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Contributions to the mathematical study of models from classical and quantum physics

Simona Rota Nodari

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UNIVERSITÉ BOURGOGNE FRANCHE-COMTÉ
ÉCOLE DOCTORALE CARNOT-PASTEUR

**Contributions to the mathematical study of models from classical
and quantum physics**

THÈSE D'HABILITATION À DIRIGER DES RECHERCHES

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INTRODUCTION

In this thesis, I will describe the different research works that I have carried out since the defense of my PhD.

My PhD thesis [1] was devoted to the mathematical study of two nonlinear relativistic models from quantum physics. The goal was to give a rigorous mathematical framework to these models that are often used by chemists and physicists. In particular, the microscopic description of matter (for instance, the inside of a nucleus or the core electrons of a heavy atom) requires the addition of special relativity to quantum mechanics. Mathematically, it amounts to analyzing partial differential equations (PDEs) involving a relativistic kinetic energy operator: the Dirac operator. The Dirac operator is a matrix-differential operator of first order whose spectrum contains an unbounded negative part. Consequently, the associated energy functionals are all strongly indefinite. Moreover, since I considered interacting systems where the interaction is modeled via a nonlinearity, all the models studied were nonlinear. As a consequence, nonlinear analysis and variational calculus methods adapted to these difficulties were used in the PhD thesis.

The first part of my PhD thesis was in particular devoted to the study of the Einstein–Dirac–Maxwell equations for a static, spherically symmetric system of two fermions in a singlet spinor state and for a weak electromagnetic coupling. By means of a perturbation method the existence of solutions of this system of equations has been proven. The results of this part of the PhD are contained in [2; 3]. However, these results, although interesting, will not be presented here because they did not give rise to further works for the moment.

In the second part of the PhD thesis, I began the study a relativistic mean-field model that describes the behavior of nucleons in the atomic nucleus. In [5], I showed the existence of solitary wave solutions for the equations of this model. That was the starting point of the research axis presented in Chapter 2.

At the same time, I started working together with S. Serfaty on the microscopic description of minimizers of the two-dimensional Coulomb gas. In particular, we were able to highlight some interesting properties of the minimizers that were later generalized to Coulomb and Riesz gases in any dimension in collaboration with M. Petrache as described in Chapter 5.

Finally, during my post-doc at the Université de Lille, I focused on the question of the (orbital) stability of stationary solutions of general PDEs. This topic will be presented in Chapter 3 in the context of general Hamiltonian PDEs and in Chapter 4 for the case of a nonlinear Schrödinger equation arising from the study of optical fibers.

The common thread in my researches is the rigorous analysis of models arising in classical and quantum physics. The mathematical tools are that of partial differential equations, nonlinear analysis, calculus of variations, and numerical analysis.

For each chapter of this thesis, I will now give a very short summary together with a list of the corresponding publications. Note that the chapters are independent and can be read separately.

Chapter 2: Relativistic Quantum Dynamics in Nuclear Physics

In [4] (see also [1]), we observed that in nuclear physics the behavior of particles inside the atomic nucleus can be described by a system of nonlinear Schrödinger type equations obtained, at least formally, as the non-relativistic limit in a strong coupling regime of a relativistic mean-field model where Dirac equations are linearly coupled to Klein-Gordon equations. In particular, in the simplest case where we consider only one particle in spatial dimension 3, we obtain the following quasi-linear Schrödinger equation

$$i\partial_t\psi = -\boldsymbol{\sigma} \cdot \nabla \left(\frac{\boldsymbol{\sigma} \cdot \nabla\psi}{1-|\psi|^2} \right) + \frac{|\boldsymbol{\sigma} \cdot \nabla\psi|^2}{(1-|\psi|^2)^2}\psi - a|\psi|^2\psi$$

where $\psi : \mathbb{R}_+ \times \mathbb{R}^3 \rightarrow \mathbb{C}^2$ is a spinor that represents the state of the particle and a is a positive coupling constant.

A first step in the study of this equation consists in looking for particular solitary wave solutions of the form $\Psi(t, x) = e^{ibt}\psi(x)$ with ψ a solution to the stationary equation

$$-\boldsymbol{\sigma} \cdot \nabla \left(\frac{\boldsymbol{\sigma} \cdot \nabla\psi}{1-|\psi|^2} \right) + \frac{|\boldsymbol{\sigma} \cdot \nabla\psi|^2}{(1-|\psi|^2)^2}\psi - a|\psi|^2\psi + b\psi = 0 \quad (1.0.1)$$

and where b is a positive constant. This equation can be further simplified by assuming that $\psi(x) = \varphi(x) \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, *i.e.* the state of the nucleon is an eigenfunction of the spin operator. In particular, φ is then a solution to the stationary equation

$$-\nabla \cdot \left(\frac{\nabla\varphi}{1-|\varphi|^2} \right) + \frac{|\nabla\varphi|^2}{(1-|\varphi|^2)^2}\varphi - a|\varphi|^2\varphi + b\varphi = 0. \quad (1.0.2)$$

In [4; 7], we investigated the existence of square integrable radial positive solutions to (1.0.2). We proved that if $a - 2b \leq 0$ equation (1.0.2) has no non-trivial positive radial solution such that $\varphi(x) \rightarrow 0$ as $|x| \rightarrow +\infty$. If $a - 2b > 0$ we showed the existence of positive radial solutions with any given number of nodes and that go to 0 exponentially as $|x| \rightarrow +\infty$. Moreover, we observed that for a good choice of the parameters a and b the shape of the mesonic potentials inside and outside the atomic nucleus is well described by the solution of this effective model. This property has been mathematically justified in [15].

In [6], via a variational method, we showed the existence of solutions to (1.0.1) without any ansatz on the particular form of the particle wave function.

Finally, in [8], we studied the uniqueness and the non-degeneracy of positive solutions to (1.0.2). We proved that the nonlinear equation (1.0.2) has no nontrivial solution $0 < \varphi < 1$ in $L^2(\mathbb{R}^3)$ whenever $0 < a \leq 2b$. If $a > 2b > 0$, the nonlinear equation (1.0.2) has a unique solution $0 < \varphi < 1$ that tends to 0 at infinity, modulo translations and multiplication by a phase factor. Moreover, this solution is radial, decreasing and non-degenerate. The non-degeneracy property allowed us to rigorously justify the formal derivation of this model in the stationary case. Moreover, by means of a perturbation argument, we were able to construct starting from a solution to (1.0.2) a family of solutions to the equations of the underlying relativistic model.

In [15], we generalized the result of uniqueness and non-degeneracy to the positive radial solutions of a class of semilinear elliptic equations of the form $-\Delta u = g(u)$ in \mathbb{R}^d for any dimension $d \geq 2$. This property plays an important role in the study of the orbital stability of the associated evolution equation as we will see in Chapter 3.

The next step consists in analyzing, from an analytical and numerical point of view, the evolution equation (1). The main difficulty comes from the fact that the nonlinearity is present in the main order of the equation.

In [14], we started the analysis of equation (1) from a numerical point of view. We consider the model in spatial dimension 1 and we generalized it to any power nonlinearity. This gives

$$i\partial_t\phi = -\partial_x \left(\frac{\partial_x\phi}{1-|\phi|^{2\alpha}} \right) + \alpha|\phi|^{2\alpha-2} \frac{|\partial_x\phi|^2}{(1-|\phi|^{2\alpha})^2} \phi - a|\phi|^{2\alpha}\phi \quad (1.0.3)$$

with $\phi : \mathbb{R}_+ \times \mathbb{R} \rightarrow \mathbb{C}$ et $\alpha \in \mathbb{N}^*$. We proved the existence of a unique (modulo translations) positive solution for any $a > (\alpha + 1)b > 0$ and we observed numerically its stability.

List of publications: [5], [4], [6], [7], [8], [14], [15]

Chapter 3: Orbital stability in Hamiltonian PDEs with symmetry

In [16], we presented an introduction to the orbital stability of relative equilibria of Hamiltonian dynamical systems in finite and infinite dimensional Banach spaces. We suggested a convenient formulation of the theory of Hamiltonian dynamics with symmetry and of the corresponding momentum maps that allows us to highlight the interplay between (symplectic) geometry and (functional) analysis in the proofs of orbital stability of relative equilibria via the so-called *energy-momentum method*. The idea was to use the geometric intuition gained from the study of finite dynamical systems as a guide when dealing with the infinite dimensional ones that were the main focus of our interest, but that demand more sophisticated technical tools from functional analysis and PDE theory.

In simple terms, the energy-momentum method consists in seeing the relative equilibria of Hamiltonian systems with symmetries as constrained critical points of the Hamiltonian energy of the system. Using the theory of Lagrange multipliers, we can conclude that they are indeed critical points of the Lagrangian. Now, the basic intuition is that a relative equilibrium should be stable if it is not only a critical point, but a constrained local minimum of the Hamiltonian energy. For that it is then enough to prove that the Lagrangian is coercive on an appropriate space.

When the symmetry group is one-dimensional, the coercivity of the Lagrangian follows from what is usually called *Vakhitov-Kolokolov slope condition*. In [13], we generalized this condition to a higher dimensional setting. Moreover, we showed what we call the *persistence of relative equilibria*, *i.e.* the existence of a family of relative equilibria in a neighborhood of a given relative equilibrium.

List of publications: [16], [13].

Chapter 4: Schrödinger equation in nonlinear optics

The propagation of a wave packet in a nonlinear optical fiber is described by a general nonlinear Schrödinger equation of the form

$$i\frac{\partial u}{\partial z} - \frac{\beta_2(z)}{2} \frac{\partial^2 u}{\partial t^2} + \gamma(z)|u|^2u = 0 \quad (1.0.4)$$

where z and t are the spatial and time coordinates respectively, β_2 is a function that describes the group-velocity dispersion (GVD) and γ is a function that models the intensity of the nonlinear interaction.

The interplay between dispersion and nonlinearity can give rise to a physical phenomenon called *modulational instability* (MI). More precisely, the modulational instability refers to a process where a weak periodic perturbation of a solitary wave grows exponentially during the propagation.

In [9; 17], we consider optical fibers where the GVD is given by

$$\beta_2(z) = 1 + \beta_m \left(\sum_{n \in \mathbb{Z}} \delta(z/Z - n\Lambda) - 1 \right),$$

with δ the Dirac function and such that strength of the nonlinearity is constant equal to 1. This kind of fibers is called dispersion-kicked fibers. We provide a simple argument allowing to determine the central

frequencies of the unstable sidebands which remains true also for general periodically modulated fibers. Then, using Floquet theory, we compute analytically the width of the unstable bands as well as their maximum gain. These results are illustrated by some experimental investigations.

In [11; 18; 19], we investigated the nonlinear stage of modulational instability in the more general case of optical fibers with periodic dispersion. We used a truncation approach, the so-called *three-mode truncations* and suitable phase transformations and averaging. We highlighted the presence of breather-type solutions which divide the phase-plane into two types of dynamical recurrent behaviors.

List of publications: [9], [11], [17], [18], [19].

Chapter 5: Microscopic description of minimizers for Coulomb and Riesz gases

In [12], we considered a system of n points in the full space of dimension $d \geq 1$, interacting via repulsive interactions and confined by an external field or potential V . The interacting kernels taken into account are the Riesz kernel $|x|^{-s}$ with $\max(0, d-2) \leq s < d$ and the logarithmic kernel in dimension one and two. In particular, this includes the Coulomb interaction which corresponds to $s = d-2$ for $d \geq 3$ and to $-\log|x|$ in dimension $d = 2$. More precisely, the Hamiltonian is given by

$$H_n(x_1, \dots, x_n) = \sum_{i \neq j} g(x_i - x_j) + n \sum_{i=1}^n V(x_i) \quad (1.0.5)$$

where x_1, \dots, x_n are n points in \mathbb{R}^d and the interaction kernel is given by either

$$g(x) = \frac{1}{|x|^s} \quad \max(0, d-2) \leq s < d, \quad (1.0.6)$$

or

$$g(x) = -\log|x| \quad \text{in dimension } d = 1, \quad (1.0.7)$$

or

$$g(x) = -\log|x| \quad \text{in dimension } d = 2. \quad (1.0.8)$$

The goal was to understand the behavior of point configurations which minimize H_n when the number of points n tends to $+\infty$.

It is well-known that, if V is sufficiently smooth and grows fast enough at infinity, then the leading order of $\min H_n$ is given by

$$n^2 I(\mu_V) + o(n^2)$$

with μ_V a minimizer of

$$I(\mu) = \iint_{\mathbb{R}^d \times \mathbb{R}^d} g(x-y) d\mu(x) d\mu(y) + \int_{\mathbb{R}^d} V(x) d\mu(x)$$

among the probability measures on \mathbb{R}^d . The next order in the asymptotic expansion of $\min H_n$ is given by the so-called *renormalized energy* \mathcal{W} which can be seen as the interaction energy of an infinite configuration of points in the whole space in a constant neutralizing background. Corrections to this order govern the behavior of point configurations at the microscopic scale and the crystallization phenomenon, by selecting point configurations that minimize the renormalized energy \mathcal{W} . It is therefore important to be able to identify and characterize the minimizers of \mathcal{W} among all possible point configurations. This remains an open question in general.

It is known that for the one-dimensional log-gas the minimum is achieved by the perfect lattice \mathbb{Z} and, in the case of two-dimensional Coulomb and Riesz gases, it has been proved that Abrikosov's (triangular) lattice is the unique minimizer of \mathcal{W} among lattice configurations. This leads to conjecture that, in dimension 2, the Abrikosov lattice is a minimizer of \mathcal{W} among all possible point configurations for both the Coulomb and Riesz kernels. It therefore seems natural to ask whether the minimizers of \mathcal{W} are

periodic. If this is true, we can deduce that after blow-up at the microscopic scale the minimizers of H_n have a crystalline structure, which is expected to be true at least in small dimension.

Solving this conjecture seems very difficult at the moment. However, intermediate results can be obtained in this direction. In [10], we showed that for the Coulomb interaction kernel in dimension 2, the renormalized energy of a minimizer as well as the number of points are uniformly distributed. In [12], we generalized this rigidity result to Coulomb interactions in any dimension $d > 2$.

For Riesz interactions, we proved the same equidistribution result on the renormalized energy \mathcal{W} but with an additional assumption on the decay of the local energy. This is needed because Riesz kernels are non-local operator kernels and therefore a dimension extension is necessary for their study. The difficulty is therefore to have good estimates in this additional dimension.

List of publications: [10], [12].

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RELATIVISTIC QUANTUM DYNAMICS IN NUCLEAR PHYSICS

This chapter is based on the articles [Rot12b; ER12b; ER13b; LR13b; LR15b; KR20b; LR20a] and is devoted to the mathematical study of a relativistic model from nuclear physics. In the appendices, some results obtained for this particular model are generalized to semilinear elliptic PDEs of the form $-\Delta u = g(u)$ and applied for a detailed study of the double-power nonlinear Schrödinger equation which arises in several physical situations.

2.1. THE RELATIVISTIC MEAN-FIELD EQUATIONS OF THE ATOMIC NUCLEUS

At low energies, the nuclear structure is classically described by a quantum mechanical many-body problems of fermions interacting by a non-relativistic interaction which is understood to have its origin in the exchange of mesons between the bare nucleons (see [Rin96; RS80b]). If one to take into account relativity, then one has to propose a relativistic Lagrangian describing the point-interaction between the nuclei.

One of the possible alternatives is the so-called RMFT (*Relativistic Mean-Field theory*) which describes the nucleus as a system Dirac nucleons which interact via meson fields.

The relativistic mean-field model is formulated on the basis of two approximations, the mean-field and the no-sea approximation. On the one hand, thanks to the mean-field approximation, the fields for the mesons and the photons are treated as classical fields and the nucleons behave as noninteracting particles moving in these mean fields. In particular, the nucleon field operator can be expanded in single-particle states $\psi_k(x^\mu)$, while the densities become simple bilinear sums over ψ_k . The single-particle wave functions $\psi_k(x^\mu) \in \mathbb{C}^4$ have to satisfy the constraint $\int_{\mathbb{R}^3} \psi_k^*(t, x) \psi_\ell(t, x) d^3x = \delta_{k\ell}$. On the other hand, thanks to no-sea approximation negative energy states belonging to the Dirac sea are not considered and the vacuum polarization is neglected.

The relativistic mean-field theory is an effective theory: the Lagrangian of the model is an effective Lagrangian with respect to the mean-field and no-sea approximations. Since the effective Lagrangian is not derived rigorously from the no-approximation Lagrangian, the parameters of the model must be adjusted on experimental data. Therefore, the effects of vacuum polarization as well as the correlation effects are not completely neglected but they are taken into account implicitly through the adjustment of model parameters.

During recent years, the relativistic mean-field theory has received a wide attention due to its successful

description of many nuclear phenomena. It has been shown that the relativistic mean-field model describes successfully the structure of the nucleus and provides a natural explanation for some relativistic effects observed experimentally such as the spin-orbit force or the “saturation phenomenon” (see [Rei89; Rin96; MI88]). This is why the relativistic mean-field model can be viewed as the relativistic generalization of some non-relativistic models, such as the Hartree–Fock model with Skyrme or Gogny interaction, where the effective forces, which are not appropriate in a relativistic formulation, are replaced by average potentials representing independent degrees of freedom.

Although often used in practice, the models of nuclear physics have rarely been discussed in the mathematical community. Some non-relativistic models of nuclear physics (of Hartree–Fock type) have been studied by Gogny and Lions in an article in 1986 ([GL86]). To our knowledge, the paper [Rot12b] contains the first mathematical study of a model from relativistic nuclear physics.

For simplicity, in the RMFT model presented here, we take into account only the potentials created by the mesons σ and ω , defining a medium range attractive interaction and a short range repulsive interaction respectively. In particular, we neglect the meson ρ describing the effects depending on the isospin (contraction of *isotopic spin*), and we omit the photons which are related to the electromagnetic interaction (see [Rei89; GM97] for a physical description and [Rot12b] for a mathematical study of the more general model).

The Lagrangian density of this relativistic mean-field model, which is currently known as σ - ω model ([Wal74; Wal04]), can be written as

$$\mathcal{L} = \mathcal{L}_{nucleons} + \mathcal{L}_{mesons} + \mathcal{L}_{coupling}. \quad (2.1.1)$$

The free Lagrangian for the nucleons is

$$\mathcal{L}_{nucleons} = \sum_{k=1}^N \bar{\psi}_k (i\gamma^\mu \partial_\mu - m)\psi_k \quad (2.1.2)$$

where m denotes the nucleon mass, γ^μ are the Dirac matrices, $\bar{\psi}_k = \psi_k^* \gamma^0$ and N is the number of nucleons. Recall that

$$\gamma^0 = \beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}, \quad \gamma^k = \beta \alpha_k \quad \text{with} \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \quad (2.1.3)$$

for $k = 1, 2, 3$, and

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2.1.4)$$

the Pauli matrices.

