time τ by $P_\tau \in U(n)$ and the flow of the equation $\frac{dx(\tau)}{d\tau} = A_\epsilon(\tau)x(\tau)$ at time τ by $P_\tau^\epsilon \in U(n)$. If

$$\int_0^\tau A_\epsilon(s)ds = \int_0^\tau A(s)ds + O(\epsilon)$$

then

$$P_\tau^\epsilon = P_\tau + O(\epsilon),$$

both estimates being uniform w.r.t. $\tau \in [0, 1]$.

We state Theorem 6.2.3 without proof because it is a particular case of next result, Theorem 6.2.4. In the following, we do not assume the boundedness of A_ϵ with respect to ϵ . We refer to [57, 58, 59, 66, 77] for more informations on the case of averaging of a general class of dynamical systems with non-bounded and highly oscillatory inputs. Our result provides an estimate of the error in the special case of quantum systems.

Theorem 6.2.4. Consider A and $(B_\epsilon)_{\epsilon>0}$ in $C^\infty([0, 1], u(n))$. Assume that

$$\int_0^\tau B_\epsilon(s)ds = O(\epsilon)$$

and

$$\int_0^\tau |B_\epsilon(s)| \left| \int_0^s B_\epsilon(x)dx \right| ds = O(\epsilon^k)$$

uniformly w.r.t. $\tau \in [0, 1]$, with $k > 0$. Set $A_\epsilon = A + B_\epsilon$. Denote the flow of the equation $\frac{dx(\tau)}{d\tau} = A(\tau)x(\tau)$ at time τ by $P_\tau \in U(n)$ and the flow of the equation $\frac{dx(\tau)}{d\tau} = A_\epsilon(\tau)x(\tau)$ at time τ by $P_\tau^\epsilon \in U(n)$. Then we have

$$P_\tau^\epsilon = P_\tau + O(\epsilon^{\min(k,1)}),$$

uniformly w.r.t. $\tau \in [0, 1]$.

Proof. Under the hypotheses of the theorem, there exists $K > 0$ such that for every $\tau \in [0, 1]$, $|\int_0^\tau B_\epsilon(s)ds| < K\epsilon$. Let Q_τ^ϵ be the flow associated with B_ϵ . We have $Q_\tau^\epsilon = \text{Id} + \int_0^\tau B_\epsilon(s)Q_s^\epsilon ds$. By integration by parts, $Q_\tau^\epsilon = \text{Id} + (\int_0^\tau B_\epsilon(s)ds) Q_\tau^\epsilon - \int_0^\tau (\int_0^s B_\epsilon(\theta)d\theta) B_\epsilon(s)Q_s^\epsilon ds$. Moreover, Q_τ^ϵ is bounded uniformly w.r.t. (τ, ϵ) , since it evolves in $U(n)$. By the triangular inequality, we get

$$\begin{aligned} |Q_\tau^\epsilon - \text{Id}| &\leq \left| \int_0^\tau B_\epsilon(s)ds \right| |Q_\tau^\epsilon| + \int_0^\tau \left| \int_0^s B_\epsilon(\theta)d\theta \right| |B_\epsilon(s)Q_s^\epsilon| ds \\ &\leq C_1\epsilon + C_2\epsilon^k, \end{aligned}$$

where C_1, C_2 are positive constants which do not depend on (ϵ, τ) . Hence, we deduce that $Q_\tau^\epsilon = \text{Id} + O(\epsilon^q)$ uniformly w.r.t. $\tau \in [0, 1]$, where $q = \min(k, 1)$. The variation formula (Proposition 6.2.1) provides $P_\tau^\epsilon = Q_\tau^\epsilon W_\tau^\epsilon$, where $W_\tau^\epsilon \in U(n)$ is the flow of the equation $\frac{dx(\tau)}{d\tau} = (Q_\tau^\epsilon)^{-1} A(\tau) Q_\tau^\epsilon x(\tau)$ at time τ . By the previous estimate, we have $(Q_\tau^\epsilon)^{-1} A(\tau) Q_\tau^\epsilon = A(\tau) + O(\epsilon^q)$ uniformly w.r.t. $\tau \in [0, 1]$. By an easy application of Gronwall's Lemma, we get that $W_\tau^\epsilon = P_\tau + O(\epsilon^q)$ and we can conclude. \square

6.2.4 Perturbation of an adiabatic trajectory

Consider $A, B_\epsilon \in C^\infty([0, 1], u(n))$. Fix $\psi_0 \in \mathbb{C}^n$. Let X_ϵ be the solution of $\frac{dX_\epsilon(\tau)}{d\tau} = (\frac{1}{\epsilon}A(\tau) + B_\epsilon(\tau)) X_\epsilon(\tau)$ such that $X_\epsilon(0) = X_0$ and let \hat{X}_ϵ be the solution of $\frac{d\hat{X}_\epsilon(\tau)}{d\tau} = \frac{1}{\epsilon}A(\tau)\hat{X}_\epsilon(\tau)$ such that $\hat{X}_\epsilon(0) = X_0$, that we call the *adiabatic trajectory associated with* A . The goal of this section is to understand under which conditions on $B_\epsilon(\cdot)$ we have

$$\|X_\epsilon(\tau) - \hat{X}_\epsilon(\tau)\| \rightarrow 0 \quad (\text{T})$$

uniformly with respect to $\tau \in [0, 1]$. By the variation formula (Proposition 6.2.1), one can show that if the flow of $\frac{dx(\tau)}{d\tau} = B_\epsilon(\tau)x(\tau)$, $x(\tau) \in \mathbb{C}^n$, is equal to $\text{Id} + O(\epsilon^k)$ uniformly w.r.t. $\tau \in [0, 1]$ with $k > 1$, then Property (T) is satisfied. However this condition is too conservative for our needs. We restrict our study to the class of perturbations $(B_\epsilon)_{\epsilon > 0} \in S(\alpha)$ introduced in the Definition 6.1.2. We give below a sufficient condition on α such that Property (T) is satisfied for every A satisfying Condition (GAP) and every finite sum $(B_\epsilon)_{\epsilon > 0}$ of elements of $S(\alpha)$ (Proposition 6.2.9). Based on such a result we then provide a proof of Theorem 6.1.3.