The Lagrangian for the free meson fields is

$$\mathcal{L}_{mesons} = \frac{1}{2}(\partial^\mu \sigma \partial_\mu \sigma - m_\sigma^2 \sigma^2) - \frac{1}{2}(\overline{\partial^\mu \omega^\nu} \partial_\mu \omega_\nu - m_\omega^2 \omega^\mu \omega_\mu) \quad (2.1.5)$$

where σ and ω^μ describe respectively the σ and ω meson field. Moreover, an antisymmetrized derivative is defined via

$$\overline{\partial^\mu \omega^\nu} = \partial^\mu \omega^\nu - \partial^\nu \omega^\mu.$$

Finally, the Lagrangian for the coupling is

$$\mathcal{L}_{coupling} = -g_\sigma \sigma \rho_s - g_\omega \omega^\mu j_\mu - U(\sigma) \quad (2.1.6)$$

where $U(\sigma) = \frac{1}{3}b_2\sigma^3 + \frac{1}{4}b_3\sigma^4$ represents a nonlinear self-coupling of the σ meson. In what follows, we will assume $b_2 = b_3 = 0$. Here

$$\rho_s = \sum_{k=1}^N \bar{\psi}_k \psi_k \quad (2.1.7)$$

is a scalar density, while

$$j^\mu = \sum_{k=1}^N \bar{\psi}_k \gamma^\mu \psi_k \quad (2.1.8)$$

is the baryon current. Note that this four-current $j^\mu = (\rho_v, \mathbf{j})$ contains the usual three-current density \mathbf{j} and the usual density of the nucleons ρ_v . Similarly, we define $\omega^\mu = (\omega_0, \boldsymbol{\omega})$. The model contains as free parameters the meson masses m_σ and m_ω , as well as the coupling constants g_σ and g_ω . For the nucleon mass m the free value is usually employed.

Varying the action integral with respect to the wave functions and to the fields yields to a Dirac equation for each wave function ψ_k ,

$$i\partial_t \psi_k = \boldsymbol{\alpha} \cdot (-i\nabla - g_\omega \boldsymbol{\omega}) \psi_k + \beta(m + S) \psi_k + V \psi_k \quad (2.1.9)$$

with relativistic fields $S = g_\sigma \sigma$, $V = g_\omega \omega_0$ and $\boldsymbol{\omega}$ which satisfies (after using the Lorentz gauge for the vector meson $\boldsymbol{\omega}$) the following Klein-Gordon equations

$$(\partial_t^2 - \Delta + m_\sigma^2) S = -g_\sigma^2 \rho_s \quad (2.1.10)$$

$$(\partial_t^2 - \Delta + m_\omega^2) V = g_\omega^2 \rho_v \quad (2.1.11)$$

$$(\partial_t^2 - \Delta + m_\omega^2) \boldsymbol{\omega} = g_\omega \mathbf{j}. \quad (2.1.12)$$

Most applications of the relativistic mean-field model are concerned with the static case. In this static approximation, one can assume that the meson fields are time-independent and each single-particle wave function can be written as

$$\psi_k(t, x) = e^{-i\varepsilon_k t} \psi_k(x) \quad (2.1.13)$$

where the ε_k are the single-particle energies and $\varepsilon_k > 0$. Moreover, time reversal symmetry implies that the space-like components of the current j^μ , *i.e.* $\mathbf{j} = (j_1, j_2, j_3)$, vanish. As a consequence, the stationary equations of the relativistic mean-field model are

$$\begin{aligned} \varepsilon_k \psi_k &= -i\boldsymbol{\alpha} \cdot \nabla \psi_k + \beta(m + S) \psi_k + V \psi_k \\ (-\Delta + m_\sigma^2) S &= -g_\sigma^2 \rho_s \\ (-\Delta + m_\omega^2) V &= g_\omega^2 \rho_v \end{aligned} \quad (2.1.14)$$

with $k = 1, \dots, N$, $\rho_s = \sum_{k=1}^N \psi_k^* \beta \psi_k$ and $\rho_v = \sum_{k=1}^N \psi_k^* \psi_k$.

Note that the fields S and V are respectively focusing and defocusing, which can be seen from the different signs in the two Klein-Gordon equations.

2.2. RESULTS ON THE RELATIVISTIC MEAN-FIELD MODEL

In the paper [Rot12b], the existence of solutions to (2.1.14) is discussed in a weakly relativistic regime and in a more general setting. More precisely, we consider a minimization problem with constraints that involve negative spectral projectors and we apply a concentration-compactness argument to prove the existence of minimizers for this problem. Then, we show that a minimizer is a solution of the relativistic mean-field equations (2.1.14) at least in a weakly relativistic regime. The results of this paper are presented here in the simplest case where only σ and ω mesons are considered.

First of all, we remark that the Klein-Gordon equations for the fields S and V can be solved explicitly. In particular, we have

$$S = -\frac{g_\sigma^2}{4\pi} \left(\frac{e^{-m_\sigma |\cdot|}}{|\cdot|} \star \rho_s \right), \quad (2.2.1)$$

$$V = \frac{g_\omega^2}{4\pi} \left(\frac{e^{-m_\omega |\cdot|}}{|\cdot|} \star \rho_v \right) \quad (2.2.2)$$

Hence, equation (2.1.14) becomes

$$\varepsilon_k \psi_k = \left[H_0 - \beta \frac{g_\sigma^2}{4\pi} \left(\frac{e^{-m_\sigma |\cdot|}}{|\cdot|} \star \rho_s \right) + \frac{g_\omega^2}{4\pi} \left(\frac{e^{-m_\omega |\cdot|}}{|\cdot|} \star \rho_v \right) \right] \psi_k \quad (2.2.3)$$

for $k = 1, \dots, N$ and where $H_0 = -i\alpha \cdot \nabla + \beta m$ is the free Dirac operator.

The operator H_0 acts on 4-spinors, i.e. functions $\psi \in \mathcal{H} := L^2(\mathbb{R}^3, \mathbb{C}^4)$. It is self-adjoint on \mathcal{H} , with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$ and form-domain $E := H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. Moreover, it is defined to ensure

$$H_0^2 = -\Delta + m^2$$

The spectrum of H_0 is $(-\infty, -m] \cup [m, +\infty)$, and the projector associated with the negative (resp. positive) part of the spectrum of H_0 will be denoted by Λ^- (resp. Λ^+). Finally, we endow the space E with the norm $\|\psi\|_E^2 := (\psi, |H_0| \psi)_{L^2}$.

The nonlinear Dirac equation (2.2.3) can be written as

$$H_\Psi \psi_k = \varepsilon_k \psi_k$$

with $H_\Psi = H_0 + V_\Psi$ and V_Ψ defined as

$$V_\Psi = -\beta \frac{g_\sigma^2}{4\pi} \left(\frac{e^{-m_\sigma |\cdot|}}{|\cdot|} \star \rho_s \right) + \frac{g_\omega^2}{4\pi} \left(\frac{e^{-m_\omega |\cdot|}}{|\cdot|} \star \rho_v \right). \quad (2.2.4)$$

The scalars ε_k can be seen as Lagrange multipliers; indeed, the nonlinear Dirac equations are the Euler-Lagrange equations of the energy functional

$$\begin{aligned} \mathcal{E}(\Psi) &= \sum_{j=1}^A \int_{\mathbb{R}^3} \psi_j^* H_0 \psi_j - \frac{g_\sigma^2}{8\pi} \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_s(x) \rho_s(y)}{|x-y|} e^{-m_\sigma |x-y|} dx dy \\ &\quad + \frac{g_\omega^2}{8\pi} \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_v(x) \rho_v(y)}{|x-y|} e^{-m_\omega |x-y|} dx dy \end{aligned} \quad (2.2.5)$$

under the constraints $\int_{\mathbb{R}^3} \psi_i^* \psi_j = \delta_{ij}$ for $1 \leq i, j \leq N$. Here we can suppose that the matrix of Lagrange multipliers is diagonal because of the fact that $\mathcal{E}(\Psi)$ is invariant under unitary transformations. In the energy functional, we remark that only the σ meson provides an attractive interaction. Indeed, if f is a real function,

$$\int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(x) f(y)}{|x-y|} e^{-\lambda |x-y|} dx dy = C \int_{\mathbb{R}^3} |\hat{f}(k)|^2 \frac{1}{k^2 + \lambda^2} dk$$

with C a positive constant and \hat{f} the Fourier transform of f . As a consequence, the term

$$-\frac{g_\sigma^2}{8\pi} \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_s(x) \rho_s(y)}{|x-y|} e^{-m_\sigma |x-y|} dx dy$$

is negative and describes an attractive interaction.

Since the functional (2.2.5) is not bounded from below under the constraints $\int_{\mathbb{R}^3} \psi_i^* \psi_j = \delta_{ij}$, as in [ES01] (see also [ELS08]), we introduce the following minimization problem

$$I = \inf \left\{ \mathcal{E}(\Psi); \Psi \in (H^{1/2})^N, \int_{\mathbb{R}^3} \psi_i^* \psi_j = \delta_{ij}, 1 \leq i, j \leq N, \Lambda_\Psi^- \Psi = 0 \right\} \quad (2.2.6)$$

together with its extension

$$I(\lambda_1, \dots, \lambda_N) = \inf \left\{ \mathcal{E}(\Psi); \Psi \in (H^{1/2})^N, \int_{\mathbb{R}^3} \psi_i^* \psi_j = \lambda_i \delta_{ij}, 1 \leq i, j \leq N, \Lambda_\Psi^- \Psi = 0 \right\} \quad (2.2.7)$$

where $\Lambda_{\Psi}^{-} = \chi_{(-\infty, 0)}(H_{\Psi})$ is the negative spectral projector of the operator H_{Ψ} and

$$\Lambda_{\Psi}^{-}\Psi = (\Lambda_{p, \Psi}^{-}\psi_1, \dots, \Lambda_{p, \Psi}^{-}\psi_N).$$

The idea of using a constraint of the form $\Lambda_{\Psi}^{-}\Psi = 0$ is due to M.J. Esteban and E. Séré in the case of the Dirac-Fock equations (see [ELS08]). This constraint has a physical meaning; more precisely, if we neglect the vacuum polarization, the Dirac sea is represented by the negative spectral projector Λ_{Ψ}^{-} . Indeed, according to Dirac's original ideas, the vacuum is composed of infinitely many particles, which completely fill up the negative spectral subspace of H_{Ψ} : these particles form the Dirac sea. So, by Pauli exclusion principle, the single-particle energies ε_k should be strictly positive and, as a consequence, Ψ should be in the positive spectral subspace of H_{Ψ} . On the one hand, the use of the constraint $\Lambda_{\Psi}^{-}\Psi = 0$ is very helpful since it transforms a strongly indefinite problem into a minimization problem; on the other hand, dealing with this constraint is the main difficulty of the proof of our results.

In [Rot12b], we prove that, for g_{σ} and g_{ω} sufficiently small, a solution of the equations (2.2.3) can be obtained as a solution of the minimization problem (2.2.6).

Theorem 2.2.1. *If g_{σ} and g_{ω} are sufficiently small, a minimizer of (2.2.6) is a solution of the equations (2.2.3).*

Moreover, the application of the concentration-compactness method ([Lio85a], [Lio85b]) to the minimization problem (2.2.6) yields the following theorem which is the main result of [Rot12b].

Theorem 2.2.2. *If g_{σ} and g_{ω} are sufficiently small, any minimizing sequence of (2.2.6) is relatively compact up to a translation if and only if the following condition holds*

$$I < I(\lambda_1, \dots, \lambda_N) + I(1 - \lambda_1, \dots, 1 - \lambda_N) \quad (2.2.8)$$

for all $\lambda_k \in [0, 1]$, $k = 1, \dots, N$, such that $\sum_{k=1}^A \lambda_k \in (0, N)$.

In particular, if (2.2.8) holds, there exists a minimum of (2.2.6).

This result is relevant both from mathematical and physical point of view since it provides a condition that ensures the existence of a ground state solution of the equations (2.2.3). Furthermore, this is the first result relating the existence of critical points of a strongly indefinite energy functional to strict concentration-compactness inequalities.

The condition g_{σ} and g_{ω} sufficiently small means that we are in a weakly relativistic regime. In our proof of Theorems 2.2.1 and 2.2.2, this condition is required for several reasons. First of all, if g_{σ} and g_{ω} are sufficiently small, we can show that H_{Ψ} is a self-adjoint isomorphism between $H^{1/2}$ and its dual $H^{-1/2}$, whose inverse is bounded independently of Ψ . Moreover, we need this condition to prove that a minimizing sequence of (2.2.6) is bounded in $(H^{1/2}(\mathbb{R}^3))^N$. We remark that the estimates on g_{σ} and g_{ω} are explicit up to this point. Finally, in both theorems, we have to apply the implicit function theorem with g_{σ} and g_{ω} as parameters.

This result is different from that obtained by Esteban–Séré on the Dirac–Fock equations (see [ES01], [ES99]). In [ES99], by a more sophisticated variational method, Esteban–Séré found an infinite sequence of solutions of the Dirac-Fock equations and, in [ES01], they showed that, in a weakly relativistic regime, the “first” solution of the Dirac–Fock equations found in [ES99] can be viewed as an electronic ground state in the sense that it minimizes the Dirac–Fock energy among all electronic configurations which are orthogonal to the Dirac sea. Their variational method takes advantage of the fact that the Dirac–Fock energy functional is not translation invariant: it contains an attractive interaction term, due to the nucleus, which confines the electrons. The nonlinear interaction is rather purely repulsive so that the use of concentration-compactness is not necessary. On the contrary, the energy functional that we consider is invariant under translations and one of the nonlinear interaction terms is attractive; because of the translation invariance, we are naturally led to use the concentration-compactness argument.

The main difficulty in the application of the concentration-compactness argument to the minimization problem (2.2.6) is to deal with the nonlinear constraint $\Lambda_{\Psi}^{-}\Psi = 0$. As usual, to conclude to compactness up to translation of minimizing sequences $\{\Psi^n\}_n$, one has to rule out the vanishing and the dichotomy cases.

Roughly speaking if dichotomy occurs then Ψ^n can be split into two parts $\Psi_1^n = (\psi_{1,1}^n, \dots, \psi_{N,1}^n)$ and $\Psi_2^n = (\psi_{1,1}^n, \dots, \psi_{N,1}^n)$ such that

$$\begin{cases} \text{dist}(\text{supp}\psi_{k,1}^n, \text{supp}\psi_{k,2}^n) > 0 \\ \|\psi_k^n - (\psi_{k,1}^n + \psi_{k,2}^n)\|_{L^p} \xrightarrow[n]{} 0 & \text{for } 2 \leq p < 3 \\ \|\psi_k^n - (\psi_{k,1}^n + \psi_{k,2}^n)\|_{H^{1/2}} \xrightarrow[n]{} 0 \\ \int_{\mathbb{R}^3} \psi_{i,1}^n * \psi_{j,1}^n = \lambda_i \delta_{ij}, & 1 \leq i, j \leq N \\ \int_{\mathbb{R}^3} \psi_{i,1}^n * \psi_{j,1}^n = (1 - \lambda_i) \delta_{ij} & 1 \leq i, j \leq N \end{cases}$$

However, Ψ_1^n and Ψ_2^n do not necessarily satisfy the constraints of $I(\lambda_1, \dots, \lambda_N)$ and $I(1 - \lambda_1, \dots, 1 - \lambda_N)$ respectively. Then, one has to prove that Ψ_1^n and Ψ_2^n “almost” satisfy the spectral constraint, *i.e.* prove that

$$\begin{cases} \Lambda_{\Psi_1^n}^{-} \Psi_1^n \xrightarrow[n]{} 0 & \text{in } (H^{1/2}(\mathbb{R}^3))^N \\ \Lambda_{\Psi_2^n}^{-} \Psi_2^n \xrightarrow[n]{} 0 & \text{in } (H^{1/2}(\mathbb{R}^3))^N \end{cases}$$

and then, using the implicit function theorem, construct Φ_1^n and Φ_2^n small perturbations of Ψ_1^n and Ψ_2^n in $(H^{1/2}(\mathbb{R}^3))^N$ which satisfies the constraints of $I(\lambda_1, \dots, \lambda_N)$ and $I(1 - \lambda_1, \dots, 1 - \lambda_N)$ respectively.

As a conclusion, thanks to the continuity of \mathcal{E} in $H^{1/2}(\mathbb{R}^3)$, we obtain

$$\begin{aligned} I &= \lim_{n \rightarrow \infty} \mathcal{E}(\Psi^n) \geq \underline{\lim}_{n \rightarrow \infty} \mathcal{E}(\Psi_1^n) + \underline{\lim}_{n \rightarrow \infty} \mathcal{E}(\Psi_2^n) \\ &= \underline{\lim}_{n \rightarrow \infty} \mathcal{E}(\Phi_1^n) + \underline{\lim}_{n \rightarrow \infty} \mathcal{E}(\Phi_2^n) \\ &\geq I(\lambda_1, \dots, \lambda_N) + I(1 - \lambda_1, \dots, 1 - \lambda_N) \end{aligned}$$

that clearly contradicts (2.2.8). We remind that the first inequality is obtained by using the properties of localization of $\Psi_1^k, \Psi_2^k, \nabla \Psi_1^k$ and $\nabla \Psi_2^k$.

The vanishing case is ruled out as usual, by using the fact that if vanishing occurs then $\psi_1^n, \dots, \psi_N^n$ converge strongly to 0 in $L^p(\mathbb{R}^3)$ for $2 < p < 3$.

Hence, the application of the concentration-compactness lemma and the remark that the problem is translation invariant, implies that there exists a sequence $y^n \in \mathbb{R}^3$ such that the sequence $\tilde{\Psi}^n = \Psi^n(\cdot + y^n)$ is a minimizing sequence that converges strongly in $(L^p(\mathbb{R}^3))^N$ for $2 \leq p < 3$ and weakly in $(H^{1/2}(\mathbb{R}^3))^N$. As a consequence its limit $\tilde{\Psi}$ satisfies the constraints of the minimization problem (2.2.6) and is such that

$$\mathcal{E}(\tilde{\Psi}) \leq \liminf_{n \rightarrow +\infty} \mathcal{E}(\tilde{\Psi}^n).$$

As a conclusion, $\tilde{\Psi}$ is a minimizer of (2.2.6) and the minimizing sequence Ψ^n is relatively compact in $(H^{1/2})^A$ up to a translation.

The proof of Theorem 2.2.1 is done by contradiction. Indeed, we show that if $\tilde{\Psi}$, a minimizer of (2.2.6), is not a solution of (2.2.3), we can construct a test function which satisfies the constraints of the minimization problem and has smaller energy.

2.3. AN EFFECTIVE NUCLEAR NONLINEAR SCHRÖDINGER EQUATION

The relativistic mean-field model has some conceptual advantages compared to non-relativistic models such as the Hartree-Fock model with Skyrme or Gogny interaction. In particular, it includes the spin

properties in a natural way and it distinguishes two fields in the nucleus, a large attractive scalar field S and a large repulsive vector field V . The difference in structure of these two fields leads to a purely relativistic saturation effect, which corresponds to a strongly density dependent repulsion at small distances (see [Rin96]).

Nevertheless, the mathematical study of this model is quite complicated and the results described in the previous section are interesting but not completely satisfactory. The idea is then to derive a new effective model as a specific non-relativistic limit of the relativistic mean-field model that takes into account the relativistic effects described above.

In the case of one nucleon ($N = 1$), the equation of this effective model is given by

$$\begin{cases} i\partial_t\psi = -\boldsymbol{\sigma} \cdot \nabla \left(\frac{\boldsymbol{\sigma} \cdot \nabla\psi}{1 - |\psi|^2} \right) + \frac{|\boldsymbol{\sigma} \cdot \nabla\psi|^2}{(1 - |\psi|^2)^2}\psi - a|\psi|^2\psi \\ \psi(0, x) = \psi(x) \end{cases} \quad (2.3.1)$$

with ψ a time-dependent 2-spinor and a a strictly positive constant.

The corresponding stationary equation is given by

$$-\boldsymbol{\sigma} \cdot \nabla \left(\frac{\boldsymbol{\sigma} \cdot \nabla\psi}{1 - |\psi|^2} \right) + \frac{|\boldsymbol{\sigma} \cdot \nabla\psi|^2}{(1 - |\psi|^2)^2}\psi - a|\psi|^2\psi + b\psi = 0 \quad (2.3.2)$$

with $b > 0$. In this equation spin is taken into account since ψ takes values in \mathbb{C}^2 . In what follows, we refer to this equation as *nuclear nonlinear Schrödinger equation with spin*.

Under the additional hypothesis that the state of a nucleon is an eigenfunction of the spin operator, the equation can be restricted to function of the special form

$$\psi(x) = \varphi(x) \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

leading to the equation

$$-\nabla \cdot \left(\frac{\nabla\varphi}{1 - |\varphi|^2} \right) + \frac{|\nabla\varphi|^2}{(1 - |\varphi|^2)^2}\varphi - a|\varphi|^2\varphi + b\varphi = 0 \quad (2.3.3)$$

that can be study in \mathbb{R}^d for any space dimension $d \geq 1$.

2.3.1. DERIVATION OF THE EFFECTIVE NUCLEAR NONLINEAR SCHRÖDINGER EQUATION

In this subsection, we present the formal derivation of the equation (2.3.1) as the non-relativistic limit of the relativistic mean-field model described above. This formal argument was first presented in the stationary case in [ER12b] and made rigorous in [LR15b].

Consider the relativistic mean-field model described by the following system of equations

$$\begin{cases} i\partial_t\Psi = \boldsymbol{\alpha} \cdot (-i\nabla - \boldsymbol{\omega})\Psi + \beta(m + S)\Psi + V\Psi \\ (\partial_t^2 - \Delta + m_\sigma^2)S = -g_\sigma^2\Psi^*\beta\Psi \\ (\partial_t^2 - \Delta + m_\omega^2)V = g_\omega^2|\Psi|^2 \\ (\partial_t^2 - \Delta + m_\omega^2)\boldsymbol{\omega} = g_\omega^2\Psi^*\boldsymbol{\alpha}\Psi \end{cases} \quad (2.3.4)$$

In our units, the non-relativistic limit corresponds to $m, m_\sigma, m_\omega \rightarrow \infty$ with all masses being on the same order. On the contrary to atomic physics, in nuclear physics the coupling constants g_σ and g_ω are very large, comparable to the masses. It is therefore customary to work in a regime where g_σ/m_σ and g_ω/m_ω are fixed or, even, large.

When the sources are large, retardation effects can be neglected, *i.e.* the fields S and V are time-independent, and the classical three-vector field $\boldsymbol{\omega}$ can be taken equal to 0 (see [SW86; Rin96]). Moreover, in the Klein-Gordon equations for S and V , the Laplacian can also be neglected in such way that

$$S \simeq -\frac{g_\sigma^2}{m_\sigma^2} \Psi^* \beta \Psi \text{ and } V \simeq \frac{g_\omega^2}{m_\omega^2} |\Psi|^2.$$

This leads to the following nonlinear Dirac equation

$$i\partial_t \Psi = (-i\boldsymbol{\alpha} \cdot \nabla + \beta m) \Psi - \kappa_1 \langle \beta \Psi, \Psi \rangle \beta \Psi + \kappa_2 |\Psi|^2 \Psi \quad (2.3.5)$$

with $\kappa_1 = \frac{g_\sigma^2}{m_\sigma^2}$ and $\kappa_2 = \frac{g_\omega^2}{m_\omega^2}$. Note that the nonlinearity coming from the field S is focusing while the one from the field V is defocusing.

For the σ - ω model, the interesting regime is when the parameters κ_1 and κ_2 behave like m , whereas $\kappa_1 - \kappa_2$ stays bounded. More precisely, let $\kappa_1 = \theta m$ and $\kappa_1 - \kappa_2 = \lambda$ with θ and λ positive constants. As a consequence, the nonlinear Dirac equation (2.3.5) can be written as

$$\begin{cases} i\partial_t \phi = -i\boldsymbol{\sigma} \cdot \nabla \zeta + m\phi - \theta m(|\phi|^2 - |\zeta|^2)\phi + (\theta m - \lambda)(|\phi|^2 + |\zeta|^2)\phi \\ i\partial_t \zeta = -i\boldsymbol{\sigma} \cdot \nabla \phi - m\zeta + \theta m(|\phi|^2 - |\zeta|^2)\zeta + (\theta m - \lambda)(|\phi|^2 + |\zeta|^2)\zeta \end{cases} \quad (2.3.6)$$

where we decompose the 4-spinor Ψ in upper and lower 2-spinors ϕ and ζ , *i.e.* $\Psi = (\phi, \zeta)$.

Hence, by writing

$$\tilde{\psi}(t, x) = e^{imt} \phi(t, x) \text{ and } \tilde{\chi}(t, x) = e^{imt} \zeta(t, x),$$

we obtain

$$\begin{cases} i\partial_t \tilde{\psi} = -i\boldsymbol{\sigma} \cdot \nabla \tilde{\chi} - \lambda |\tilde{\psi}|^2 \tilde{\psi} + 2\theta m |\tilde{\chi}|^2 \tilde{\psi} - \lambda |\tilde{\chi}|^2 \tilde{\psi} \\ i\partial_t \tilde{\chi} = -i\boldsymbol{\sigma} \cdot \nabla \tilde{\psi} - 2m \tilde{\chi} + 2\theta m |\tilde{\psi}|^2 \tilde{\chi} - \lambda |\tilde{\psi}|^2 \tilde{\chi} - \lambda |\tilde{\chi}|^2 \tilde{\chi} \end{cases}$$

As usual, in the non-relativistic regime, the lower spinor $\tilde{\chi}$ is of order $1/\sqrt{m}$. Hence, we have to perform the following change of scale

$$\tilde{\psi}(t, x) = \frac{1}{\sqrt{\theta}} \psi \left(\frac{t}{2}, \sqrt{m}x \right) \text{ and } \tilde{\chi}(t, x) = \frac{1}{2\sqrt{\theta}} \frac{1}{\sqrt{m}} \chi \left(\frac{t}{2}, \sqrt{m}x \right)$$

which leads to

$$\begin{cases} i\partial_t \psi = -i\boldsymbol{\sigma} \cdot \nabla \chi - a|\psi|^2 \psi + |\chi|^2 \psi - \frac{1}{m} \frac{a}{4} |\chi|^2 \psi \\ \frac{1}{m} \frac{1}{4} i\partial_t \chi = -i\boldsymbol{\sigma} \cdot \nabla \psi - \chi + |\psi|^2 \chi - \frac{1}{m} \frac{a}{4} |\psi|^2 \chi - \frac{1}{m^2} \frac{a}{16} |\chi|^2 \chi \end{cases}$$

with $a = \frac{2\lambda}{\theta}$. Finally, denoting $\varepsilon = \frac{1}{m}$ the perturbative parameter, we obtain

$$\begin{cases} i\partial_t \psi + i\boldsymbol{\sigma} \cdot \nabla \chi - |\chi|^2 \psi + a|\psi|^2 \psi + \varepsilon \frac{a}{4} |\chi|^2 \psi = 0 \\ i\boldsymbol{\sigma} \cdot \nabla \psi + (1 - |\psi|^2) \chi + \varepsilon \frac{1}{4} i\partial_t \chi + \varepsilon \frac{a}{4} |\psi|^2 \chi + \varepsilon^2 \frac{a}{16} |\chi|^2 \chi = 0 \end{cases} \quad (2.3.7)$$

In particular, when $\varepsilon = 0$, we have

$$\begin{cases} i\partial_t \psi = -i\boldsymbol{\sigma} \cdot \nabla \chi + |\chi|^2 \psi - a|\psi|^2 \psi \\ i\boldsymbol{\sigma} \cdot \nabla \psi + (1 - |\psi|^2) \chi = 0 \end{cases} \quad (2.3.8)$$

which leads at least formally to the time-dependent quasilinear Schrödinger type equation

$$\begin{cases} i\partial_t \psi = -\boldsymbol{\sigma} \cdot \nabla \left(\frac{\boldsymbol{\sigma} \cdot \nabla \psi}{1 - |\psi|^2} \right) + \frac{|\boldsymbol{\sigma} \cdot \nabla \psi|^2}{(1 - |\psi|^2)^2} \psi - a|\psi|^2 \psi \\ \psi(0, x) = \psi_0(x) \end{cases} \quad (2.3.9)$$

We remark that in the static approximation, the system (2.3.4) reduces to

$$\begin{cases} (m - \mu)\Psi = -i\boldsymbol{\alpha} \cdot \nabla\Psi + \beta(m + S)\Psi + V\Psi \\ (-\Delta + m_\sigma^2)S = -g_\sigma^2\Psi^*\beta\Psi \\ (-\Delta + m_\omega^2)V = g_\omega^2|\Psi|^2 \end{cases} \quad (2.3.10)$$

and the non-relativistic limit is given by

$$-\boldsymbol{\sigma} \cdot \nabla \left(\frac{\boldsymbol{\sigma} \cdot \nabla \psi}{1 - |\psi|^2} \right) + \frac{|\boldsymbol{\sigma} \cdot \nabla \psi|^2}{(1 - |\psi|^2)^2} \psi - a|\psi|^2\psi + b\psi = 0$$

with $b = 2\mu$. Note that this equation can be recovered from (2.3.9) by taking $\psi(t, x) = e^{ibt}\psi(x)$.

2.3.2. EXISTENCE OF SOLUTIONS FOR THE NUCLEAR SCHRÖDINGER EQUATION WITH SPIN

In [ER12b; LR13b; ER13b], we prove the existence of solutions to the equation (2.3.2). More precisely, in [ER12b] and [LR13b], we look for spherically symmetric solutions and we prove the existence of infinitely many solutions for a large class of value of a and b . In [ER13b], we consider a variational problem related to (2.3.2) for which we prove the existence of minimizers for a large class of values of the parameter a . This proves the existence of solutions to (2.3.2) without considering any particular ansatz for the nucleon's wave function.

Spherically symmetric solutions

First of all, as we have seen in the formal derivation described above, we remark that equation (2.3.2) is a equivalent to the system

$$\begin{cases} i\boldsymbol{\sigma} \cdot \nabla \chi + |\chi|^2\psi - a|\psi|^2\psi + b\psi = 0, \\ -i\boldsymbol{\sigma} \cdot \nabla \psi + (1 - |\psi|^2)\chi = 0. \end{cases} \quad (2.3.11)$$

In [ER12b; LR13b], we look for square integrable solutions to (2.3.11) which are spherically symmetric, *i.e.* which can be written in the particular form

$$\begin{pmatrix} \psi(x) \\ \chi(x) \end{pmatrix} = \begin{pmatrix} g(r) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ if(r) \begin{pmatrix} \cos \vartheta \\ \sin \vartheta e^{i\phi} \end{pmatrix} \end{pmatrix}, \quad (2.3.12)$$

where f and g are real valued radial functions and (r, ϑ, ϕ) are the spherical coordinates of x . This ansatz corresponds to particles with minimal angular momentum, that is, $j = 1/2$ (for instance, see [Tha04]). The equations for f and g read as follows:

$$\begin{cases} f' + \frac{2}{r}f = g(f^2 - ag^2 + b), \\ g' = f(1 - g^2). \end{cases} \quad (2.3.13)$$

In order to avoid singularities at the origin, we assume $f(0) = 0$, and, since we are interested in square integrable solutions, we look for solutions to (2.3.13) which fulfill

$$(f(r), g(r)) \longrightarrow (0, 0) \text{ as } r \longrightarrow +\infty. \quad (2.3.14)$$

One can easily show that for any given value of $g(0) = x$, there is a local solution to (2.3.13). The main difficulty is to show that this solution is globally defined and is such that (2.3.14) is satisfied.

In [ER12b], we proved the existence of ground state solutions to (2.3.13), *i.e.* nontrivial solutions to (2.3.13) which are square integrable and do not change sign.

Theorem 2.3.1 (Existence of spherically symmetric ground states). *Given $a, b > 0$ such that $a - 2b > 0$, there exists a solution $(f, g) \in \mathcal{C}^1([0, +\infty), \mathbb{R}^2)$ of the system (2.3.13) such that $f(0) = 0$, and there exists a constant C such that for $r > 0$*

$$0 < -f(r), g(r) \leq C \exp(-K_{a,b}r),$$

with $K_{a,b} = \min \left\{ \frac{b}{2}, \frac{2a-b}{2a} \right\}$.

In [LR13b], we generalized this result by showing the existence of solutions with any given number of nodes.

Theorem 2.3.2 (Existence of spherically symmetric excited states). *Let $a, b > 0$ such that $a - 2b > 0$. There exists an increasing sequence $\{x_k\}_{k \geq 0}$ in $(0, 1)$ with the following properties. For every $k \geq 0$,*

1. *the solution (f_{x_k}, g_{x_k}) of (2.3.13) is a global solution;*
2. *both f_{x_k} and g_{x_k} have exactly k zeros on $(0, +\infty)$;*
3. *(f_{x_k}, g_{x_k}) converges exponentially to $(0, 0)$ as $r \rightarrow +\infty$.*

Here we denote by (f_x, g_x) a solution to (2.3.13) such that $f_x(0) = 0$ and $g_x(0) = x$.

Note that the condition $a - 2b > 0$ is necessary for the existence of square integrable solutions. Indeed, in [ER12b], we proved the following proposition.

Proposition 2.3.3. *There is no nontrivial solution of (2.3.13) such that (2.3.14) is satisfied, unless $a - 2b > 0$. Moreover, for all the solutions of (2.3.13) satisfying (2.3.14), we have $g^2(r) < 1$ in $[0, +\infty)$. So, in particular, $g(0)$ must be chosen such that $g(0)^2 < 1$.*

Proposition 2.3.3 gives also a constraint on the initial value of g that has to be chosen in $(-1, 1)$. Moreover, we can remark that if (f_x, g_x) is a solution to (2.3.13), then $(-f_x, -g_x)$ is equal to (f_{-x}, g_{-x}) so that we can restrict the set of initial values for g at $(0, 1)$.

Theorem 2.3.1 and its proof have the same flavor as the main results and proof [CV86]. In that paper, Cazenave and Vazquez study solutions of the so-called Soler model, which consists in a nonlinear Dirac equation. They also consider solutions separable in spherical coordinates, with the same angular momentum constraint as we do, and they use a shooting method to solve the associated problem of ordinary differential equations. The main difference between their methods of proof and ours are related to the fact that, as we have seen above, in our case there is a boundedness constraint for the initial value of g . This creates additional difficulties and another strategy is necessary for the proof. More details will be given later in subsection 2.3.3.

Theorem 2.3.2 is similar to the result obtained by Balabane, Cazenave, Douady and Merle ([Bal+88]) for a nonlinear Dirac equation and, as for the ground states, the proof is based on a shooting method inspired by the one used by Balabane, Dolbeault and Ounaies ([BDO03]). As for the ground states, the first difficulty to deal with is that, to obtain a localized solution, the initial condition x must be chosen in $(0, 1)$. Second, we are looking for solutions such that each component has exactly k zeros on $(0, +\infty)$, which means, intuitively, that we have to show the existence of a solution (f_x, g_x) whose trajectory in the phase portrait winds around $(0, 0)$.

Usually in a shooting method, the localized solution with k nodes is obtained taking the solution whose initial data x is the supremum of a well-chosen open subset of $\{x : g_x \text{ has } k \text{ zeros}\}$. Hence, the main difficulty of our shooting method is to prove that for any $k \in \mathbb{N}$, there exists $\epsilon > 0$ such that

$$\{x \in (0, 1) : g_x \text{ has } k \text{ zeros}\} \subset (0, 1 - \epsilon).$$

To do this, we have to give some accurate estimates on the behavior of the solution when the initial condition x becomes close to 1. The presence of four rest points $(\pm\sqrt{a-b}, \pm 1)$ in the Hamiltonian system

$$\begin{cases} f' = g(f^2 - ag^2 + b) \\ g' = f(1 - g^2) \end{cases}, \quad (2.3.15)$$

associated with the system (2.3.13), makes this study difficult.

To have a control on the solutions (f_x, g_x) , we would like to use the continuity of the flow and compare (f_x, g_x) to (f_1, g_1) whenever x is close enough to 1. The problem is that (f_1, g_1) converges to the rest point $(-\sqrt{a-b}, 1)$ of the system (2.3.15). Thus, (f_x, g_x) stay in a neighborhood of $(-\sqrt{a-b}, 1)$ a very long time if x is sufficiently close to 1. Since (f_1, g_1) does not wind around $(0, 0)$, it is hopeless to get estimates on the speed of rotations of (f_x, g_x) around $(0, 0)$ as in [BDO03]. Hence, we have to introduce another strategy to prove that (f_x, g_x) winds around $(0, 0)$.

First of all, we prove that (f_x, g_x) exits the neighborhoods of $(-\sqrt{a-b}, 1)$ at finite time, possibly very large. Next, we control (f_x, g_x) using again the continuity of the flow by comparing (f_x, g_x) to a solution (f, g) of the Hamiltonian system (2.3.15) which satisfies

$$\lim_{t \rightarrow -\infty} (f, g) = (-\sqrt{a-b}, 1) \text{ and } \lim_{t \rightarrow +\infty} (f, g) = (-\sqrt{a-b}, -1).$$

Iterating this argument, we can show that the trajectory of (f_x, g_x) winds around $(0, 0)$ whenever x is close enough to 1.