Lemma 6.2.5. *For every $\alpha > 0$ and every $a, h \in C^\infty([0, 1], \mathbb{R})$, we have $\int_0^\tau a(s)e^{i(\frac{s}{\epsilon^{\alpha+1}} + \frac{h(s)}{\epsilon})} ds = O(\epsilon^{\alpha+1})$ uniformly with respect to $\tau \in [0, 1]$.*

Proof. Integrating by parts, for every $\tau \in [0, 1]$,

$$\begin{aligned} & \int_0^\tau a(s)e^{i(\frac{s}{\epsilon^{\alpha+1}} + \frac{h(s)}{\epsilon})} ds \\ &= i\epsilon^{\alpha+1} \int_0^\tau e^{i\frac{s}{\epsilon^{\alpha+1}}} \left(a'(s) + i\frac{h'(s)}{\epsilon} a(s) \right) e^{i\frac{h(s)}{\epsilon}} ds \\ &+ \left[-i\epsilon^{\alpha+1} e^{i\frac{s}{\epsilon^{\alpha+1}}} a(s) e^{i\frac{h(s)}{\epsilon}} \right]_0^\tau \\ &= -\epsilon^\alpha \int_0^\tau h'(s)a(s)e^{i\frac{s}{\epsilon^{\alpha+1}}} e^{i\frac{h(s)}{\epsilon}} ds + O(\epsilon^{\alpha+1}). \end{aligned}$$

Iterating the integration by parts on the integral term $\lceil \frac{1}{\alpha} \rceil$ more times, we get

$$\int_0^\tau a(s)e^{i(\frac{s}{\epsilon^{\alpha+1}} + \frac{h(s)}{\epsilon})} ds = O(\epsilon^{\alpha+1}).$$

\square

6.2. Approximation results

Definition 6.2.6. Let $\alpha > 0$ and $(B_\epsilon)_{\epsilon>0}$ be a finite sum of element in $S(\alpha)$. For every $\epsilon > 0$, $P \in C^\infty([0, 1], U(n))$, and every diagonal matrix $\Gamma(\tau) = \text{diag}(\Gamma_j(\tau))_{j=1}^n$ with $\Gamma_j \in C^\infty([0, 1], \mathbb{R})$, $j = 1, \dots, n$, define

$$M(P, \Gamma, \epsilon)(\tau) = e^{i\frac{\Gamma(\tau)}{\epsilon}} P^*(\tau) B_\epsilon(\tau) P(\tau) e^{-i\frac{\Gamma(\tau)}{\epsilon}}, \quad \tau \in [0, 1].$$

Lemma 6.2.7. Let $\alpha > 1$. Consider $(B_\epsilon)_{\epsilon>0}$, P , Γ , and M as in Definition 6.2.6. Then

$$\int_0^\tau M(P, \Gamma, \epsilon)(s) ds = O(\epsilon^\alpha)$$

and

$$\int_0^\tau |M(P, \Gamma, \epsilon)(s)| \left| \int_0^s M(P, \Gamma, \epsilon)(x) dx \right| ds = O(\epsilon^{\alpha-1})$$

uniformly w.r.t. $\tau \in [0, 1]$.

Proof. Define the following matrix $C_\epsilon(\tau) = \frac{1}{\epsilon} v_{j\ell}(\tau) e^{i(\frac{\beta_{j\ell}\tau}{\epsilon^{\alpha+1}} + \frac{h_{j\ell}(\tau)}{\epsilon})} E_{j\ell}$ for fixed $j, \ell \in \{1, \dots, n\}$ where $E_{j\ell}$ is the matrix whose coefficient (j, ℓ) is equal to 1 and others are equal to 0. By direct computations, denoting $(P(\tau))_{kq} = p_{kq}(\tau)$, we get

$$\begin{aligned} & e^{i\frac{\Gamma(s)}{\epsilon}} P^*(s) C_\epsilon(s) P(s) e^{-i\frac{\Gamma(s)}{\epsilon}} \\ &= \frac{v_{j\ell}(\tau)}{\epsilon} \sum_{k,q=1}^n p_{lk}(\tau) \bar{p}_{jq}(\tau) e^{i(\Gamma_q(\tau) - \Gamma_k(\tau))} e^{i(\frac{\beta_{j\ell}\tau}{\epsilon^{\alpha+1}} + \frac{h_{j\ell}(\tau)}{\epsilon})} E_{qk}. \end{aligned}$$

By Lemma 6.2.5, we get for every $q, k \in \{1, \dots, n\}$,

$$\int_0^\tau v_{j\ell}(s) p_{lk}(s) \bar{p}_{jq}(s) e^{i(\Gamma_q(s) - \Gamma_k(s))} e^{i(\frac{\beta_{j\ell}s}{\epsilon^{\alpha+1}} + \frac{h_{j\ell}(s)}{\epsilon})} ds$$

is $O(\epsilon^{\alpha+1})$. Hence,

$$\int_0^\tau e^{i\frac{\Gamma(s)}{\epsilon}} P(s) C_\epsilon(s) P^*(s) e^{-i\frac{\Gamma(s)}{\epsilon}} ds = O(\epsilon^\alpha).$$

We deduce by linearity that the result is also true for B_ϵ . The second part of the claim follows noticing that $M(P, \Gamma, \epsilon)(\tau) = O(\frac{1}{\epsilon})$. \square

Lemma 6.2.8. Let $\alpha > 1$. Consider $(B_\epsilon)_{\epsilon>0}$, P , Γ , and M as in Definition 6.2.6. Then the flow of the equation $\frac{dx(\tau)}{d\tau} = M(P, \Gamma, \epsilon)(\tau)x(\tau)$ is equal to $\text{Id} + O(\epsilon^{\alpha-1})$, uniformly w.r.t. $\tau \in [0, 1]$.

Proof. We apply Theorem 6.2.4 using the estimates from Lemma 6.2.7. \square

The next proposition, based on Lemma 6.2.8, shows that under the condition $\alpha > 1$, an adiabatic trajectory is robust with respect to perturbations of the dynamics by a term $(B_\epsilon)_{\epsilon>0}$ which is a finite sum of elements belonging to $S(\alpha)$ for ϵ small.

Proposition 6.2.9. Consider $A \in C^\infty([0, 1], u(n))$ and $(B_\epsilon)_{\epsilon > 0}$ be a finite sum of elements in $S(\alpha)$. with $\alpha > 1$. Assume that Condition (GAP) is satisfied. Select $\lambda_j \in C^\infty([0, 1], \mathbb{R})$, $j = 1, \dots, n$, and $P \in C^\infty([0, 1], U(n))$ such that, for $j = 1, \dots, n$, $\lambda_j(\tau)$ and the j -th column of $P(\tau)$ are, respectively, an eigenvalue of $iA(\tau)$ and a corresponding eigenvector (the existence of C^∞ eigenpairs being guaranteed by Lemma 6.2.2). Define $\Lambda(\tau) = \text{diag}(\lambda_j(\tau))_{j=1}^n$, $\tau \in [0, 1]$. Fix $X_0 \in \mathbb{C}^n$ independent of ϵ . Let X_ϵ be the solution of $\frac{dX_\epsilon(\tau)}{d\tau} = \left(\frac{1}{\epsilon}A(\tau) + B_\epsilon(\tau)\right) X_\epsilon(\tau)$ such that $X_\epsilon(0) = X_0$. Set

$$\Upsilon_\epsilon(\tau) = P(\tau) \exp\left(\frac{-i}{\epsilon} \int_0^\tau \Lambda(s) ds\right) \exp\left(\int_0^\tau D(s) ds\right) P^*(0),$$

where D is equal to the diagonal part of $\frac{dP^*}{d\tau}P$. Then

$$\|X_\epsilon(\tau) - \Upsilon_\epsilon(\tau)X_0\| < c\epsilon^{\min(1, \alpha-1)}$$

for some constant $c > 0$ independent of $\tau \in [0, 1]$ and $\epsilon > 0$.

Proof. Define $\Gamma(\tau) = \int_0^\tau \Lambda(s) ds$ and $Y_\epsilon(\tau) = \exp\left(\frac{i}{\epsilon}\Gamma(\tau)\right) P^*(\tau)X_\epsilon(\tau)$. Then Y_ϵ satisfies the equation

$$\begin{aligned} & \frac{dY_\epsilon(\tau)}{d\tau} \\ &= \exp\left(\frac{i}{\epsilon}\Gamma(\tau)\right) \frac{dP^*}{d\tau}(\tau)P(\tau) \exp\left(-\frac{i}{\epsilon}\Gamma(\tau)\right) Y_\epsilon(\tau) \\ & \quad + M(P, \Gamma, \epsilon)(\tau)Y_\epsilon(\tau), \end{aligned} \tag{6.14}$$

where $M(P, \Gamma, \epsilon)$ is defined as in Definition 6.2.6. In order to simplify the notations, set $D_\epsilon(\tau) = \exp\left(\frac{i}{\epsilon}\Gamma(\tau)\right) \frac{dP^*}{d\tau}(\tau)P(\tau) \exp\left(-\frac{i}{\epsilon}\Gamma(\tau)\right)$ and denote the flow at time τ of the equations $\frac{dx(\tau)}{d\tau} = M(P, \Gamma, \epsilon)(\tau)x(\tau)$ and $\frac{dx(\tau)}{d\tau} = (P_\tau^\epsilon)^{-1}D_\epsilon(\tau)P_\tau^\epsilon x(\tau)$ by P_τ^ϵ and W_τ^ϵ , respectively. By the variation formula (Proposition 6.2.1), we get that the flow at time τ of equation (6.14) is equal to $Q_\tau^\epsilon = P_\tau^\epsilon W_\tau^\epsilon$. By Lemma 6.2.8, we have $P_\tau^\epsilon = \text{Id} + O(\epsilon^{\alpha-1})$. Hence $(P_\tau^\epsilon)^{-1}D_\epsilon(\tau)P_\tau^\epsilon = D_\epsilon(\tau) + O(\epsilon^{\alpha-1})$. Using the gap condition (GAP), we have the estimate $\int_0^\tau D_\epsilon(s) ds = \int_0^\tau D(s) ds + O(\epsilon)$ uniformly with respect to $\tau \in [0, 1]$. Indeed, $(D_\epsilon(\tau))_{jl} = q_{jl}(\tau)e^{\frac{i}{\epsilon}\int_0^\tau (\lambda_j(s) - \lambda_l(s)) ds}$, $j, l \in \{1, \dots, n\}$, where q_{jl} is C^∞ . Hence we get the expected estimation by a direct estimation of the integral of the oscillating term $e^{\frac{i}{\epsilon}\int_0^\tau (\lambda_j(s) - \lambda_l(s)) ds}$, $j, l \in \{1, \dots, n\}$. Moreover, since D_ϵ is bounded with respect to ϵ , Theorem 6.2.3 ensures that $W_\tau^\epsilon = \exp\left(\int_0^\tau D(s) ds\right) + O(\epsilon^{\min(1, \alpha-1)})$. It follows that

$$\begin{aligned} Q_\tau^\epsilon &= (\text{Id} + O(\epsilon^{\alpha-1})) \left(\exp\left(\int_0^\tau D(s) ds\right) + O(\epsilon^{\min(1, \alpha-1)}) \right) \\ &= \exp\left(\int_0^\tau D(s) ds\right) + O(\epsilon^{\min(1, \alpha-1)}). \end{aligned}$$

□

6.2. Approximation results

Proof. (Proof of Theorem 6.1.3) By an easy application of Theorem 6.2.3, we get the adiabatic estimate

$$\forall \tau \in [0, 1], \|\hat{X}_\epsilon(\tau) - \Upsilon_\epsilon(\tau)X_0\| < C\epsilon$$

where $C > 0$ is independent of τ, ϵ and Υ_ϵ is defined as in Proposition 6.2.9. The result is then obtained combining the previous inequality with the estimate of Proposition 6.2.9 by triangular inequality. \square

6.2.5 Parametric case

Definition 6.2.10. Let K be a compact of \mathbb{R}^N , where $N \in \mathbb{N}$. For $A^\delta(\tau) \in u(n)$ whose dependence on $(\tau, \delta) \in [0, 1] \times K$ is C^∞ , define $\Lambda^\delta(\tau) = \text{diag}(\lambda_j^\delta(\tau))_{j \in \{1, \dots, n\}}$ where $j \mapsto \lambda_j^\delta(\tau)$ is the nondecreasing sequence of eigenvalues of $iA^\delta(\tau)$. We say that A^δ satisfies a uniform gap condition if and only if there exists $C > 0$ such that

$$\forall l \neq j, \forall \delta \in K, \forall \tau \in [0, 1], |\lambda_l^\delta(\tau) - \lambda_j^\delta(\tau)| > C. \quad (\text{UGAP})$$