The main difficulty is to control the behavior of (f_x, g_x) when its trajectory is close to one of the rest points $(\pm\sqrt{a-b}, \pm 1)$. To do this, we introduce the so-called *Hamiltonian regularization*. More precisely, we replace the system (2.3.13) by the Hamiltonian ones (2.3.15) in a neighborhood of the points $(\pm\sqrt{a-b}, \pm 1)$. Then, we can use the qualitative properties of the solutions of the Hamiltonian system (2.3.15) to know the behavior of the solution when it is in a neighborhood of $(\pm\sqrt{a-b}, \pm 1)$.

Variational approach

Consider the minimization problem

$$I = \inf \left\{ \mathcal{E}(\psi); \psi \in X, \int_{\mathbb{R}^3} |\psi(x)|^2 dx = 1 \right\}, \quad (2.3.16)$$

where

$$X = \left\{ \psi \in L^2(\mathbb{R}^3, \mathbb{C}^2); \int_{\mathbb{R}^3} \frac{|\boldsymbol{\sigma} \cdot \nabla \psi(x)|^2}{(1 - |\psi(x)|^2)_+} < +\infty \right\} \quad (2.3.17)$$

and

$$\mathcal{E}(\psi) = \frac{1}{2} \int_{\mathbb{R}^3} \frac{|\boldsymbol{\sigma} \cdot \nabla \psi(x)|^2}{(1 - |\psi(x)|^2)_+} dx - \frac{a}{4} \int_{\mathbb{R}^3} |\psi(x)|^4 dx. \quad (2.3.18)$$

Here $x_+ = \max(x, 0)$ is the positive part and $\psi = (\psi_1, \psi_2) \in L^2(\mathbb{R}^3, \mathbb{C}^2)$ is a 2-spinor that describes the quantum state of a nucleon. The Euler-Lagrange equation of the energy functional \mathcal{E} under the L^2 normalization constraint, also called mass constraint, is given by the second order equation

$$-\boldsymbol{\sigma} \cdot \nabla \left(\frac{\boldsymbol{\sigma} \cdot \nabla \psi}{(1 - |\psi|^2)_+} \right) + \frac{|\boldsymbol{\sigma} \cdot \nabla \psi|^2}{(1 - |\psi|^2)_+^2} \psi - a|\psi|^2 \psi + b\psi = 0 \quad (2.3.19)$$

with b a Lagrange multiplier. Hence, a solution of the minimization problem (2.3.16) is a solution of the equation (2.3.19). Moreover, one can easily prove that any $\psi \in X$ is in $H^1(\mathbb{R}^3, \mathbb{C}^2)$ and satisfies $|\psi|^2 \leq 1$ a.e. in \mathbb{R}^3 (see [ER13b]). As a consequence, a minimizer of (2.3.16) is actually a solution of

$$-\boldsymbol{\sigma} \cdot \nabla \left(\frac{\boldsymbol{\sigma} \cdot \nabla \psi}{1 - |\psi|^2} \right) + \frac{|\boldsymbol{\sigma} \cdot \nabla \psi|^2}{(1 - |\psi|^2)^2} \psi - a|\psi|^2 \psi + b\psi = 0. \quad (2.3.20)$$

Solutions of (2.3.20) which are minimizers for I can be called *ground states*. In fact, equation (2.3.20) is the Euler-Lagrange equation of the energy functional

$$\mathcal{F}(\psi) = \frac{1}{2} \int_{\mathbb{R}^3} \frac{|\boldsymbol{\sigma} \cdot \nabla \psi(x)|^2}{1 - |\psi(x)|^2} dx - \frac{a}{4} \int_{\mathbb{R}^3} |\psi(x)|^4 dx$$

under the mass constraint. The problem is that the energy functional \mathcal{F} is not bounded from below.

As a conclusion, trying to find solutions of (2.3.20) which minimize the energy \mathcal{F} is hopeless and the definition of ground states for (2.3.20) based on this functional is not clear.

In the above subsection, we remark that for all the solution of (2.3.13) which are square integrable, $g^2(r) < 1$ in $[0, +\infty)$. Hence, according to this result, we conjecture that a solution to (2.3.20) has to satisfy $|\psi|^2 \leq 1$ a.e. in \mathbb{R}^3 . In this case, $\mathcal{F}(\psi) = \mathcal{E}(\psi)$, and the ground states of (2.3.20) can be defined without further specification as the minimizers of \mathcal{E} .

From a physical point of view the term $-(a/4) \int_{\mathbb{R}^3} |\psi|^4$ in (2.3.18) is the usual nonlinear Schrödinger attraction which describes here the confinement of the nucleons. On the other hand, the denominator $(1 - |\psi|^2)_+$ can be interpreted as a mass depending on the state ψ of the nucleon, and it describes a phenomenon of saturation in the system. A high density $|\psi|^2$ generates a lower mass, which itself prevents from having a too high density.

The main result in [ER13b] is the following:

Theorem 2.3.4 (Existence of minimizers in the spin case). *If $I < 0$ there exists a minimizer of (2.3.16). Moreover, $I < 0$ if and only if $a > a_0$ where a_0 is a strictly positive constant. In particular, $10.96 \approx \frac{2}{S^2} < a_0 < 48.06$, where S is the best constant in the Sobolev embedding of $H^1(\mathbb{R}^3)$ into $L^6(\mathbb{R}^3)$.*

The proof of this theorem is an application of the concentration-compactness principle [Lio85a; Lio85b] with some new ingredients. The main new difficulty is due to the presence of the term $\int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \psi|^2}{(1 - |\psi|^2)_+} dx$ in the energy functional. In particular, to rule out the dichotomy case in the concentration-compactness lemma we have to choose ad-hoc cut-off functions allowing us to deal with possible singularities of the integrand. This is also necessary in order to show the localization properties of $\int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \psi|^2}{(1 - |\psi|^2)_+} dx$. More precisely, we have to establish a slightly modified concentration-compactness lemma in the functional set X that reads as follows.

Lemma 2.3.5. *Let $\{\psi_n\}_n$ be a X -bounded sequence such that $\int_{\mathbb{R}^3} |\psi_n|^2 dx = 1$ for all $n \geq 0$. Then there exists a subsequence that we still denote by $\{\psi_n\}_n$ such that one of the following properties holds:*

1. *Compactness up to a translation: there exists a sequence $\{y_n\}_n \subset \mathbb{R}^3$ such that, for every $\varepsilon > 0$, there exists $0 < R < \infty$ with*

$$\int_{B(y_n, R)} |\psi_n|^2 dx \geq 1 - \varepsilon;$$

2. *Vanishing: for all $0 < R < \infty$*

$$\sup_{y \in \mathbb{R}^3} \int_{B(y, R)} |\psi_n|^2 dx \xrightarrow{n} 0;$$

3. *Dichotomy: there exist $\alpha \in (0, 1)$ and $n_0 \geq 0$ such that there exist two X -bounded sequences, $\{\psi_1^n\}_{n \geq n_0}$ and $\{\psi_2^n\}_{n \geq n_0}$, satisfying the following properties:*

$$\|\psi_n - (\psi_1^n + \psi_2^n)\|_{L^p} \xrightarrow{n} 0, \text{ for } 2 \leq p < 6, \quad (2.3.21)$$

and

$$\int_{\mathbb{R}^3} |\psi_1^n|^2 dx \xrightarrow{n} \alpha \text{ and } \int_{\mathbb{R}^3} |\psi_2^n|^2 dx \xrightarrow{n} 1 - \alpha, \quad (2.3.22)$$

$$\text{dist}(\text{supp } \psi_1^n, \text{supp } \psi_2^n) \xrightarrow{n} +\infty. \quad (2.3.23)$$

Moreover, in this case we have that

$$\liminf_{n \rightarrow +\infty} \mathcal{E}(\psi_n) - \mathcal{E}(\psi_1^n) - \mathcal{E}(\psi_2^n) \geq 0, \quad (2.3.24)$$

which implies $I \geq I_\alpha + I_{1-\alpha}$.

Here, a sequence $\{\psi_n\}_n$ is X -bounded if there exists a positive constant C independent of n such that

$$\|\psi_n\|_{L^2}^2 + \int_{\mathbb{R}^3} \frac{|\boldsymbol{\sigma} \cdot \nabla \psi_n|^2}{(1 - |\psi_n|^2)_+} dx \leq C \quad (2.3.25)$$

and, for any $\nu > 0$,

$$I_\nu = \inf \left\{ \mathcal{E}(\psi) ; \psi \in X, \int_{\mathbb{R}^3} |\psi|^2 dx = \nu \right\}. \quad (2.3.26)$$

Note that $I_1 = I$.

Assume that $I < 0$. The vanishing case is easily ruled out. Indeed, if vanishing occurs, $\{\psi_n\}_n$ converges strongly to 0 in $L^p(\mathbb{R}^3)$ for $2 < p < 6$ and, as a consequence, $I \geq 0$.

Next, by a scaling argument, we can show that $I < 0$ is equivalent to the strict inequality

$$I < I_\alpha + I_{1-\alpha}$$

for all $\alpha \in (0, 1)$. Hence, dichotomy can not occur.

As a consequence, there exists a sequence $\{y_n\}_n \subset \mathbb{R}^3$ such that the sequence of $\tilde{\psi}_n = \psi_n(\cdot + y_n)$ is a minimizing sequence that converges strongly in L^p for $2 \leq p < 6$ and weakly in H^1 to some $\tilde{\psi}$. Note that the weak convergence in H^1 implies that $\{\boldsymbol{\sigma} \cdot \nabla \tilde{\psi}_n\}$ converges weakly to $\boldsymbol{\sigma} \cdot \nabla \tilde{\psi}$ in L^2 . This allows us to prove that

$$\int_{\mathbb{R}^3} \frac{|\boldsymbol{\sigma} \cdot \nabla \tilde{\psi}|^2}{(1 - |\tilde{\psi}|^2)_+} dx \leq \liminf_{n \rightarrow +\infty} \int_{\mathbb{R}^3} \frac{|\boldsymbol{\sigma} \cdot \nabla \tilde{\psi}_n|^2}{(1 - |\tilde{\psi}_n|^2)_+} dx$$

and conclude that the minimum of I is achieved by $\tilde{\psi}$.

Finally, it is clear that $I < 0$ for a large enough. Moreover, since the function $a \rightarrow I$ is concave non-increasing, we may denote by a_0 the least positive constant such that $I < 0$. The lower bound for a_0 is obtained by using the Sobolev embedding of $H^1(\mathbb{R}^3)$ into $L^6(\mathbb{R}^3)$ and Hölder inequality, while the upper bound is obtained by means of a test function.

2.3.3. RESULTS FOR THE NUCLEAR SCHRÖDINGER EQUATION IN THE NO-SPIN CASE

To go further in the study of the properties of solutions to the nuclear Schrödinger equation (2.3.20), we assume that the state of the nucleon is an eigenfunction of the spin operator. This leads to equation (2.3.3) that can be seen as the Euler-Lagrange equation of the simpler functional

$$\mathcal{E}_a(\varphi) = \frac{1}{2} \int_{\mathbb{R}^d} \frac{|\nabla \varphi(x)|^2}{(1 - |\varphi(x)|^2)_+} dx - \frac{a}{4} \int_{\mathbb{R}^d} |\varphi(x)|^4 dx \quad (2.3.27)$$

under the mass constraint. Note that the mass term $(1 - |\varphi|^2)_+$ allows us to consider the minimization of the energy (2.3.27) in space dimensions $d \geq 1$ without any limitation on d and $a > 0$.

Note that it remains an open problem to show that minimizers of the original energy (2.3.18) are necessarily eigenfunctions of the spin operator. In principle, the spin symmetry could be broken.

In [LR15b], we remarked that the approach of [ER13b] applies as well to the simplified no-spin model and the proof works in any dimension. The result in this case is the following.

Theorem 2.3.6 (Existence of minimizers in the no-spin case). *Let $d \geq 1$ and*

$$E(a) := \inf \left\{ \mathcal{E}_a(\varphi) : \int_{\mathbb{R}^d} \frac{|\nabla \varphi|^2}{(1 - |\varphi|^2)_+} < \infty, \int_{\mathbb{R}^d} |\varphi|^2 = 1 \right\}. \quad (2.3.28)$$

There exists a universal number $0 \leq a_d < \infty$ such that

- *For $a \leq a_d$, $E(a) = 0$ and there is no minimizer;*

• For $a > a_d$, $E(a) < 0$ and all the minimizing sequences are precompact in $H^1(\mathbb{R}^d)$, up to translations. There is at least one minimizer φ for the minimization problem $E(a)$ and it can be chosen such that $0 \leq \varphi \leq 1$, after multiplication by an appropriate phase factor. It solves the nonlinear equation

$$-\nabla \cdot \left(\frac{\nabla \varphi}{1 - |\varphi|^2} \right) + \frac{|\nabla \varphi|^2}{(1 - |\varphi|^2)^2} \varphi - a|\varphi|^2 \varphi + b\varphi = 0 \quad (2.3.29)$$

for some $b > 0$.

As above, the critical strength a_d of the nonlinear attraction is the largest for which $E(a) = 0$ and it can simply be defined by

$$a_d = \inf_{\substack{\varphi \in H^1(\mathbb{R}^d) \\ 0 \leq |\varphi| \leq 1}} \left\{ \frac{2 \left(\int_{\mathbb{R}^d} |\varphi|^2 \right)^{\frac{2}{d}} \left(\int_{\mathbb{R}^d} \frac{|\nabla \varphi|^2}{(1 - |\varphi|^2)_+} \right)}{\int_{\mathbb{R}^d} |\varphi|^4} \right\}.$$

It can easily be verified that $a_1 = 0$ in dimension $d = 1$, that

$$a_2 = \inf_{\substack{\varphi \in H^1(\mathbb{R}^2) \\ 0 \leq |\varphi| \leq 1}} \left\{ 2 \frac{\|\varphi\|_{L^2(\mathbb{R}^2)}^2 \|\nabla \varphi\|_{L^2(\mathbb{R}^2)}^2}{\|\varphi\|_{L^4(\mathbb{R}^2)}^4} \right\} > 0$$

is related to the Gagliardo-Nirenberg-Sobolev constant in dimension $d = 2$, and that $a_d > 0$ in higher dimensions. Estimates on a_d have been provided in dimension $d = 3$ in [ER13b] and similar bounds can be derived in higher dimensions by following the same method.

After the two works [ER12b; ER13b], it remained an open problem to show that minimizers are all radial and unique, up to a possible translation and multiplication by a phase factor. The purpose of [LR15b] was to answer this question. The main result obtained is the following.

Theorem 2.3.7 (Uniqueness and non-degeneracy in the no-spin case). *The nonlinear equation (2.3.29) has no non-trivial solution $0 < \varphi < 1$ in $L^2(\mathbb{R}^d)$ when $0 < a \leq 2b$. For $a > 2b > 0$, the nonlinear equation (2.3.29) has a unique solution $0 < \varphi < 1$ that tends to 0 at infinity, modulo translations and multiplication by a phase factor. It is radial, decreasing, and non-degenerate.*

This theorem is the analogue of a celebrated similar result for the nonlinear Schrödinger equation (see, e.g., [Tao06, App. B] and [Fra13] for references). Our main contribution was the remark that the equation (2.3.29) can be rewritten in terms of $u := \arcsin(\varphi)$ as a simpler nonlinear Schrödinger equation

$$-\Delta u + b \sin(u) \cos(u) - a \sin^3(u) \cos(u) = 0. \quad (2.3.30)$$

Applying the the moving plane method [GNN81; LN93] allows us to conclude that any positive solution of (2.3.29) is necessarily radial decreasing.

Radial solutions to the equation (2.3.30) solve

$$\begin{cases} u'' + \frac{d-1}{r} u' + \frac{a}{2} \sin(2u) \left(\sin^2(u) - \frac{b}{a} \right) = 0 & \text{on } \mathbb{R}_+ \\ u'(0) = 0 \end{cases} \quad (2.3.31)$$

and, since we look for solutions which are square integrable, we concentrate on showing the existence and the uniqueness of positive solutions such that $(u(r), u'(r)) \rightarrow 0$ when $r \rightarrow \infty$. In dimensions $d \geq 2$, the condition $u'(0) = 0$ is necessary to avoid a singularity at the origin. In dimension $d = 1$, the solution is known to be even about one point and, after a suitable translation we may always assume $u'(0) = 0$ as well.

More precisely, to prove the existence of solutions in dimension $d = 1$, we use the fact that in this case the local energy

$$H(r) = \frac{u'(r)^2}{2} + a \frac{\sin^4(u(r))}{4} - b \frac{\sin^2(u(r))}{2} \quad (2.3.32)$$

is conserved along the trajectories. However, in dimension $d \geq 2$, the energy H defined by (2.3.32), decreases:

$$H'(r) = -\frac{(d-1)}{r} u'(r)^2.$$

The solutions u_y to (2.3.31) are parametrized by $u_y(0) := y \in (0, \pi/2)$. Using the same arguments as in the proof of [ER12b, Lem. 2.6] and in particular the fact that the energy H is non-increasing, we can easily show that a solution starting at $y \geq \pi/2$ stays bigger than $\pi/2$ and hence cannot tend to 0 at infinity. Moreover, note that the equation (2.3.31) has the three stationary solutions $u \equiv 0$, $u \equiv \pi/2$ and $u \equiv \arcsin(\sqrt{b/a})$. Hence $u(0) \notin \{0, \arcsin(\sqrt{b/a}), \pi/2\}$ is necessary. The following is a reformulation of the result of [ER12b] that was expressed in terms of $\varphi = \sin(u)$.

Theorem 2.3.8 (Existence of solutions). *For $0 < a \leq 2b$, there is no non-trivial solution u to (2.3.31), such that $u \rightarrow 0$ at infinity. For $a > 2b > 0$, there exists one positive solution Q to (2.3.31), such that $(Q, Q') \rightarrow (0, 0)$ at infinity. It is decreasing, starts at*

$$\begin{aligned} Q(0) &= \bar{y} = \arcsin(\sqrt{2b/a}) && \text{for } d = 1, \\ Q(0) &= \bar{y} \in (\arcsin(\sqrt{2b/a}), \pi/2) && \text{for } d \geq 2, \end{aligned}$$

and has the following behavior at infinity:

$$Q(r) \underset{r \rightarrow \infty}{\sim} C \frac{e^{-\sqrt{b}r}}{r^{\frac{d-1}{2}}} \quad Q'(r) \underset{r \rightarrow \infty}{\sim} -\sqrt{b} C \frac{e^{-\sqrt{b}r}}{r^{\frac{d-1}{2}}}, \quad (2.3.33)$$

for some $C > 0$.

The proof used in [ER12b], which is presented for $d = 3$ but can be generalized for all $d \geq 2$, is based on a shooting method consisting in increasing y continuously starting from 0. More precisely, we introduce the set

$$S_+ = \{y \in (0, \pi/2) : \min_{\mathbb{R}_+} u_y > 0\},$$

and we define $\bar{y} = \sup S_+$. It is clear that $\bar{y} \in (0, \pi/2]$ and, as explained in Section 2.3.2, the main difficulty is to prove that $\bar{y} \in (0, \pi/2)$. This is done by using a contradiction argument: we assume that there exists a sequence of initial data $y_n \in S_+$ such that $\lim_{n \rightarrow +\infty} y_n = \pi/2$ and we show, with a careful analysis of u_{y_n} , that this leads to a contradiction (see [ER12b] for more details). The explicit decay rate (2.3.33) was not stated in [ER12b], but it is a classical fact whose proof can for instance be read in [GNN81].

Note that in dimension $d \geq 2$, one can also apply the results of [BGK83; BL83] to equation (2.3.30) and deduce the existence of a positive radial decreasing solution Q such that $(Q, Q') \rightarrow (0, 0)$ at infinity whenever $a > 2b > 0$.

The non-existence part in Theorem 2.3.8 is a consequence of the fact that the local energy (2.3.32) is non-increasing. Indeed, this implies that any solution satisfying $u'(0) = 0$ and $(u, u') \rightarrow (0, 0)$ at infinity must be such that

$$1 > \sin^2(u(0)) \geq \frac{2b}{a}.$$

Hence, $a/2b > 1$ is a necessary condition for the existence of u . Moreover, we see that $\bar{y} > \arcsin(\sqrt{2b/a})$ which is strictly above the stationary solution $\arcsin(\sqrt{b/a})$.

To prove the non-degeneracy and uniqueness in the radial case, we follow a classical argument of McLeod [McL93] (reviewed in [Tao06, App. B] and in [Fra13]). Our proof can be applied to more general

semilinear elliptic equations of the form $-\Delta u = g(u)$ as explained in Appendix A.1 (see also [LR20a]). Here $g(u) = a \sin^3(u) \cos(u) - b \sin(u) \cos(u)$.

Finally, we conclude the non-degeneracy in $L^2(\mathbb{R}^d)$, *i.e.* the fact that the kernel of the linearized operator at our solution φ is spanned by the generators of the symmetries of the problem (space translation and multiplication by a phase factor). The linearized operators at our solution $\varphi = \sin(Q)$ are defined by

$$L_1(\eta) = -\nabla \cdot \left(\frac{\nabla \eta}{1 - \varphi^2} \right) + \left\{ -2\nabla \cdot \left(\frac{\varphi \nabla \varphi}{(1 - \varphi^2)^2} \right) + 4 \frac{\varphi^2 (\varphi')^2}{(1 - \varphi^2)^3} + \frac{(\varphi')^2}{(1 - \varphi^2)^2} - 3a\varphi^2 + b \right\} \eta \quad (2.3.34)$$

and

$$L_2(\eta) = -\nabla \cdot \left(\frac{\nabla \eta}{1 - \varphi^2} \right) + \left\{ \frac{(\varphi')^2}{(1 - \varphi^2)^2} - a\varphi^2 + b \right\} \eta. \quad (2.3.35)$$

More precisely, the linearized operator is $\mathcal{L}(\eta_1 + i\eta_2) = L_1\eta_1 + iL_2\eta_2$. The operator L_1 describes variations with respect to φ for real functions, whereas L_2 is related to the invariance of our problem under multiplication by a phase factor. It is easy to verify that both L_1 and L_2 are self-adjoint operators on $L^2(\mathbb{R}^d)$, with domain $H^2(\mathbb{R}^d)$ and form domain $H^1(\mathbb{R}^d)$.

Theorem 2.3.9 (Non-degeneracy of the unique ground state φ). *In $L^2(\mathbb{R}^d)$, we have*

$$\ker(L_1) = \text{span}(\partial_{x_1}\varphi, \dots, \partial_{x_d}\varphi)$$

and $\ker(L_2) = \text{span}(\varphi)$.

The proof of this theorem is based on the fact that the first eigenvalue of L_1 and L_2 , when it exists, is necessarily simple with a positive eigenfunction. Since $L_2\varphi = 0$ and φ is positive, it is clear that $\ker(L_2) = \text{span}(\varphi)$. Next, in dimension $d = 1$, we know that $\partial_x\varphi \in \ker(L_1)$ and $\partial_x\varphi$ has a constant sign. Hence, 0 is the first eigenvalue of L_1 and it is non-degenerate which implies $\ker(L_1) = \text{span}(\partial_x\varphi)$.

The argument for L_1 in dimension $d \geq 2$ is slightly more complicated. A lengthy but straightforward computation shows that

$$L_1(\eta) = -\frac{\Delta v + g'(Q)v}{\cos(Q)}, \quad \text{with } v = \frac{\eta}{\cos(Q)}.$$

Since $0 < Q \leq Q(0) < \pi/2$, the multiplier $\cos(Q)$ is bounded away from 0 and we deduce that $v \in L^2(\mathbb{R}^d)$ if and only if $\eta \in L^2(\mathbb{R}^d)$. Hence $\eta \in \ker(L_1)$ if and only if $v = \eta/\cos(Q) \in \ker(\Delta + g'(Q))$. The argument is now classical will explained in more details in Appendix A.1.

To conclude, let us remark that, since equation (2.3.29) is invariant under multiplications by a phase factor, we can always suppose that a solution φ is real-valued. Hence, in [ER13b, Appendix A.1] it has been proved that any solution $\varphi \in H^1(\mathbb{R}^d)$ is such that $|\varphi|^2 \leq 1$ a.e. in \mathbb{R}^d whenever $a \geq b > 0$. As a consequence, the change of variables $u = \arcsin(\varphi)$ makes sense whenever $a \geq b > 0$.

2.3.4. BRANCH OF SOLUTIONS TO THE RELATIVISTIC MEAN-FIELD MODEL IN THE STATIC CASE

As an application of Theorem 2.3.7, we are able to construct a branch of solutions of the underlying Dirac equation (2.3.10), that converges to the non-relativistic solution φ in the limit $m \rightarrow +\infty$, thereby justifying in the static case the formal arguments given above (see also [ER12b]). We explain this now.

As explained above, for the σ - ω model, the interesting regime is when the parameters g_σ^2/m_σ^2 and g_ω^2/m_ω^2 behave like m , whereas $g_\sigma^2/m_\sigma^2 - g_\omega^2/m_\omega^2$ stays bounded. Even if g_σ^2/m_σ^2 diverges, the model still has a nice bounded limit φ , which is precisely the non-relativistic ground state studied in the previous subsection.

Theorem 2.3.10 (Non-relativistic limit of the σ - ω model in the static case). *Let $\theta, \lambda, \mu, C, D$ be positive constants such that $\lambda > 2\mu\theta$. Then for m large enough, the equation (2.3.10) admits a branch of solutions of the special form*

$$\Psi_m(x) = \begin{pmatrix} \phi_m(|x|) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ -i\chi_m(|x|) \boldsymbol{\sigma} \cdot \frac{x}{|x|} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix}, \quad (2.3.36)$$

with

$$m_\sigma^2 = Cm^2, \quad m_\omega^2 - m_\sigma^2 = D, \quad \left(\frac{g_\sigma}{m_\sigma}\right)^2 = \theta m, \quad \left(\frac{g_\sigma}{m_\sigma}\right)^2 - \left(\frac{g_\omega}{m_\omega}\right)^2 = \lambda. \quad (2.3.37)$$

In the limit $m \rightarrow \infty$, we have

$$\sqrt{\theta} \phi_m(\cdot/\sqrt{m}) \rightarrow \phi \quad \text{and} \quad 2\sqrt{\theta m} \chi_m(\cdot/\sqrt{m}) \rightarrow \frac{\phi'}{1-\phi^2}$$

strongly in $H^2(\mathbb{R}^3)$, where ϕ is the unique positive solution of (2.3.29) with $a = 2\lambda/\theta$ and $b = 2\mu$.

The proof of Theorem 2.3.10 is based on the implicit function theorem. In other words, we see (2.3.10) as a small perturbation of (2.3.11) and we use the non-degeneracy of φ to construct a solution. Remark that, thanks to the non-degeneracy property, this argument gives also the local uniqueness of the solution to (2.3.10) around φ , modulo translations and multiplication by a phase factor. A similar argument has for instance been used in [Len09].

The idea of is the following. We want to prove the existence of a branch of solutions to the Dirac equation which can be rewritten for $\Psi = (\psi, \zeta)$ as

$$\begin{cases} -i\boldsymbol{\sigma} \cdot \nabla \zeta + (S + V + \mu)\psi = 0, \\ -i\boldsymbol{\sigma} \cdot \nabla \psi = (2m - \mu + S - V)\zeta, \\ (-\Delta + m_\sigma^2)S = -g_\sigma^2(|\psi|^2 - |\zeta|^2), \\ (-\Delta + m_\omega^2)V = g_\omega^2(|\psi|^2 + |\zeta|^2). \end{cases} \quad (2.3.38)$$

It will be convenient to introduce the new fields

$$\tilde{W}_+ = \frac{S+V}{2} \quad \text{and} \quad \tilde{W}_- = \frac{S-V}{2} \quad (2.3.39)$$

Then, imposing the special form

$$\psi(x) = \tilde{\varphi}(|x|) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \zeta(x) = -i\tilde{\chi}(|x|) \boldsymbol{\sigma} \cdot \frac{x}{|x|} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (2.3.40)$$

with real-valued functions $\tilde{\varphi}$ and $\tilde{\chi}$, and using (2.3.38) and (2.3.39), we obtain the following system

$$\begin{cases} \tilde{\varphi}' - (2m + 2\tilde{W}_- - \mu)\tilde{\chi} = 0 \\ \tilde{\chi}' + \frac{2}{r}\tilde{\chi} - (2\tilde{W}_+ + \mu)\tilde{\varphi} = 0 \\ \tilde{W}_+ = \frac{1}{2} \left(\frac{1}{m_\sigma^2} + \frac{1}{m_\omega^2} \right) \Delta \tilde{W}_+ + \frac{1}{2} \left(\frac{1}{m_\sigma^2} - \frac{1}{m_\omega^2} \right) \Delta \tilde{W}_- - \frac{\lambda}{2}(\tilde{\varphi}^2 + \tilde{\chi}^2) + \theta m \tilde{\chi}^2 \\ \tilde{W}_- = \frac{1}{2} \left(\frac{1}{m_\sigma^2} - \frac{1}{m_\omega^2} \right) \Delta \tilde{W}_+ + \frac{1}{2} \left(\frac{1}{m_\sigma^2} + \frac{1}{m_\omega^2} \right) \Delta \tilde{W}_- + \frac{\lambda}{2}(\tilde{\varphi}^2 + \tilde{\chi}^2) - \theta m \tilde{\varphi}^2 \end{cases} \quad (2.3.41)$$

which is equivalent to (2.3.38) for functions of the above form (2.3.40).

Next, we consider the following rescaling

$$\begin{aligned}\tilde{\varphi}(x) &= \frac{1}{\sqrt{\theta}}\varphi(\sqrt{m}x), & \tilde{\chi}(x) &= \frac{1}{2\sqrt{\theta}}\frac{1}{\sqrt{m}}\chi(\sqrt{m}x), \\ \tilde{W}_+(x) &= W_+(\sqrt{m}x), & \tilde{W}_-(x) &= mW_-(\sqrt{m}x),\end{aligned}\tag{2.3.42}$$

and we find

$$\begin{cases} \varphi' - \left(1 + W_- - \frac{\mu}{2m}\right)\chi = 0 \\ \chi' + \frac{2}{r}\chi - (4W_+ + 2\mu)\varphi = 0 \\ W_+ = \frac{2 + D/(Cm^2)}{2m(C + D/m^2)}\Delta W_+ + \frac{D}{2C(Cm^2 + D)}\Delta W_- - \frac{\lambda}{2}\left(\frac{\varphi^2}{\theta} + \frac{\chi^2}{4\theta m}\right) + \frac{\chi^2}{4} \\ W_- = \frac{D}{2Cm^2(Cm^2 + D)}\Delta W_+ + \frac{2 + D/(Cm^2)}{2m(C + D/m^2)}\Delta W_- + \frac{\lambda}{2m}\left(\frac{\varphi^2}{\theta} + \frac{\chi^2}{4\theta m}\right) - \varphi^2 \end{cases}$$

Finally, denoting $\varepsilon = 1/m$ the perturbative parameter and recalling that

$$a = 2\lambda/\theta, \quad b = 2\mu,$$

we obtain

$$\begin{cases} \varphi' - \left(1 + W_- - \varepsilon\frac{b}{4}\right)\chi = 0 \\ \chi' + \frac{2}{r}\chi - (4W_+ + b)\varphi = 0 \\ \left(-\varepsilon\mathcal{R}(\varepsilon)\Delta + \mathbb{1}_2\right)\begin{pmatrix} W_+ \\ W_- \end{pmatrix} + \mathcal{F}(\varphi, \chi) + \mathcal{H}(\varepsilon, \varphi, \chi) = 0 \end{cases}\tag{2.3.43}$$

with

$$\begin{aligned}\mathcal{R}(\varepsilon) &= \frac{1}{2(C + D\varepsilon^2)}\begin{pmatrix} 2 + \varepsilon^2 D/C & \varepsilon D/C \\ \varepsilon^3 D/C & 2 + \varepsilon^2 D/C \end{pmatrix}, \\ \mathcal{F}(\varphi, \chi) &= \begin{pmatrix} a\varphi^2/4 - \chi^2/4 \\ \varphi^2 \end{pmatrix}, \quad \mathcal{H}(\varepsilon, \varphi, \chi) = \varepsilon\frac{a}{4}\begin{pmatrix} \chi^2/4 \\ -\varphi^2 - \varepsilon\chi^2/4 \end{pmatrix}.\end{aligned}$$

When $\varepsilon = 0$, we obtain the system of equations

$$\begin{cases} \varphi' = \chi(1 - \varphi^2) \\ \chi' + \frac{2}{r}\chi = \varphi(\chi^2 - a\varphi^2 + b) \end{cases}\tag{2.3.44}$$

presented above.

We introduce the map $\mathcal{K} : \mathbb{R} \times \mathcal{H}_{\text{rad}}^2 \times (H_{\text{rad}}^2)^2 \longrightarrow \mathcal{H}_{\text{rad}}^1 \times (H_{\text{rad}}^2)^2$ defined by

$$\mathcal{K}(\varepsilon, \varphi, \chi, W_+, W_-) = \left(\begin{pmatrix} \varphi' - (1 + W_- - \varepsilon b/4)\chi \\ \chi' + 2\chi/r - (4W_+ + b)\varphi \end{pmatrix}, \begin{pmatrix} W_+ \\ W_- \end{pmatrix} + \frac{1}{\varepsilon\mathcal{R}(\varepsilon)(-\Delta) + \mathbb{1}_2}(\mathcal{F}(\varphi, \chi) + \mathcal{H}(\varepsilon, \varphi, \chi)) \right).\tag{2.3.45}$$

Here the spaces

$$\mathcal{H}_{\text{rad}}^k := \left\{ (\varphi, \chi) : \begin{pmatrix} \varphi(|x|) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ -i\chi(|x|) \boldsymbol{\sigma} \cdot \frac{x}{|x|} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} \in H^k(\mathbb{R}^3, \mathbb{C}^4) \right\}$$

are the projections of the usual Sobolev spaces $H^k(\mathbb{R}^3, \mathbb{C}^4)$ to the sector of minimal total angular momentum (they in particular contain a boundary condition at $r = 0$), whereas H_{rad}^2 is the usual projection of $H^2(\mathbb{R}^3, \mathbb{R})$ to the subspace of radial functions.

In what follows, we let $X = \mathcal{H}_{\text{rad}}^2 \times (H_{\text{rad}}^2)^2$, $Y = \mathcal{H}_{\text{rad}}^1 \times (H_{\text{rad}}^2)^2$ and $\Xi = (\phi, \chi, W_+, W_-)$. Solving the system (2.3.43) is equivalent to solving $\mathcal{K}(\varepsilon, \Xi) = 0$. We construct a branch of solutions, by means of an implicit function-type argument.

The first step is to prove that \mathcal{K} is a smooth operator from $\mathbb{R} \times X$ into Y .

Next, we consider the linearization $\partial_{\Xi}\mathcal{K}(0, \Xi_0)$ of the operator \mathcal{K} at our non-relativistic solution $\Xi_0 = (\varphi, \chi, W_+, W_-) \in X$ with

$$\chi = \varphi'/(1 - \varphi^2), \quad W_+ = -\frac{a}{4}\varphi^2 + \frac{1}{4}\chi^2, \quad W_- = -\varphi^2,$$

which is defined by

$$\partial_{\Xi}\mathcal{K}(0, \Xi_0)(f, g, h_+, h_-) = \begin{pmatrix} f' - (1 + W_-)g - \chi h_- \\ g' + \frac{2}{r}g - 4W_+f - 4\varphi h_+ - bf \\ h_+ + \frac{a}{2}\varphi f - \frac{1}{2}\chi g \\ h_- + 2\varphi f \end{pmatrix}, \quad (2.3.46)$$

and we prove that it is an isomorphism from X onto Y .

In particular, to prove that the operator $\partial_{\Xi}\mathcal{K}(0, \Xi_0)$ is one-to-one as an operator from X to Y , we use the fact that the unique radial solution $0 < \varphi < 1$ to (2.3.29) is non-degenerate. More precisely, we remark that if $(f, g, h_+, h_-) \in X$ is a nontrivial solution to $\partial_{\Xi}\mathcal{K}(0, \Xi_0)(f, g, h_+, h_-) = 0$, then the radial function f solves $L_1 f = 0$ where L_1 is the linearized operator defined in (2.3.34).

Since the restriction of L_1 to radial functions is invertible by Theorem 2.3.9, we conclude that $f = 0$ and $\partial_{\Xi}\mathcal{K}(0, \Xi_0)$ is one-to-one.

To conclude it is enough to remark that $\partial_{\Xi}\mathcal{K}(0, \Xi_0)$ is a one-to-one operator that can be written as a sum of an isomorphism and a compact perturbation and it is then an isomorphism.

Hence, we can apply the implicit function theorem to find that there exists $\delta > 0$ and a function $\Xi \in \mathcal{C}([0, \delta) \times X)$ such that

$$\Xi(0) = \left(\phi, \frac{\phi'}{1 - \phi^2}, -\frac{a}{4}\phi^2 + \frac{1}{4}\chi^2, -\phi^2 \right)$$

and $\mathcal{K}(\varepsilon, \Xi(\varepsilon)) = 0$ for $0 \leq \varepsilon < \delta$. This concludes the proof of Theorem 2.3.10.

2.3.5. SATURATION PHENOMENON FOR NUCLEAR MATTER AND QUALITATIVE PROPERTIES OF MESON FIELDS

In computations carried out in physics it has been observed that the fields of mesons σ and ω are proportional to the scalar and the vector density. In models for finite nuclei these fields approximately assume a ‘‘plateau’’-like Saxon–Woods shape: they vanish outside the nucleus and they are more or less constant inside it. Moreover, the intensity of the potential for the antinucleons $V - S$ is much more higher than that of the potential for the nucleons $V + S$ (see for instance [Rin96]).