We say that A^δ has a conical uniform intersection of eigenvalues if and only if there exists $j \in \{1, \dots, n\}$ such that $\lambda_j^\delta, \lambda_{j+1}^\delta$ is separated from the rest of the spectrum for every $\delta \in K$, and for every $\delta \in K, l \neq j, \lambda_l^\delta(\tau) \neq \lambda_{l+1}^\delta(\tau)$ for every $\tau \in [0, 1]$, and there exists $\tau_\delta \in [0, 1]$ such that for every $l \neq j$,

$$\lambda_j^\delta(\tau_\delta) = \lambda_{j+1}^\delta(\tau_\delta), \quad \forall \tau \neq \tau_\delta, \lambda_j^\delta(\tau) \neq \lambda_{j+1}^\delta(\tau), \quad \text{and} \quad \frac{d(\lambda_{j+1}^\delta - \lambda_j^\delta)}{d\tau}(\tau_\delta) \neq 0, \quad (\text{Conical-UGAP})$$

the associated eigenvectors are C^2 w.r.t $\tau \in [0, 1]$, and their derivatives w.r.t. τ until order 2 are bounded w.r.t. $\delta \in K$.

Using uniform estimates with respect to $\delta \in K$ in the proof of the propositions 6.2.9, we get the following theorem.

Theorem 6.2.11. Let $K = [a, b]$ where $a, b \in \mathbb{R}$. Consider $(B_\epsilon)_{\epsilon > 0} \in S(\alpha)$ with $\alpha > 1$. Let $(A^\delta(\tau))_{\delta \in K}$ be a family of matrices in $u(n)$ whose dependence in $(\tau, \delta) \in [0, 1] \times K$ is C^∞ . Assume that $A^\delta(\tau)$ satisfies (UGAP). Fix $X_0 \in \mathbb{C}^n$ independent of ϵ . Let $X_\epsilon(\delta, \tau)$ be the solution of $\frac{dX_\epsilon(\tau)}{d\tau} = (\frac{1}{\epsilon}A^\delta(\tau) + \delta B_\epsilon(\tau))X_\epsilon(\tau)$ such that $X_\epsilon(0) = X_0$ and $\hat{X}_\epsilon(\delta, \tau)$ be the solution of $\frac{d\hat{X}_\epsilon(\tau)}{d\tau} = \frac{1}{\epsilon}A^\delta(\tau)\hat{X}_\epsilon(\tau)$ such that $\hat{X}_\epsilon(0) = X_0$. Then there exists $c > 0$ independent of τ, δ, ϵ such that for every $(\tau, \delta) \in [0, 1] \times K$,

$$\|X_\epsilon(\delta, \tau) - \hat{X}_\epsilon(\delta, \tau)\| \leq c\epsilon^{\min(1, \alpha-1)}.$$

Theorem 6.2.12. Let K be a compact of \mathbb{R}^{N^2} and $\delta = (\delta_{k,q})_{k,q \in \{1 \dots N\}} \in K$. Consider a family $(B_\epsilon^\delta)_{\epsilon > 0}$ of matrices in $u(n)$ such that, for every $\epsilon > 0, \tau \in [0, 1]$ and $\delta \in K$, $B_\epsilon^\delta(\tau) = \sum_{k,q=1}^N \delta_{k,q} B_\epsilon^{k,q}(\tau)$, where for every $k, q \in \{1 \dots N\}, (B_\epsilon^{k,q})_{\epsilon > 0} \in S(\alpha)$ with $\alpha > 1$.

Let $(A^\delta(\tau))_{\delta \in K}$ be a family of matrices in $u(n)$ whose dependence in $(\tau, \delta) \in [0, 1] \times K$ is C^∞ . Assume that $A(\tau)$ satisfies (UGAP). Fix $X_0 \in \mathbb{C}^n$. Let $X_\epsilon(\delta, \tau)$ be the solution of $\frac{dX_\epsilon(\tau)}{d\tau} = (\frac{1}{\epsilon}A^\delta(\tau) + B_\epsilon^\delta(\tau))X_\epsilon(\tau)$ such that $X_\epsilon(0) = X_0$ and $\hat{X}_\epsilon(\delta, \tau)$ be the solution of $\frac{d\hat{X}_\epsilon(\tau)}{d\tau} = \frac{1}{\epsilon}A^\delta(\tau)\hat{X}_\epsilon(\tau)$ such that $\hat{X}_\epsilon(0) = X_0$. Then there exists $c > 0$ independent of τ, δ, ϵ such that for every $(\tau, \delta) \in [0, 1] \times K$,

$$\|X_\epsilon(\delta, \tau) - \hat{X}_\epsilon(\delta, \tau)\| \leq c\epsilon^{\min(1, \alpha-1)}.$$

Remark 6.2.13. In the case $A^\delta(\tau)$ satisfies (Conical-UGAP), the theorems 6.2.11 and 6.2.12 remain valid replacing the error of order $\epsilon^{\min(1, \alpha-1)}$ by $\epsilon^{\min(\frac{1}{2}, \alpha-1)}$.

6.3 Control of two-level systems

6.3.1 Control strategy for two-level systems and simulations

Let $v, \varphi \in C^\infty([0, 1], \mathbb{R})$ be such that $v(0) = v(1) = 0$, $\varphi(0) = 0$, $\varphi'(0)\varphi'(1) < 0$, and $v(\tau) \neq 0$ for $\tau \in (0, 1)$. Let $e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. By adiabatic approximation, the solution $x_\epsilon : [0, 1] \rightarrow \mathbb{C}^2$ of

$$\frac{dx_\epsilon(\tau)}{d\tau} = -\frac{i}{\epsilon} \begin{pmatrix} -\varphi'(\tau)/2 & v(\tau) \\ v(\tau) & \varphi'(\tau)/2 \end{pmatrix} x_\epsilon(\tau), \quad x_\epsilon(0) = e_1,$$

satisfies $\|x_\epsilon(1) - e^{i\xi_\epsilon}e_2\| \leq C\epsilon$ where $C > 0$ is independent of ϵ and $\xi_\epsilon \in \mathbb{R}$. Consider the solution $\psi_\epsilon(\tau)$ of Equation (6.7) such that $\psi_0 = e_1$ and corresponding to the controls (v, φ) . Applying Theorem 6.1.5, we have

$$\|\psi_\epsilon(1) - e^{i\theta_\epsilon}e_2\| \leq c\epsilon^{\min(1, \alpha-1)}$$

where $c > 0$ is independent of ϵ and $\theta_\epsilon \in \mathbb{R}$.