These properties are nicely described by the solutions of the effective model presented above.

In our seminal work [ER12b], we had run some numerical calculations for the ground state solution to (2.3.3), trying to see how the values of the parameters in the problem affect the shapes of the meson fields and the intensity of the potentials. We observed that the results depend a lot on the values of a and b , which are related to the physical values of the meson masses and of the coupling constants, as we have seen above. More precisely, we remarked that even in this very particular case where only one nucleon is taken into account and where we assume that its state is an eigenfunction of the spin operator, the

Saxon–Woods shape for the potentials V and S is perfectly observable and the magnitude of $|V - S|$ is much larger than that of $|V + S|$, if the parameters a and b are well-chosen.

Recall that in the regime of parameters which is relevant in nuclear physics

$$S \simeq -m|\varphi|^2 + \frac{1}{4}|\chi|^2 \text{ and } V \simeq m|\varphi|^2 - \frac{a}{2}|\varphi|^2 + \frac{1}{4}|\chi|^2 - \frac{a}{8}|\chi|^2$$

as m goes to ∞ . As a consequence,

$$V - S \simeq 2m|\varphi|^2 - \frac{a}{2}|\varphi|^2 - \frac{a}{8}|\chi|^2 \text{ and } V + S \simeq -\frac{a}{2}|\varphi|^2 + \frac{1}{2}|\chi|^2 - \frac{a}{8}|\chi|^2$$

so that the intensity of $|V - S|$ is much higher than that of $|V + S|$. Moreover, the above asymptotics show that V and S behave like a plateau if φ does.

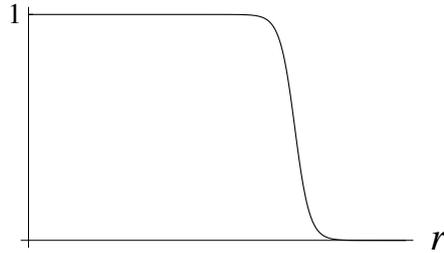


Figure 2.1: Plot of φ^2 , $\frac{2b}{a} \sim 1$

In Figure 2.1, we plot the shape of φ^2 for the values $a = 9$ and $b = 4$ and the “plateau”-like profile is perfectly clear.

A less clear case is the next one, see figure 2.2, where the values of a and b are respectively of 4 and 1. Here the “plateau” is much less visible and its edge are much less sharp. Practically there is no “plateau” in this case.

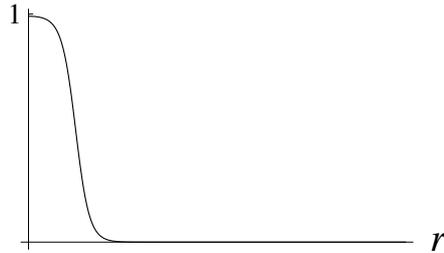


Figure 2.2: Plot of φ^2 , $\frac{2b}{a} \not\sim 1$

Actually, other computations that we have run show that the “plateau” shape is more and more present when $2b/a$ approaches 1. This property has been mathematically clarified in [LR20a]. More precisely, using the same arguments presented in [LR20a] for the double-power nonlinear Schrödinger equation, we can prove the following theorem (see also Appendix A.2).

Theorem 2.3.11 (Behavior when $\frac{2b}{a} \nearrow 1$). *Let $d \geq 2$ and $u_{a,b}$ the unique positive solution to (2.3.30). Let $\mu = \frac{2b}{a}$ and $u_\mu(x) = u_{a,b}((a/2)^{-1/2}x)$. Then u_μ is the unique positive solution to*

$$-\Delta u = g_\mu(u) \text{ in } \mathbb{R}^d \tag{2.3.47}$$

with $g_\mu(s) = 2 \sin^3(s) \cos(s) - \mu \sin(s) \cos(s)$.

Let $\gamma \in (0, \beta_*)$ be any constant and call R_μ the unique radius such that $u_\mu(R_\mu) = \gamma$. Then we have

$$R_\mu = \frac{d-1}{1-\mu} + o\left(\frac{1}{1-\mu}\right), \quad (2.3.48)$$

and the uniform convergence

$$\lim_{\mu \rightarrow 1} \|u_\mu - U_*(|x| - R_\mu)\|_{L^\infty(\mathbb{R}^d)} = 0, \quad (2.3.49)$$

where U_* is the unique solution to the one-dimensional limiting problem

$$\begin{cases} U_*'' + g_1(U_*) = 0 & \text{on } \mathbb{R} \\ U_*(-\infty) = \pi/2 \\ U_*(+\infty) = 0 \\ U_*(0) = \gamma \in (0, \pi/2) \end{cases} \quad (2.3.50)$$

In particular, $U_*(r) = \cot^{-1}(\cot(\gamma)e^r)$.

This result says u_μ resemble a radial translation of the one-dimensional solution U_* , which links the two unstable stationary solutions $\pi/2$ and 0 of the underlying Hamiltonian system. Since U_* tends to $\pi/2$ at $-\infty$, we see that $u_\mu(r)$ tends to $\pi/2$ for any fixed r as $\mu \rightarrow 1$, i.e. $u_{a,b}(r)$ tends to $\pi/2$ for any fixed r as $\frac{2b}{a} \rightarrow 1$.

Recalling that $\varphi = \sin(u)$ we obtain $\varphi^2(r)$ tends to 1 for any fixed r as $\frac{2b}{a} \rightarrow 1$. The convergence of the solution to a constant is interpreted as a saturation phenomenon for nuclear matter (see [BM84])

2.3.6. NUMERICAL ANALYSIS IN ONE SPACE DIMENSION

To have a first insight on the behavior of the ground state solution to (2.3.3) in the context of the time-dependent Schrödinger equation, in [KR20b] we analyze its stability from a numerical point of view.

In particular, in space dimension $d = 1$, we consider the equation

$$i\partial_t \phi = -\partial_x \left(\frac{\partial_x \phi}{1 - |\phi|^{2\alpha}} \right) + \alpha |\phi|^{2\alpha-2} \frac{|\partial_x \phi|^2}{(1 - |\phi|^{2\alpha})^2} \phi - a |\phi|^{2\alpha} \phi \quad (2.3.51)$$

which is the generalization of (2.3.9) to any power nonlinearity $\alpha \in \mathbb{N}^*$ ($\alpha = 1$ being the most relevant case in physical literature).

Solitary wave solutions for this equation can be constructed by taking $\phi(t, x) = e^{ibt} \varphi(x)$ with φ a real positive square integrable solution to the stationary equation

$$-\partial_x \left(\frac{\partial_x \varphi}{1 - \varphi^{2\alpha}} \right) + \alpha \frac{(\partial_x \varphi)^2}{(1 - \varphi^{2\alpha})^2} \varphi^{2\alpha-1} - a \varphi^{2\alpha+1} + b \varphi = 0. \quad (2.3.52)$$

In spatial dimension $d = 1$, the results of [LR15b] can be straightforward generalized for any $\alpha \in \mathbb{N}^*$ and we obtain the following theorem.

Theorem 2.3.12. *Let $\alpha \in \mathbb{N}^*$. The nonlinear equation (2.3.52) has no non-trivial solution $0 \leq \varphi < 1$ such that $\lim_{x \rightarrow \pm\infty} \varphi(x) = 0$ when $0 < a \leq (\alpha+1)b$. For $a > (\alpha+1)b > 0$, the nonlinear equation (2.3.52) has a unique solution $0 < \varphi < 1$ that tends to 0 at $\pm\infty$, modulo translations. This solution is given by*

$$\varphi(x) = \left(\frac{1}{2} \left(\frac{a}{(\alpha+1)b} + 1 \right) + \frac{1}{2} \left(\frac{a}{(\alpha+1)b} - 1 \right) \cosh(2\alpha\sqrt{bx}) \right)^{-\frac{1}{2\alpha}}. \quad (2.3.53)$$

In particular, the following holds

1. $\varphi \in C^1(\mathbb{R})$;
2. $\varphi(x) = \varphi(-x)$;
3. $\varphi'(x) < 0$ for all $x > 0$;
4. $\varphi(x) \sim_{x \rightarrow +\infty} C e^{-\sqrt{b}x}$;
5. φ is non-degenerate.

The core of paper [KR20b] is however devoted to the numerical study of the time evolution of initial data for the equation (2.3.51). In particular, we study the stability of the ground state and the time evolution of general initial data in the Schwartz class of smooth rapidly decreasing functions for various parameters.

The results of [KR20b] can be summarized in the following

Conjecture 1. *The ground states of equation (2.3.51) are asymptotically stable if the perturbed initial data satisfy $|\phi(x, 0)| < 1$. The long time behavior of solutions for general localized initial data is characterized by ground states and radiation.*

This conjecture is supported by the numerical simulations that we have run. Note that because of the exponential decay of the stationary solutions, the use of Fourier spectral methods is quite natural. The solution ϕ is approximated via a truncated Fourier series where the coefficients $\hat{\phi}$ are computed efficiently via a *fast Fourier transform* (FFT). On the other hand, if FFT techniques are used we have to deal with a *stiff* system of ODEs. However, the main problem of equation (2.3.51) is not the stiffness, but the singular term for $|\phi| \rightarrow 1$. Since the equation is focusing, it is to be expected that for initial data with modulus close to 1 it will be numerically challenging since the focusing nature of the equation might lead for some time to even higher values of $|\phi|$. Obviously the regime $\phi \sim 1$ is the most interesting from a mathematical point of view since here the strongest deviation from the standard NLS equation is to be expected.

To study the stability of the ground states (2.3.53), we perturb it first in the form $\phi(x, 0) = \lambda\varphi(x)$, where $\lambda \sim 1$.

Remark 1. *Numerically one cannot consider arbitrary small perturbations as in analytical work since one would have to wait for very large times in order to get meaningful results. But using long times would imply that numerical errors of even high order schemes pile up. Thus, in practice, one always considers perturbations of the order of 1%. This implies, however, that the final state of a perturbed ground state is not the exact ground state even for asymptotically stable ground states, but a nearby one.*

The cubic case $\alpha = 1$

In Fig. 2.3 we show the solution for the perturbed ground state with $\lambda = 0.99$. It can be seen that after a short phase of focusing a ground state with slightly larger maximum than the initial data is reached. In addition, there is some radiation towards infinity.

As stated in remark 1, we expect a ground state of slightly different b as the final state since we have a perturbation of the order of 1%. On the right of Fig. 2.3, we show the solution at the final time in blue together with a fitted ground state in green. The good agreement shows that the final state is indeed a very nearby ground state, $b = 4.388$, which can be already identified (the difference is of the order of 10^{-3}) at an early time.

If we perturb the same ground state as in Fig. 2.3 with a factor $\lambda > 1$ (such that $\|\lambda\varphi\|_\infty < 1$), we observe a similar behavior.

The same initial data as above are perturbed with a localized perturbation of the form $\phi(x, 0) = \varphi(x) \pm 0.001 \exp(-x^2)$.

In Fig. 2.4 we show the solutions for both cases at the final time in blue together with fitted ground states. In both cases the agreement is so good that a difference (again of the order of 10^{-3}) can hardly be recognized. Thus, the ground states appear to be asymptotically stable also in this case.

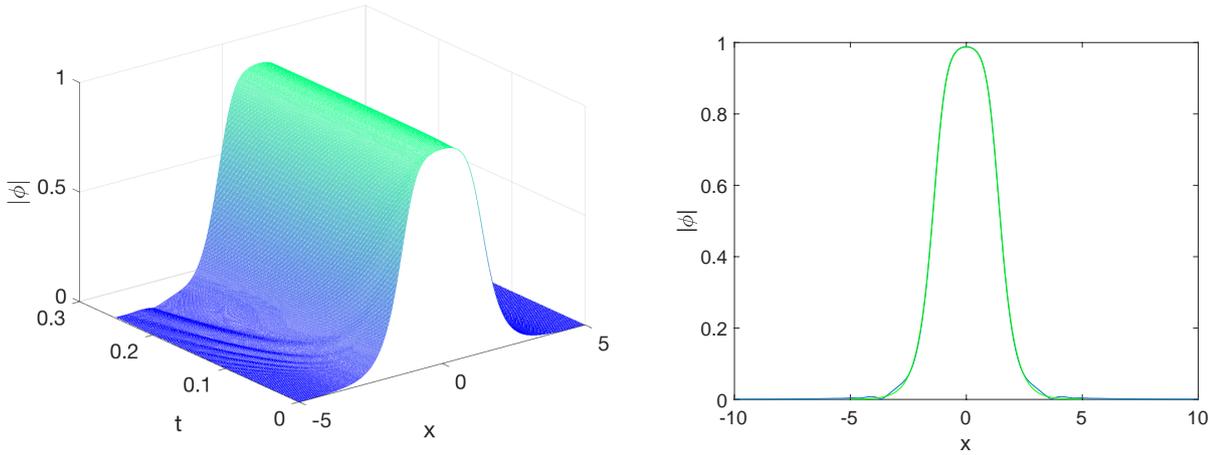


Figure 2.3: Solution to the equation (2.3.51) for the initial data $\phi(x, 0) = 0.99\varphi(x, a = 9, b = 4.4)$ and $\alpha = 1$ on the left, and on the right the solution at the final time in blue and a fitted ground state in green.

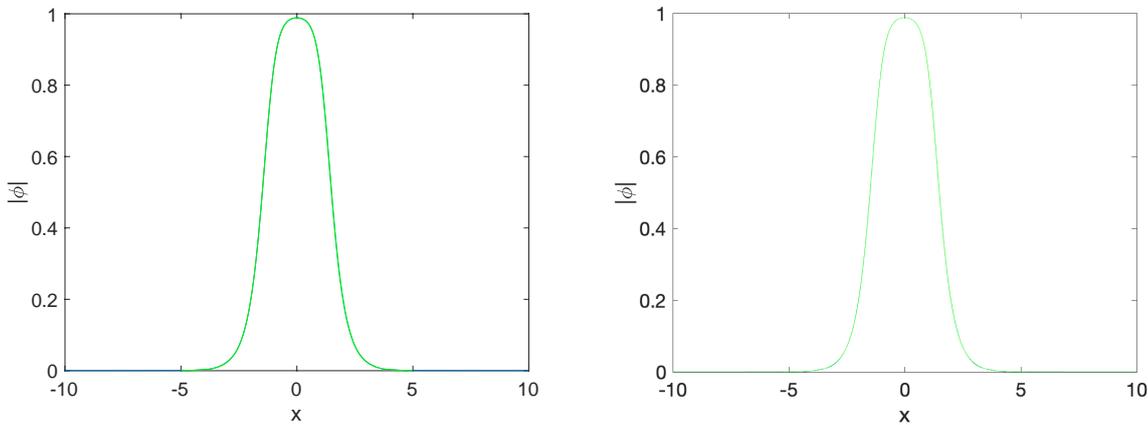


Figure 2.4: Solutions of (2.3.51) for the initial data $\phi(x, 0) = \varphi(x) \pm 0.001 \exp(-x^2)$, on the left for the minus sign, on the right for the plus sign in the initial data in blue together with a fitted ground state in green.

Higher nonlinearities

We repeat the experiments done before for $\alpha = 2, 3$, i.e., a higher nonlinearity. As can be seen below in Fig. 2.5, the ground states still appear to be stable, but take a considerably longer time to settle to a final state. This means we will need much higher numerical resolution in order to avoid too much interaction between the radiation and the bulk on a torus (we simply choose a larger period), and have to solve for longer times.

Schwartz class initial data

An interesting question in this context is whether these stable ground states appear in the long time behavior of solutions to generic localized initial data. To address this question we consider initial data of the form $\phi(x, 0) = \mu \exp(-x^2)$ with $0 < \mu < 1$, again for $a = 9$. In Fig. 2.6 it can be seen that the L^∞ norm of the solution appears to oscillate around some asymptotic values, and that some radiation is emitted towards infinity. On the right of the same figure we show the solution at the final time of the computation in blue together with an estimated ground state ($b \sim 2.7188$) in green.

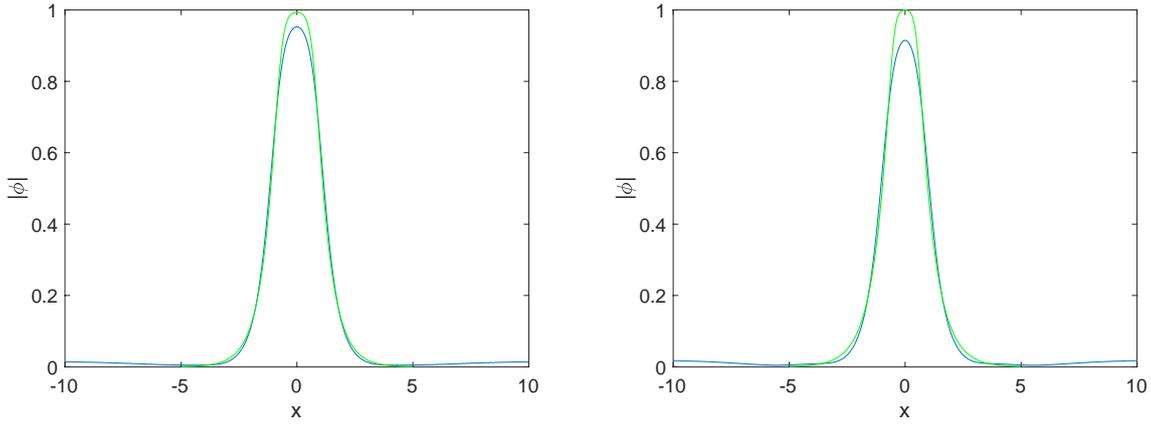


Figure 2.5: Solutions of (2.3.51) for the initial data $\phi(x, 0) = 0.99\varphi(x)$ and $a = 9$, $b = 2.9$ and $\alpha = 2$ on the left, $a = 9$, $b = 2.1$ and $\alpha = 3$ on the right in blue together with an estimated ground state in green.

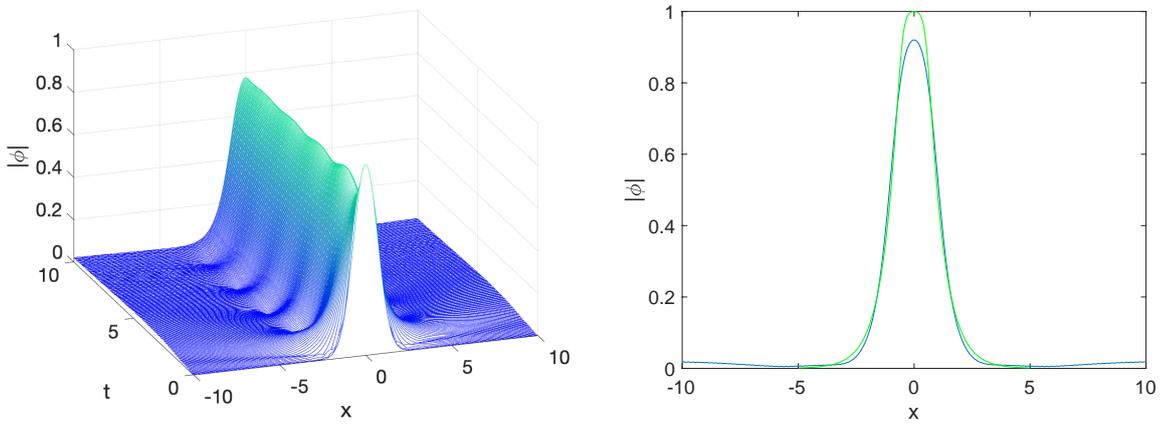


Figure 2.6: Solution to the equation (2.3.51) with $a = 9$, $\alpha = 1$, for the initial data $\phi(x, 0) = 0.9 \exp(-x^2)$ on the left, on the right the solution at the final time in blue together with a fitted ground state in green.

The situation is similar for higher nonlinearity (see [KR20b]).

A.1. UNIQUENESS AND NON-DEGENERACY FOR A CLASS OF SEMILINEAR ELIPTIC EQUATION

In [LR20a], we state an abstract result about the uniqueness and non-degeneracy of solutions of

$$\Delta u + g(u) = 0 \text{ in } \mathbb{R}^d \text{ with } d \geq 2, \quad (\text{A.1.1})$$

where $\Delta u = \sum_{i=1}^d \partial_{x_i}^2 u$ is the Laplacian. We assume that the nonlinearity g is gauge-invariant under the action of the group \mathbb{S}^1 , that is

$$g(|u|e^{i\theta}) = g(|u|)e^{i\theta} \quad (\text{A.1.2})$$

for any $u, \theta \in \mathbb{R}$. In other words, without loss of generality we may assume that $g : \mathbb{R} \rightarrow \mathbb{R}$ is a real odd function such that $g(0) = 0$. Then (A.1.1) is invariant under translations and multiplications by a phase factor.

The study of the *existence* and *uniqueness* of positive solutions to equations of the type (A.1.1) has a very long history. Of particular interest is the (focusing) *nonlinear Schrödinger equation* (NLS) corresponding to

$$g(u) = u^q - u, \quad 1 < q < 2^* - 1 \quad (\text{A.1.3})$$

where $2^* = 2d/(d-2)$ is the critical Sobolev exponent in dimensions $d \geq 3$ and $2^* = \infty$ in dimensions $d = 1, 2$. Here and everywhere else in the paper we use the convention that $u^q := |u|^{q-1}u$ to ensure that (A.1.2) is satisfied. In the particular case (A.1.3), the uniqueness of positive solutions was proved first by Coffman [Cof72] for $q = 3$ and $d = 3$, and then by Kwong [Kwo89] in the general case. These results have been extended to a larger class of nonlinearities by many authors, including for instance [PS83; MS87; KZ91; CL91; McL93; PS98; ST00; Jan10].

Another important property for applications is the *non-degeneracy* of these solutions, which means that the kernel of the linearized operators is trivial, modulo phase and space translations:

$$\ker \left(\Delta + \frac{g(u)}{u} \right) = \text{span}\{u\}, \quad \ker (\Delta + g'(u)) = \text{span}\{\partial_{x_1} u, \dots, \partial_{x_d} u\}.$$

This property plays a central role for the stability or instability of these stationary solutions [Wei85; SS85; GSS87a; GSS90a; DGR15b; DR19b] in the context of the time-dependent Schrödinger equation

$$i\partial_t u = \Delta u + g(u).$$

See Chapter 3 for a detailed description of [DGR15b; DR19b]. In the NLS case (A.1.3) non-degeneracy was shown first in [Cof72; Kwo89; Wei85], but for general nonlinearities it does not necessarily follow from the method used to show uniqueness.

Theorem A.1.1 (Uniqueness and non-degeneracy). *Let $0 < \alpha < \beta$ and g be a continuously differentiable function on $[0, \beta]$. Assume that the following conditions hold:*

(H1) *We have $g(0) = g(\alpha) = g(\beta) = 0$, g is negative on $(0, \alpha)$ and positive on (α, β) with $g'(0) < 0$, $g'(\alpha) > 0$ and $g'(\beta) \leq 0$.*

(H2) *For every $\lambda > 1$, the function*

$$I_\lambda(x) := xg'(x) - \lambda g(x) \quad (\text{A.1.4})$$

has exactly one root x_ on the interval $(0, \beta)$, which belongs to (α, β) .*

Then equation (A.1.1) admits at most one positive radial solution with $\|u\|_\infty < \beta$ and such that

$$u(x), u'(x) \rightarrow 0$$

when $|x| \rightarrow \infty$. Moreover, when it exists, this solution is non-degenerate in the sense that

$$\ker (\Delta + g'(u)) = \text{span}\{\partial_{x_1} u, \dots, \partial_{x_d} u\}, \quad \ker \left(\Delta + \frac{g(u)}{u} \right) = \text{span}\{u\}. \quad (\text{A.1.5})$$

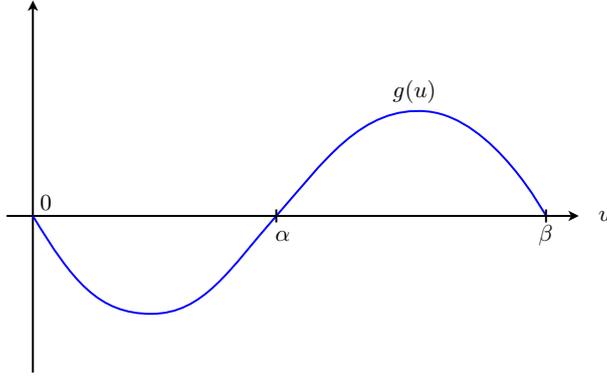


Figure A.1: Typical form of the admissible nonlinearity g in (A.1.1).

Remark 2. *The assumption (H2) can be replaced by the two stronger conditions*

(H2') *there exists $x^* \in (0, \beta)$ such that $g'' > 0$ on $(0, x^*)$ and $g'' < 0$ on (x^*, β) ;*

(H2'') *the function $x \mapsto \frac{xg'(x)}{g(x)}$ is strictly decreasing on (α, β) .*

Remark 3. *In the proof we use (H2) only for one (unknown) particular $\lambda > 1$. Should one be able to localize better this λ for a concrete nonlinearity g , one would then only need to verify (H2) in this region.*

Remark 4. *If g is defined on the half line \mathbb{R}_+ and negative on (β, ∞) , then all the positive solutions satisfy $u < \beta$. This follows from the maximum principle since $-\Delta u = g(u) \leq 0$ on $\{u \geq \beta\}$.*

As we have mentioned, Theorem A.1.1 was indeed proved in [LR15b] although perhaps only implicitly since we were there mainly concerned with a special case for g (see [LR15b, Lemma 3] and the comments after the statement).

The operators appearing in (A.1.5) are the two linearized operators (for the real and imaginary parts of u , respectively) at the solution u and the non-degeneracy means that their kernel (at the solution u) is spanned by the generators of the two symmetries of the problem (space translations and multiplication by a phase).

Note that our assumptions (H1)–(H2) require the existence of three successive zeroes for g as in Figure A.1. In the traditional NLS case there are only two and this corresponds to taking $\beta = +\infty$ in our theorem, a situation where the same result is valid, as proved by McLeod in [McL93] and reviewed in [Tao06; Fra13].

In the article [ST00] by Serrin and Tang, uniqueness is proved under similar assumptions as in Theorem A.1.1. More precisely, the authors assume instead of (H2) that $xg'(x)/g(x)$ is non-increasing on (α, β) , in dimensions $d \geq 3$. We assume less on (α, β) but put the additional assumption that I_λ does not vanish on $(0, \alpha)$. The function I_λ in (A.1.4) appears already in [MS87; McL93]. The method of proof in [ST00] does not seem to provide the non-degeneracy of solutions. Here we clarify this important point by providing a self-contained proof in the spirit of McLeod [McL93]. Similar arguments were independently used in [Kil+17; ASW18].

Theorem A.1.1 does not ensure the existence of solutions to (A.1.1). However, let g satisfy the condition (H1) of Theorem A.1.1 on $[0, \beta]$ and extend it as a continuously differentiable function over \mathbb{R} such that g is odd and $g < 0$ on (β, ∞) . Then we know from [BL83; BGK83] that, in dimension $d \geq 2$, there exists at least one radial decreasing positive solution u to (A.1.1) which is C^2 and decays exponentially at infinity, if and only if

$$G(\eta) := \int_0^\eta g(s) ds > 0 \text{ for some } \eta > 0. \tag{A.1.6}$$

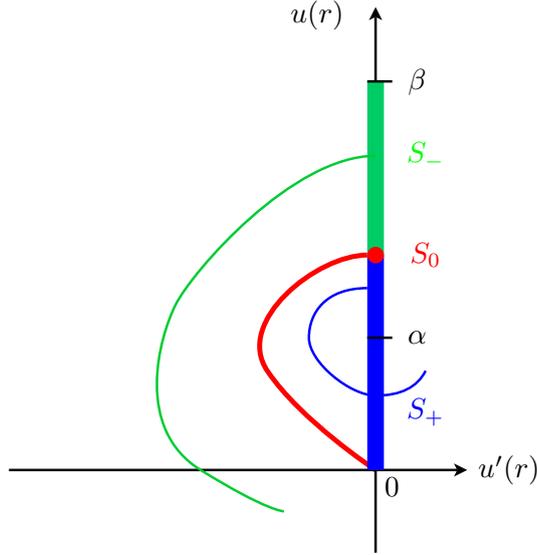


Figure A.2: Phase portrait of the solutions in the plane (u', u) . The interval $(0, \beta)$ is partitioned into the sets S_+ , S_- and S_0 . Solutions with an initial datum in S_+ cross first the vertical axis and stay positive for all times, whereas solutions in S_- cross first the horizontal axis. The set S_0 contains the solutions that stay in the quadrant for all times and converge to the origin. The goal is to prove that S_0 is reduced to one point as in the picture.

That this condition is necessary follows from the Pohozaev identity

$$\frac{d-2}{2d} \int_{\mathbb{R}^d} |\nabla u|^2 dx = \int_{\mathbb{R}^d} G(u(x)) dx \quad (\text{A.1.7})$$

which implies that $G(u(x))$ has to take positive values, it cannot be always negative (as it is for $x \rightarrow \infty$ since $G(s) \sim g'(0)s^2/2 < 0$ for $s \rightarrow 0$).

Finally, we recall that if $g \in C^{1+\varepsilon}$ for some $\varepsilon > 0$ and since $g(0) = 0$ and $g'(0) < 0$, it follows from the moving plane method [GNN81] that all the positive solutions to (A.1.1) are radial decreasing about some point in \mathbb{R}^d .

To conclude this Appendix, we give an idea of the proof of Theorem A.1.1. Since we are interested in proving the uniqueness and the non-degeneracy of positive radial solution to (A.1.1), we consider the associated ordinary differential equation

$$\begin{cases} u'' + \frac{d-1}{r}u' + g(u) = 0 \text{ on } \mathbb{R}_+^* \\ u'(0) = 0 \end{cases} \quad (\text{A.1.8})$$

and we focus on showing the uniqueness and non-degeneracy of positive solutions such that $(u(r), u'(r)) \rightarrow 0$ when $r \rightarrow \infty$. This system has a local energy, given by

$$H(r) = \frac{u'(r)^2}{2} + G(u(r)), \quad \text{with } G(\eta) = \int_0^\eta g(s) ds, \quad (\text{A.1.9})$$

which decreases along the trajectories, since

$$H'(r) = -\frac{d-1}{r}u'(r)^2 \leq 0.$$

We parametrize the solutions u_y to (A.1.8) by $u_y(0) = y$. Since we are interested in positive solution with $\|u_y\|_\infty < \beta$, then $y < \beta$. Hence, following [McL93; LR15b; LR20a], we introduce the three sets

$$\begin{aligned} S_+ &= \{y \in (0, \beta) : \min_{\mathbb{R}} u_y > 0\}, \\ S_0 &= \{y \in (0, \beta) : u_y > 0 \text{ and } \lim_{r \rightarrow +\infty} u_y(r) = 0\}, \\ S_- &= \{y \in (0, \beta) : u_y(r_y) = 0 \text{ for some (first) } r_y > 0\}, \end{aligned}$$

which form a partition of $(0, \beta)$. In case $y \in S_0$, we set $r_y = +\infty$. One should think of plotting the solution in the plane (u', u) as in Figure A.2. Then, as we will show, S_+ exactly correspond to all the solutions that cross the vertical axis, while staying above the horizontal axis at all times. On the other hand, S_- consists of those crossing the horizontal axis first (we will show they cannot cross the vertical axis before). We are particularly interested in the set S_0 containing the remaining solutions which are converging to the point $(0, 0)$ at infinity while staying in the quadrant $(u' < 0, u > 0)$. Our goal is indeed to show that S_0 is reduced to one point. A transition between S_- and S_+ is typically a point in S_0 and this is actually how one can prove the existence of solutions by the shooting method. Here we *assume* the existence of one such solution, hence we have $S_0 \neq \emptyset$. Points in S_0 typically occur as transition points between S_- and S_+ . The main idea of the proof is to show that for any $y \in S_0$, we must have

$$(y - \eta, y) \in S_+ \quad \text{and} \quad (y, y + \eta) \in S_- \quad (\text{A.1.10})$$

for some sufficiently small $\eta > 0$. In other words, there can only exist transitions from S_- to S_+ and never the other way around, when y is increased starting from $y = 0$. This will imply uniqueness. The way to show (A.1.10) is to prove that the variation with respect to the initial condition y ,

$$v_y := \frac{\partial}{\partial y} u_y, \quad (\text{A.1.11})$$

tends to $-\infty$ at infinity, as well as its derivative v_y' . This implies that the curves move enough to cross either the horizontal or the vertical axis when y is moved a bit, for a sufficiently large r . The function v_y in (A.1.11) turns out to be the zero-energy solution of the linearized operator $\Delta + g'(u)$ with $v(0) = 1$. The fact that v_y diverges implies $v_y \notin L^2(\mathbb{R}_+, r^{d-1} dr)$, which means that the kernel of $\Delta + g'(u)$ cannot contain any non-trivial radial function. It is then classical [Wei85] that this implies the non-degeneracy (A.1.5).

A.2. THE DOUBLE-POWER NONLINEAR SCHRÖDINGER EQUATION

The result described in Appendix A.1 applies to the nonlinear elliptic equation

$$-\Delta u = -u^p + u^q - \mu u \quad (\text{A.2.1})$$

with $p > q > 1$ and $\mu > 0$ and $u^p := |u|^{p-1}u$. This equation appears in a variety of practical situations, including density functional theory in quantum chemistry and condensed matter physics [Le 95; Ric18], Bose-Einstein condensates with three-body repulsive interactions [MI88], heavy-ion collisions processes [Kar84] and nonclassical nucleation near spinodal in mesoscopic models of phase transitions [MV04; CH59; vH92; CH93]. Uniqueness in this case was shown in [ST00], but the non-degeneracy of the solutions does not seem to follow from the proof. In the case of the cubic-quintic nonlinearity $q = 3, p = 5$, non-degeneracy was shown in [Kil+17] for $d = 3$ and in [CS20] for $d = 2$. On the other hand, the case $p = 7/3$ and $q = 5/3$ in dimension $d = 3$ was considered in [Ric18] in the context of symmetry breaking for a model of Density Functional Theory for solids. A general result which covers (A.2.1) appeared later in [ASW18].

The non-degeneracy property of the unique positive solution u_μ for the double-power nonlinearity (A.2.1) allows us to discuss the behavior of the L^2 mass

$$M(\mu) = \int_{\mathbb{R}^d} u_\mu(x)^2 dx$$

of this solution.

In particular, we are able to determine its exact behavior in the two regimes $\mu \rightarrow 0^+$ and $\mu \rightarrow \mu_*^-$, where μ_* is the threshold for existence of solutions.

One important motivation for studying the variations of M concerns the uniqueness of energy minimizers at fixed mass

$$I(\lambda) = \inf \left\{ \frac{1}{2} \int_{\mathbb{R}^d} |\nabla u|^2 dx + \frac{1}{p+1} \int_{\mathbb{R}^d} |u|^{p+1} dx - \frac{1}{q+1} \int_{\mathbb{R}^d} |u|^{q+1} dx : \right. \\ \left. u \in H^1(\mathbb{R}^d) \cap L^{p+1}(\mathbb{R}^d), \int_{\mathbb{R}^d} |u|^2 dx = \lambda \right\}, \quad (\text{A.2.2})$$

which naturally appears in physical applications. Any minimizer, when it exists, is positive and solves the double-power NLS equation for some Lagrange multiplier μ , hence equals u_μ after an appropriate space translation. The difficulty here is that several μ 's could in principle give the same mass λ and the same energy $I(\lambda)$, so that the uniqueness of solutions to the equation at fixed μ does not at all imply the uniqueness of energy minimizers.

The nonlinearity

$$g_\mu(u) = -u^p + u^q - \mu u \quad (\text{A.2.3})$$

satisfies the condition (H1) of Theorem A.1.1 hence, due to the Pohozaev identity (A.1.7), there exists a $\mu_* > 0$ such that (A.2.1) admits no nontrivial solutions for $\mu \geq \mu_*$, whereas it always has at least one positive solution for $\mu \in (0, \mu_*)$. The value of μ_* is given by

$$\mu_* = \frac{2(p+1)^{\frac{q-1}{p-q}} (q-1)^{\frac{q-1}{p-q}} (p-q)}{(q+1)^{\frac{p-1}{p-q}} (p-1)^{\frac{p-1}{p-q}}}. \quad (\text{A.2.4})$$

For $\mu = \mu_*$ what is happening is that the primitive

$$G_\mu(u) := -\frac{|u|^{p+1}}{p+1} + \frac{|u|^{q+1}}{q+1} - \frac{\mu}{2}|u|^2$$

becomes non-positive over the whole half line \mathbb{R}_+ , with a double zero at

$$\beta_* := \left(\frac{(q-1)(p+1)}{(q+1)(p-1)} \right)^{\frac{1}{p-q}} < 1. \quad (\text{A.2.5})$$

For all $0 < \mu \leq \mu_*$, the function g_μ is seen to have two zeroes $0 < \alpha_\mu < \beta_\mu$ such that

$$\begin{cases} \lim_{\mu \rightarrow 0^+} \alpha_\mu = 0, & \lim_{\mu \rightarrow \mu_*^-} \alpha_\mu = \alpha_* \in (0, \beta_*), \\ \lim_{\mu \rightarrow 0^+} \beta_\mu = 1, & \lim_{\mu \rightarrow \mu_*^-} \beta_\mu = \beta_*. \end{cases}$$

In addition, $\mu \mapsto \beta_\mu$ is *decreasing* over $(0, \mu_*)$.