On Figure 6.1, we have plotted the projection of the wave function onto e_2 for

$$v(\tau) = \sin(\pi\tau), \quad \varphi(\tau) = -\frac{1}{\pi} \sin(\pi\tau),$$

with $\epsilon = 0.01$, $\alpha = 1.5$ and $E = 1$ in the fast time scale, that is, as a function of $\tau \in [0, 1]$. The total time needed by our control strategy in the variable $t = \frac{\tau}{\epsilon^{\alpha+1}}$ is $T = \frac{1}{\epsilon^{\alpha+1}}$. On Figure 6.2, we have plotted the norm of the difference between ψ_ϵ and the solution of Equation (6.10) with the same initial condition and parameters as a function of $\tau \in [0, 1]$.

6.3. Control of two-level systems

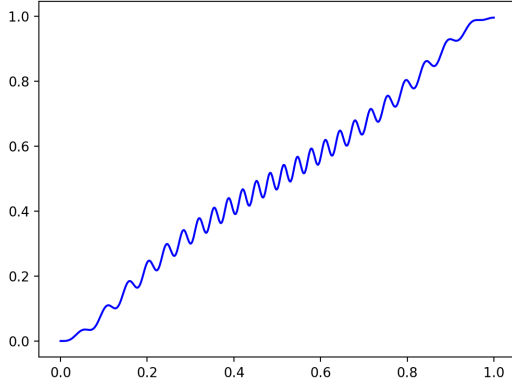


Figure 6.1 – Fidelity $|\langle \psi_\epsilon(\tau), e_2 \rangle|^2$ as a function of the time variable $\tau \in [0, 1]$ with $\epsilon = 0.01$, $\alpha = 1.5$, and $E = 1$.

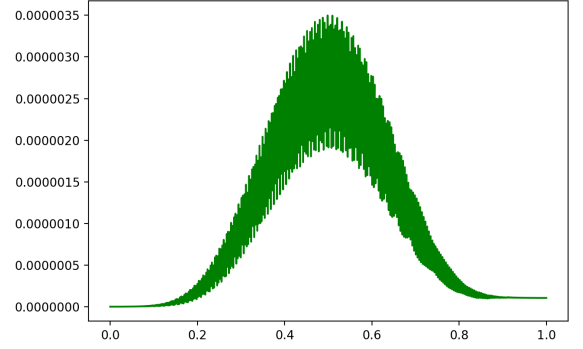


Figure 6.2 – Squared norm of the difference between ψ_ϵ and $\hat{\psi}_\epsilon$ as a function of the time variable $\tau \in [0, 1]$ with $\epsilon = 0.01$, $\alpha = 1.5$, and $E = 1$.

6.3.2 Robustness of the control strategy with respect to amplitude of control inhomogeneities

Let U be a connected open set of \mathbb{R} containing 0.

Theorem 6.3.1. *Let $E \in \mathbb{R} \setminus \{0\}$. The equation*

$$i \frac{d\psi}{dt} = \begin{pmatrix} E & \delta u \\ \delta u & -E \end{pmatrix} \psi \quad (6.15)$$

is approximately ensemble controllable between the eigenstates of $H_0 = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$ uniformly with respect to $\delta \in [a, b] \subset (0, +\infty)$ and $u \in U$.

Proof. Let $\alpha > 1$ and $v, \varphi \in C^\infty([0, 1], \mathbb{R})$ be such that $v(0) = v(1) = 0$, $\varphi(0) = 0$, $\varphi'(0)\varphi'(1) < 0$, and $v(\tau) \neq 0$ for $\tau \in (0, 1)$. Let us consider $\tau = \epsilon^{\alpha+1}t \in [0, 1]$ and $u_\epsilon(\tau) = \frac{2}{\epsilon}v(\tau) \cos(\frac{2E\tau}{\epsilon^{\alpha+1}} + \frac{1}{\epsilon}\varphi(\tau))$. For each $\delta \in [a, b]$, let $\psi_\epsilon(\delta, \tau)$ be the solution of

$$i \frac{d\psi(\delta, \tau)}{d\tau} = \begin{pmatrix} \frac{E}{\epsilon^{\alpha+1}} & \delta u_\epsilon(\tau) \\ \delta u_\epsilon(\tau) & -\frac{E}{\epsilon^{\alpha+1}} \end{pmatrix} \psi(\delta, \tau), \quad \psi_\epsilon(\delta, 0) = e_1.$$

Apply the unitary transformation $X_\epsilon(\delta, \tau) = U_\epsilon(\tau)\psi_\epsilon(\delta, \tau)$ where

$$U_\epsilon(\tau) = \begin{pmatrix} e^{-i(\frac{E\tau}{\epsilon^{\alpha+1}} + \frac{\varphi(\tau)}{2\epsilon})} & 0 \\ 0 & e^{i(\frac{E\tau}{\epsilon^{\alpha+1}} + \frac{\varphi(\tau)}{2\epsilon})} \end{pmatrix}.$$

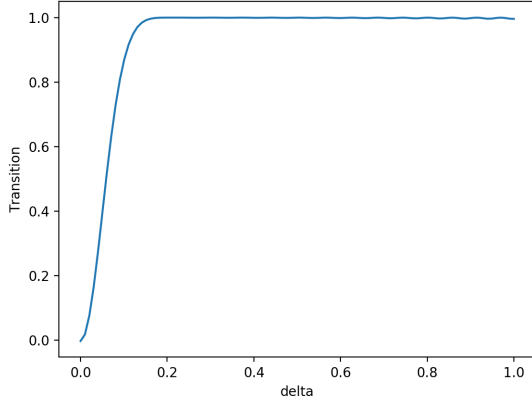


Figure 6.3 – Fidelity $|\langle \psi_\epsilon(\delta, 1), e_2 \rangle|^2$ as a function of the amplitude inhomogeneity δ , with $\epsilon = 0.01$, $\alpha = 1.5$, and $E = 1$.