A.2.1. BRANCH PARAMETRIZED BY THE LAGRANGE MULTIPLIER μ

The following result from [LR20a] is a corollary of Theorem A.1.1.

Theorem A.2.1 (Uniqueness and non-degeneracy). *Let $d \geq 2$, $p > q > 1$ and g_μ as in (A.2.3). For all $\mu \in (0, \mu_*)$, the nonlinear equation (A.2.1) has a unique positive solution u_μ tending to 0 at infinity, modulo space translations. It can be chosen radial-decreasing. It is non-degenerate:*

$$\begin{cases} \ker(-\Delta + pu_\mu^{p-1} - qu_\mu^{q-1} + \mu) = \text{span}\{\partial_{x_1}u_\mu, \dots, \partial_{x_d}u_\mu\}, \\ \ker(-\Delta + u_\mu^{p-1} - u_\mu^{q-1} + \mu) = \text{span}\{u_\mu\}. \end{cases} \quad (\text{A.2.6})$$

This solution satisfies

$$0 < u_\mu(x) < \beta_\mu < 1, \quad \forall x \in \mathbb{R}^d$$

and $u_\mu(0) \rightarrow \beta_*$ when $\mu \nearrow \mu_*$.

Existence was proved in [BL83; BGK83], while the uniqueness and the non-degeneracy of the solution follows from Theorem A.1.1. In particular, $g_\mu(u)$ satisfies the hypotheses of [GNN81] therefore all the positive solutions to (A.2.1) are radial decreasing about some point in \mathbb{R}^d . The function g_μ also satisfies hypothesis (H1) for some $0 < \alpha_\mu < \beta_\mu$ and it is negative on (β_μ, ∞) . Since g is C^∞ on $(0, \infty)$ and $u > 0$, we deduce from regularity theory that u is real-analytic on \mathbb{R}^d . We have $-\Delta u = g_\mu(u) < 0$ on the open ball $\{u > \beta_\mu\}$, hence u must be constant on this set, by the maximum principle. This definitely cannot happen for a real analytic function tending to 0 at infinity and therefore $u \leq \beta_\mu$ everywhere. The maximum of u can also not be equal to β_μ since otherwise $u \equiv \beta_\mu$ which is the unique corresponding solution to (A.2.1). We have therefore proved that all the positive solutions must satisfy $u < \beta_\mu$ and we are in position to apply Theorem A.1.1. A straightforward calculation show that g satisfies hypothesis (H2) (see [LR20a]).

This gives the proof of the uniqueness and non-degeneracy in Theorem A.2.1.

Since $\mu \mapsto \beta_\mu$ is decreasing and its limit at $\mu = 0$ is 1, we deduce that the family $(u_\mu)_\mu$ of solutions to (A.2.1) is uniformly bounded: $0 < u_\mu < \beta_\mu < 1$. If we denote by η_μ the first positive zero of G_μ , then we also have $u_\mu(0) \geq \eta_\mu$, since $G_\mu(u_\mu(0)) > 0$ by (A.1.7). Since $\eta_\mu \rightarrow \beta_*$ when $\mu \nearrow \mu_*$, we obtain $u_\mu(0) \rightarrow \beta_*$ when $\mu \nearrow \mu_*$.

Later in Theorem A.2.3 we will see that $u_\mu(x) \rightarrow \beta_*$ when $\mu \nearrow \mu_*$, for every $x \in \mathbb{R}^d$. The behavior of u_μ when $\mu \searrow 0$ depends on the parameters p and q , however, and will be given in Theorem A.2.2.

A.2.2. BEHAVIOR OF THE MASS

As we will see in Chapter 3, it is very important to understand how the mass of the solution u_μ

$$M(\mu) := \int_{\mathbb{R}^d} u_\mu(x)^2 dx \quad (\text{A.2.7})$$

varies with μ . In the case of the usual focusing NLS equation with one power nonlinearity q (which formally corresponds to $p = +\infty$ when $q < 2^* - 1$ since $u < 1$), the mass is an explicit function of μ by scaling:

$$M_{\text{NLS}}(\mu) = \mu^{\frac{4+d-dq}{2(q-1)}} \int_{\mathbb{R}^d} Q(x)^2 dx$$

where $-\Delta Q - Q^q + Q = 0$. There is no such simple relation for the double-power nonlinearity.

The importance of $M(\mu)$ is for instance seen in the Grillakis-Shatah-Strauss theory [Wei85; SS85; GSS87a; GSS90a; DGR15b] of stability for these solutions within the time-dependent Schrödinger equation. The latter says that the solution u_μ is *orbitally stable* when $M'(\mu) > 0$ and that it is *unstable* when $M'(\mu) < 0$. Therefore the intervals where M is increasing furnish stable solutions whereas those where M is decreasing correspond to unstable solutions. The Grillakis-Shatah-Strauss theory relies on another

conserved quantity, the energy, which is discussed in the next section and for which the variations of M also play a crucial role.

Note that the derivative can be expressed in terms of the linearized operator

$$\mathcal{L}_\mu := -\Delta - g'_\mu(u_\mu) = -\Delta + pu_\mu^{p-1} - qu_\mu^{q-1} + \mu$$

by

$$M'(\mu) = 2\Re \left\langle u_\mu, \frac{\partial}{\partial \mu} u_\mu \right\rangle = -2 \langle u_\mu, (\mathcal{L}_\mu)_{\text{rad}}^{-1} u_\mu \rangle. \quad (\text{A.2.8})$$

Here $(\mathcal{L}_\mu)_{\text{rad}}^{-1}$ denotes the inverse of \mathcal{L}_μ when restricted to the subspace of radial functions, which is well defined and bounded due to the non-degeneracy (A.2.6) of the solution.¹ This is why the non-degeneracy is crucial for understanding the variations of M . From the implicit function theorem, note that M is a real-analytic function on $(0, \mu_*)$.

Our main goal in [LR20a] was to understand the number of sign changes of M' , which tells us how many stable and unstable branches there are.

In order to make a conjecture concerning the number of roots of M' in terms of the exponents p and q and the dimension $d \geq 2$, it is useful to analyze the two regimes $\mu \rightarrow 0$ and $\mu \rightarrow \mu_*$, where one can expect some simplification.

In particular, in [LR20a] we obtain the following result which is an extension of results from [MM14], where the limit of u_μ in the regime $\mu \rightarrow 0$ was studied, but not that of M and M' .

Theorem A.2.2 (Behavior when $\mu \searrow 0$). *Let $d \geq 2$ and $p > q > 1$.*

• **(Sub-critical case)** *If $d = 2$, or if $d \geq 3$ and*

$$q < 1 + \frac{4}{d-2},$$

then the rescaled function

$$\frac{1}{\mu^{\frac{1}{q-1}}} u_\mu \left(\frac{x}{\sqrt{\mu}} \right) \quad (\text{A.2.9})$$

converges strongly in $H^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ in the limit $\mu \rightarrow 0$ to the function Q which is the unique positive radial-decreasing solution to the nonlinear Schrödinger (NLS) equation

$$\Delta Q + Q^q - Q = 0. \quad (\text{A.2.10})$$

We have

$$M(\mu) = \mu^{\frac{4+d-dq}{2(q-1)}} \int_{\mathbb{R}^d} Q^2 + \frac{2(p-1) + 4 + d - dq}{(p+1)(q-1)} \mu^{\frac{2(p-q)+4+d-dq}{2(q-1)}} \int_{\mathbb{R}^d} Q^{p+1} + o \left(\mu^{\frac{2(p-q)+4+d-dq}{2(q-1)}} \right)_{\mu \searrow 0} \quad (\text{A.2.11})$$

and

$$M'(\mu) = \frac{4+d-dq}{2(q-1)} \mu^{\frac{4+d-dq}{2(q-1)}-1} \int_{\mathbb{R}^d} Q^2 + \frac{(2(p-1) + 4 + d - dq)(2(p-q) + 4 + d - dq)}{2(p+1)(q-1)^2} \mu^{\frac{2(p-q)+4+d-dq}{2(q-1)}-1} \int_{\mathbb{R}^d} Q^{p+1} + o \left(\mu^{\frac{2(p-q)+4+d-dq}{2(q-1)}-1} \right)_{\mu \searrow 0}. \quad (\text{A.2.12})$$

¹The functions $\partial_{x_j} u_\mu$ spanning the kernel of \mathcal{L}_μ are orthogonal to the radial sector, hence 0 is not an eigenvalue of $(\mathcal{L}_\mu)_{\text{rad}}$. But then 0 belongs to its resolvent set, since the essential spectrum starts at $\mu > 0$.

In particular, M is increasing for $q \leq 1 + 4/d$ and decreasing for $q > 1 + 4/d$, in a neighborhood of the origin.

• **(Critical case)** If $d \geq 3$ and

$$q = 1 + \frac{4}{d-2},$$

then the rescaled function

$$\frac{1}{\epsilon_\mu^{\frac{d-2}{2}}} u_\mu \left(\frac{x}{\epsilon_\mu} \right) \quad (\text{A.2.13})$$

converges strongly in $\dot{H}^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ in the limit $\mu \rightarrow 0$ to the Sobolev optimizer

$$S(x) = \left(1 + \frac{|x|^2}{d(d-2)} \right)^{-\frac{d-2}{2}},$$

which is also the unique positive radial-decreasing solution (up to dilations) to the Emden-Fowler equation $\Delta S + S^q = 0$, where

$$\epsilon_\mu \sim c \begin{cases} \mu^{\frac{1}{p-3}} & \text{if } d = 3, \\ (\mu \log \mu^{-1})^{\frac{1}{p-1}} & \text{if } d = 4, \\ \mu^{\frac{q-1}{2(p-1)}} & \text{if } d \geq 5. \end{cases} \quad (\text{A.2.14})$$

Furthermore, we have

$$\lim_{\mu \searrow 0} M(\mu) = \lim_{\mu \searrow 0} -M'(\mu) = \infty. \quad (\text{A.2.15})$$

In particular, M is decreasing in a neighborhood of the origin.

• **(Super-critical case)** If $d \geq 3$ and

$$q > 1 + \frac{4}{d-2},$$

then u_μ converges strongly in $\dot{H}^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ in the limit $\mu \rightarrow 0$ to the unique positive radial-decreasing solution $u_0 \in \dot{H}^1(\mathbb{R}^d) \cap L^{p+1}(\mathbb{R}^d)$ of the ‘zero-mass’ double-power equation

$$-\Delta u_0 = -u_0^p + u_0^q$$

decaying like $u_0(x) = O(|x|^{2-d})$ at infinity. We have the limits

$$\lim_{\mu \searrow 0} M(\mu) = \int_{\mathbb{R}^d} u_0(x)^2 dx \begin{cases} = \infty & \text{if } d \in \{3, 4\}, \\ < \infty & \text{if } d \geq 5 \end{cases} \quad (\text{A.2.16})$$

and

$$\lim_{\mu \searrow 0} M'(\mu) = \begin{cases} -\infty & \text{if } d \in \{3, 4, 5, 6\}, \\ M'(0) \in \mathbb{R} & \text{if } d \geq 7. \end{cases} \quad (\text{A.2.17})$$

In particular, M is decreasing in a neighborhood of the origin when $d \in \{3, \dots, 6\}$. In dimensions $d \geq 7$, we have $M'(0) < 0$ under the additional condition

$$1 + \frac{4}{d-2} < q < p < 1 + \frac{4}{d-2} + \frac{32}{d(d-2)((d-2)q - d - 2)}. \quad (\text{A.2.18})$$

The condition (A.2.18) in the super-critical case is not at all expected to be optimal and it is only provided as an illustration. Although we are able to prove that M' admits a finite limit when $\mu \rightarrow 0$ in dimensions $d \geq 7$, we cannot determine its sign in the whole range of parameter. Numerical simulations provided in [LR20a] seem to indicate that $M'(0)$ can be positive. The limit $\mu \rightarrow 0$ for $M'(\mu)$ is quite delicate in the super-critical case, since the limiting linearized operator

$$\mathcal{L}_0 = -\Delta + p(u_0)^{p-1} - q(u_0)^{q-1}$$

has no gap at the origin. Its essential spectrum starts at 0. Nevertheless, we show in [LR20a] that u_0 is still *non-degenerate* in the sense that $\ker(\mathcal{L}_0) = \text{span}\{\partial_{x_1}u_0, \dots, \partial_{x_d}u_0\}$. This allows us to define $(\mathcal{L}_0)_{\text{rad}}^{-1}$ by the functional calculus and to prove that, as expected,

$$M'(0) = -2\langle u_0, (\mathcal{L}_0)_{\text{rad}}^{-1}u_0 \rangle,$$

where the right side is interpreted in the sense of quadratic forms. In dimensions $d \geq 5$ there are no resonances and $(\mathcal{L}_0)_{\text{rad}}^{-1}$ essentially behaves like $(-\Delta)_{\text{rad}}^{-1}$ at low momenta [Jen80]. Since $\langle u_0, (-\Delta)^{-1}u_0 \rangle$ is finite only in dimensions $d \geq 7$ due to the slow decay of u_0 at infinity, $M'(0)$ is only finite in those dimensions.

Next, in [LR20a], we studied the behavior of the branch of solutions in the limit $\mu \nearrow \mu_*$.

Theorem A.2.3 (Behavior when $\mu \nearrow \mu_*$). *Let $d \geq 2$ and $p > q > 1$. Let μ_* and β_* be the two critical constants defined in (A.2.4) and (A.2.5), respectively. Then we have*

$$\lim_{\mu \nearrow \mu_*} (\mu_* - \mu)^d M(\mu) = \lim_{\mu \nearrow \mu_*} \frac{(\mu_* - \mu)^{d+1}}{d} M'(\mu) = \Lambda \quad (\text{A.2.19})$$

where

$$\Lambda := 2^{\frac{3d}{2}} \frac{|\mathbb{S}^{d-1}|}{d} (\beta_*)^{2(1-d)} (d-1)^d \left(\int_0^{\beta_*} |G_{\mu_*}(s)|^{\frac{1}{2}} ds \right)^d. \quad (\text{A.2.20})$$

Let $\gamma \in (0, \beta_*)$ be any constant and call R_μ the unique radius such that $u_\mu(R_\mu) = \gamma$. Then we have

$$R_\mu = \frac{\rho}{\mu_* - \mu} + o\left(\frac{1}{\mu_* - \mu}\right), \quad \rho = \frac{2\sqrt{2}(d-1)}{\beta_*^2} \int_0^{\beta_*} \sqrt{|G_{\mu_*}(s)|} ds, \quad (\text{A.2.21})$$

and the uniform convergence

$$\lim_{\mu \rightarrow \mu_*} \|u_\mu - U_*(|x| - R_\mu)\|_{L^\infty(\mathbb{R}^d)} = 0, \quad (\text{A.2.22})$$

where U_* is the unique solution to the one-dimensional limiting problem

$$\begin{cases} U_*'' + g_{\mu_*}(U_*) = 0 & \text{on } \mathbb{R} \\ U_*(-\infty) = \beta_* \\ U_*(+\infty) = 0 \\ U_*(0) = \gamma \in (0, \beta_*) \end{cases} \quad (\text{A.2.23})$$

This result says is that u_μ resemble a *radial translation* of the one-dimensional solution U_* , which links the two unstable stationary solutions β_* and 0 of the underlying Hamiltonian system. Since U_* tends to β_* at $-\infty$, we see that $u_\mu(r)$ tends to β_* for every fixed r , as we claimed earlier, and this is why the mass diverges like

$$M(\mu) \underset{\mu \rightarrow \mu_*}{\sim} (R_\mu)^d (\beta_*)^2 \frac{|\mathbb{S}^{d-1}|}{d}.$$

Plugging the asymptotics of R_μ from (A.2.21) then provides (A.2.19).

Upper and lower bounds on $M(\mu)$ in terms of $(\mu_* - \mu)^{-d}$ were derived in [Kil+17] in the case $d = 3$, $p = 5$ and $q = 3$ but the exact limit (A.2.19) is new, to our knowledge.

Theorem A.2.3 implies that M is always increasing close to μ_* , hence in this region we obtain an orbitally stable branch for the Schrödinger flow, for every $p > q > 1$.

As remarked in Subsection 2.3.5, the same arguments used in the proof of theorem A.2.3 can be adapted to show a saturation effect for nuclear matter.

More generally our proof of Theorem A.2.3 works the same for a function in the form $g_\mu(u) = g_0(u) - \mu u$ with

- $g_0 \in C^1([0, \infty)) \cap C^2(0, \infty)$ with $g_0(0) = g_0'(0) = 0$ and $g_0(s) \rightarrow -\infty$ when $s \rightarrow +\infty$;
- g_μ has exactly two roots $0 < \alpha_\mu < \beta_\mu$ on $(0, \infty)$ with $g_\mu'(\alpha_\mu) > 0$ and $g_\mu'(\beta_\mu) < 0$ for all $\mu \in (0, \mu_*)$ where μ_* is the first μ so that $G_\mu(r) = \int_0^r g_\mu(s) ds \leq 0$ for all $r \geq 0$;
- $\Delta u + g_\mu(u) = 0$ has a unique non-degenerate radial positive solution for every $\mu \in (0, \mu_*)$ (for instance g_μ satisfies (H2) in Theorem A.1.1 for all $\mu \in (0, \mu_*)$).

Theorems A.2.2 and A.2.3 and the fact that M is a smooth function on $(0, \mu_*)$ imply some properties of solutions to the equation $M(\mu) = \lambda$, whenever λ is either small or large. Those are summarized in the following

Corollary A.2.4 (Number of solutions to $M(\mu) = \lambda$). *Let $d \geq 2$ and $p > q > 1$. The equation*

$$M(\mu) = \lambda$$

- *admits a unique solution μ for λ small enough when $1 < q < 1 + \frac{4}{d}$, and it is stable, $M'(\mu) > 0$;*
- *admits a unique solution μ for λ large enough when*

$$\begin{cases} 1 < q \leq 1 + \frac{4}{d}, \\ q > 1 + \frac{4}{d-2} \text{ and } d \geq 5, \end{cases}$$

and it is stable, $M'(\mu) > 0$;

- *admits exactly two solutions $\mu_1 < \mu_2$ for λ large enough when*

$$\begin{cases} q > 1 + \frac{4}{d} \text{ and } d \in \{2, 3, 4\}, \\ 1 + \frac{4}{d} < q \leq 1 + \frac{4}{d-2} \text{ and } d \geq 5, \end{cases}$$

which are respectively unstable and stable: $M'(\mu_1) < 0$, $M'(\mu_2) > 0$.

Once we have determined the exact behavior of M at the two end points of its interval of definition, it seems natural to expect that the following conjecture, given in [LR20a], holds true.

Conjecture 2 (Behavior of M). *Let $d \geq 2$