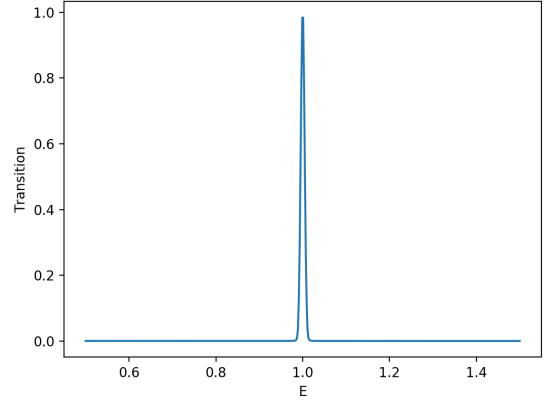


Figure 6.4 – Fidelity $|\langle \psi_\epsilon(E, 1), e_2 \rangle|^2$ as a function of the drift term E , with $\epsilon = 0.01$ and $\alpha = 1.5$.

Then $X_\epsilon(\delta, \tau)$ satisfies

$$\frac{dX_\epsilon(\delta, \tau)}{d\tau} = \left(\frac{1}{\epsilon} A^\delta(\tau) + \delta B_\epsilon(\tau) \right) X_\epsilon(\delta, \tau), \quad X_\epsilon(\delta, 0) = e_1,$$

where

$$A^\delta(\tau) = -i \begin{pmatrix} -\varphi'(\tau)/2 & \delta v(\tau) \\ \delta v(\tau) & \varphi'(\tau)/2 \end{pmatrix},$$

and

$$B_\epsilon(\tau) = \frac{-i}{\epsilon} \begin{pmatrix} 0 & v(\tau) e^{i(\frac{4E\tau}{\epsilon^{\alpha+1}} + \frac{2\varphi(\tau)}{\epsilon})} \\ v(\tau) e^{-i(\frac{4E\tau}{\epsilon^{\alpha+1}} + \frac{2\varphi(\tau)}{\epsilon})} & 0 \end{pmatrix}.$$

By our choice of v and φ , $A^\delta(\tau)$ is C^∞ w.r.t (τ, δ) and satisfies (UGAP). Applying Theorem 6.2.11, we get that $\|\psi_\epsilon(\delta, 1) - e^{i\theta_{\delta, \epsilon}} e_2\| \leq C\epsilon^{\min(1, \alpha-1)}$ where $C > 0$ is independent of δ, ϵ and $\theta_{\delta, \epsilon} \in \mathbb{R}$. The result follows. \square

Consider the same (v, φ) as those chosen in Section 6.3.1. For each $\delta \in [0, 1]$, let $\psi_\epsilon(\delta, \tau)$ be the solution of Equation (6.15) with initial condition $\psi(\delta, 0) = e_1$ and $E = 1$. We have plotted on Figure 6.3 the *fidelity*, that is $|\langle \psi_\epsilon(\delta, 1), e_2 \rangle|^2$ for a dispersion δ of the amplitude of the control in $[0, 1]$. On every sub-interval $[a, b]$ of $[0, 1]$ with $a > 0$, the fidelity converges uniformly to the constant function $\delta \mapsto 1$ when $\epsilon \rightarrow 0$.

Let now $\psi_\epsilon(E, \tau)$ be the solution of the equation

$$i \frac{d\psi_\epsilon(E, \tau)}{d\tau} = \begin{pmatrix} \frac{E}{\epsilon^{\alpha+1}} & u_\epsilon(\tau) \\ u_\epsilon(\tau) & -\frac{E}{\epsilon^{\alpha+1}} \end{pmatrix} \psi_\epsilon(E, \tau) \quad (6.16)$$

where $u_\epsilon(\tau) = \frac{2}{\epsilon}v(\tau) \cos(\frac{2\tau}{\epsilon^{\alpha+1}} + \frac{1}{\epsilon}\varphi(\tau))$, with initial condition $\psi(E, 0) = e_1$ for every $E \in [\frac{1}{2}, \frac{3}{2}]$. We have plotted on Figure 6.4 the fidelity for a dispersion of E in $[\frac{1}{2}, \frac{3}{2}]$. As already mentioned in the introduction of the thesis, numerical simulations suggest that our method of control is not robust w.r.t. inhomogeneities of the resonance frequency E .

6.4 Control of STIRAP Process

Denote the canonical basis of \mathbb{R}^3 by (e_1, e_2, e_3) . We prove the following theorem.

Theorem 6.4.1. *Let $E_1, E_2, E_3 \in \mathbb{R}$ such that $E_1 < E_2 < E_3$ and $|E_k - E_q| \neq |E_j - E_l|$, for every $k, q, j, l \in \{1 \dots 3\}$ such that $(k, q) \notin \{(j, l), (l, j)\}$. The equation*

$$i \frac{d\psi}{dt} = \begin{pmatrix} E_1 & \delta_1 u & 0 \\ \delta_1 u & E_2 & \delta_2 u \\ 0 & \delta_2 u & E_3 \end{pmatrix} \psi \quad (6.17)$$

is ensemble controllable between eigenstates of $H_0 = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix}$ uniformly with respect to $\delta_1 \in [a_1, b_1] \subset (0, +\infty)$ and $\delta_2 \in [a_2, b_2] \subset (0, +\infty)$ and $u \in U$.

Proof. For $\delta_1, \delta_2 \in \mathbb{R}$, set $\delta = (\delta_1, \delta_2) \in \mathbb{R}^2$. We prove the result for a transfer of populations between e_1 and e_3 . Let $\alpha > 1$ and $v_{12}, v_{23}, (\varphi_j)_{j \in \{1, \dots, 3\}} \in C^\infty([0, 1], \mathbb{R})$. Define, for $\epsilon > 0$ and $t \in [0, \frac{1}{\epsilon^{\alpha+1}}]$,

$$\begin{aligned} u_\epsilon(t) = & 2\epsilon^\alpha v_{12}(\epsilon^{\alpha+1}t) \cos((E_1 - E_2)t + \frac{1}{\epsilon}(\varphi_1(\epsilon^{\alpha+1}t) - \varphi_2(\epsilon^{\alpha+1}t))) \\ & + 2\epsilon^\alpha v_{23}(\epsilon^{\alpha+1}t) \cos((E_2 - E_3)t + \frac{1}{\epsilon}(\varphi_2(\epsilon^{\alpha+1}t) - \varphi_3(\epsilon^{\alpha+1}t))). \end{aligned}$$

Assume that for every $\tau \in [0, 1]$ and $j \in \{1, \dots, 3\}$, $\varphi_j(\tau) = \tilde{E}_j \tau$, where $(\tilde{E}_j)_{j \in \{1, \dots, 3\}}$ are such that $\tilde{E}_1 < \tilde{E}_2 < \tilde{E}_3$. Let us consider $\tau = \epsilon^{\alpha+1}t \in [0, 1]$ and, by a slight abuse of notations,

$$\begin{aligned} u_\epsilon(\tau) = & \frac{2}{\epsilon} v_{12}(\tau) \cos((E_1 - E_2) \frac{\tau}{\epsilon^{\alpha+1}} + \frac{1}{\epsilon}(\varphi_1(\tau) - \varphi_2(\tau))) \\ & + \frac{2}{\epsilon} v_{23}(\tau) \cos((E_2 - E_3) \frac{\tau}{\epsilon^{\alpha+1}} + \frac{1}{\epsilon}(\varphi_2(\tau) - \varphi_3(\tau))). \end{aligned}$$

For each $\delta \in [a, b]$, let $\psi_\epsilon(\delta, \tau)$ be the solution of

$$i \frac{d\psi(\delta, \tau)}{dt} = \begin{pmatrix} \frac{E_1}{\epsilon^{\alpha+1}} & \delta_1 u_\epsilon(\tau) & 0 \\ \delta_1 u_\epsilon(\tau) & \frac{E_2}{\epsilon^{\alpha+1}} & \delta_2 u_\epsilon(\tau) \\ 0 & \delta_2 u_\epsilon(\tau) & \frac{E_3}{\epsilon^{\alpha+1}} \end{pmatrix} \psi(\delta, \tau), \quad \psi_\epsilon(\delta, 0) = e_1. \quad (6.18)$$

Apply the unitary transformation $X_\epsilon(\delta, \tau) = U_\epsilon(\tau)\psi_\epsilon(\delta, \tau)$ where

$$U_\epsilon(\tau) = \begin{pmatrix} e^{i\left(\frac{E_1\tau}{\epsilon^{\alpha+1}} + \frac{\varphi_1(\tau)}{2\epsilon}\right)} & 0 & 0 \\ 0 & e^{i\left(\frac{E_2\tau}{\epsilon^{\alpha+1}} + \frac{\varphi_2(\tau)}{2\epsilon}\right)} & 0 \\ 0 & 0 & e^{i\left(\frac{E_3\tau}{\epsilon^{\alpha+1}} + \frac{\varphi_3(\tau)}{2\epsilon}\right)} \end{pmatrix}.$$

Then $X_\epsilon(\delta, \tau)$ satisfies

$$\frac{dX_\epsilon(\delta, \tau)}{d\tau} = \left(\frac{1}{\epsilon} A^\delta(\tau) + B_\epsilon^\delta(\tau) \right) X_\epsilon(\delta, \tau), \quad X_\epsilon(\delta, 0) = e_1,$$

where for $\tau \in [0, 1]$, $A^\delta(\tau) = \begin{pmatrix} \tilde{E}_1 & \delta_1 v_{12}(\tau) & 0 \\ \delta_1 v_{12}(\tau) & \tilde{E}_2 & \delta_2 v_{23}(\tau) \\ 0 & \delta_2 v_{23}(\tau) & \tilde{E}_3 \end{pmatrix}$ is C^∞ w.r.t (τ, δ) , and $B_\epsilon^\delta(\tau)$ has the form required by Theorem 6.2.12.

Define, for $(x, y) \in \mathbb{R}^2$, $\tilde{A}^\delta(x, y) = \begin{pmatrix} \tilde{E}_1 & \delta_1 x & 0 \\ \delta_1 x & \tilde{E}_2 & \delta_2 y \\ 0 & \delta_2 y & \tilde{E}_3 \end{pmatrix}$, and its eigenvalues by $\Lambda_j^\delta(x, y)$

for $j \in \{1 \dots 2\}$. Notice that we have $A^\delta(\tau) = \tilde{A}^\delta(v_{12}(\tau), v_{23}(\tau))$. Design a control path $(v_{12}(\tau), v_{23}(\tau))_{\tau \in [0, 1]}$ passing through the conical intersections of \tilde{A}^δ between the levels Λ_1^δ and Λ_2^δ , then those between the levels Λ_2^δ and Λ_3^δ , for every $\delta \in [a_1, b_1] \times [a_2, b_2]$ as it is made in Section 3.7.2. For every $\delta \in [a_1, b_1] \times [a_2, b_2]$, at a time τ_δ where the control path passes at a conical intersection, $A^\delta(\tau)$ satisfies (Conical-UGAP) locally w.r.t. τ . Applying Theorem 6.2.12, we get that $\|\psi_\epsilon(\delta, 1) - e^{i\theta_{\delta, \epsilon}} e_3\| \leq C \epsilon^{\min(\frac{1}{2}, \alpha-1)}$ where $C > 0$ is independent of δ, ϵ and $\theta_{\delta, \epsilon} \in \mathbb{R}$. Following the same steps, we can get transfers from e_j to e_k , for every $j, k \in \{1 \dots 3\}$. The result follows. \square

Set $E_1 = 2, E_2 = 5, E_3 = 6$. On Figure 6.5, we have illustrated the robustness of our control strategy for Equation 6.17 with respect to the parameter δ_1 defined in Theorem 6.4.1, assuming that $\delta_2 = 1$, for a transfer from state 1 to state 3, with a control

$$u_\epsilon(\tau) = \frac{2}{\epsilon} v_{12}(\tau) \cos\left(\left(E_1 - E_2\right) \frac{\tau}{\epsilon^{\alpha+1}} + \frac{1}{\epsilon} (\varphi_1(\tau) - \varphi_2(\tau))\right) + \frac{2}{\epsilon} v_{23}(\tau) \cos\left(\left(E_2 - E_3\right) \frac{\tau}{\epsilon^{\alpha+1}} + \frac{1}{\epsilon} (\varphi_2(\tau) - \varphi_3(\tau))\right),$$

where τ is the normalized time. We have chosen piecewise affine functions v_{12} and v_{23} as on Figure 6.6, and linear functions $(\varphi_k)_{k \in \{1, \dots, 3\}}$ as in the proof of Theorem 6.4.1 with $\tilde{E}_1 = 0, \tilde{E}_2 = 1, \tilde{E}_3 = 3$, and we have considered the solution $\psi_\epsilon(\delta, \tau)$ of Equation 6.17.

On Figure 6.7, we have illustrated the failure of our control strategy with fixed parameters $\delta_1 = \delta_2 = 1$ and $0 < \alpha < 1$. On Figure 6.8, we have illustrated the failure of our control strategy with fixed parameters $\delta_1 = \delta_2 = 1$, $\alpha > 1$ and $|E_1 - E_2| = |E_2 - E_3|$.

6.4. Control of STIRAP Process

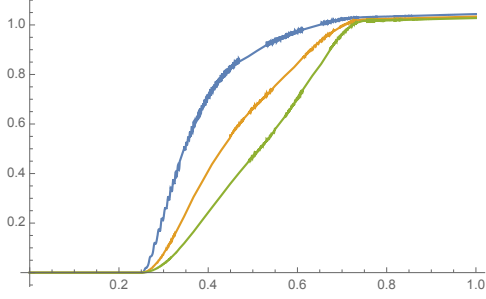


Figure 6.5 – Time-evolution of $|\langle \psi_\epsilon(\delta, \tau), e_3 \rangle|^2$ where τ is the renormalized time, with $\delta_1 = 0.5$ in blue, $\delta_1 = 1$ in orange, $\delta_1 = 1.5$ in green, with $\epsilon = 0.02$ and $\alpha = 1.5$.

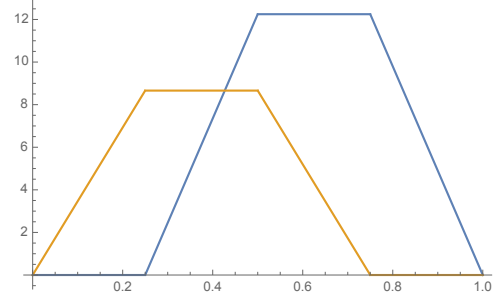


Figure 6.6 – Time-evolution of $v_{12}(\tau)$ in blue, and of $v_{23}(\tau)$ in orange

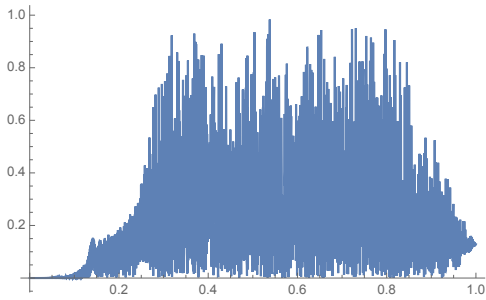


Figure 6.7 – Time-evolution of $|\langle \psi_\epsilon(\delta, \tau), e_3 \rangle|^2$ where τ is the renormalized time, with $\delta_1 = \delta_2 = 1$, $\epsilon = 0.02$ and $\alpha = 0.5$.

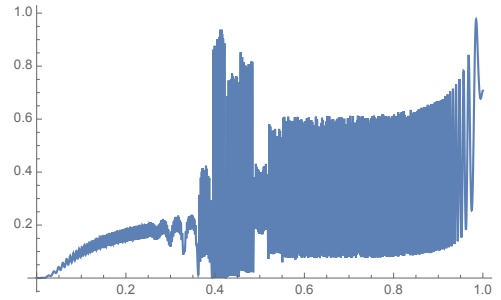


Figure 6.8 – Time-evolution of $|\langle \psi_\epsilon(\delta, \tau), e_3 \rangle|^2$ where τ is the renormalized time, with $\delta_1 = \delta_2 = 1$, $\epsilon = 0.02$ and $\alpha = 1.5$, in the resonant case $|E_1 - E_2| = |E_2 - E_3|$.

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Références

Titre : Contrôle adiabatique des systèmes quantiques

Mots clés : Contrôle quantique, théorie adiabatique, approximation rotating wave, contrôle robuste, singularités, champs de direction, moyennisation de systèmes dynamiques

Résumé : Le but principal de la thèse est d'étudier les liens entre les singularités du spectre d'un Hamiltonien quantique contrôlé et les questions de contrôlabilité de l'équation Schrödinger associée.

La question que l'on se pose est de savoir comment contrôler une famille de systèmes quantiques dépendant d'un paramètre avec une entrée de commande commune. Grâce à l'étude des familles à un paramètre de Hamiltoniens et de leurs singularités génériques, on donne une stratégie de contrôle explicite pour le problème de contrôlabilité d'ensemble lorsque certaines conditions géométriques sur le spectre des Hamiltoniens de la famille à un paramètre sont satisfaites, en particulier l'existence d'intersections coniques ou semi-coniques, en se basant sur la théorie adiabatique.

Pour l'étude d'un système unique non-paramétrique, on se concentre sur une classe de courbes dans l'espace des contrôles, appelées les courbes non-mixantes, qui peuvent optimiser la dynamique adiabatique près des intersections coniques et semi-coniques. Elles sont liées à la géométrie des espaces propres du Hamiltonien contrôlé et l'approximation adiabatique possède une meilleure précision le long de celles-ci.

On étudie ensuite la compatibilité de l'approximation adiabatique avec l'approximation rotating wave. De telles approximations sont généralement combinées par les physiciens. On montre que cela ne se justifie que dans certaines conditions sur les échelles de temps. On étudie également les questions de contrôle d'ensemble dans ce cas.

Title : Adiabatic control of quantum systems

Keywords : Quantum control, adiabatic theory, rotating wave approximation, robust control, singularities, line fields, averaging of dynamical systems

Abstract : The main purpose of the thesis is to study the links between the singularities of the spectrum of a controlled quantum Hamiltonian and the controllability issues of the associated Schrödinger equation.

The principal issue that is developed is how to control a parameter-dependent family of quantum systems with a common control input. Thanks to the study one-parametric families of Hamiltonians and their generic singularities, we give an explicit control strategy for the ensemble controllability problem when geometric conditions on the spectrum of the Hamiltonian are satisfied, in particular the existence of conical or semi-conical intersections, using adiabatic theory.

For the study of a single system, we focus on a class

of curves in the space of controls, called the non-mixing curves, that can optimize the adiabatic dynamics near conical and semi-conical intersections. They are linked to the geometry of the eigenspaces of the controlled Hamiltonian and the adiabatic approximation holds with higher precision along them.

We propose to study the compatibility of the adiabatic approximation with the rotating wave approximation. Such approximations are usually done in cascade by physicists. It is shown in this work that this is justified for finite dimensional quantum systems only under certain conditions on the time scales. We also study ensemble control issues in this case.

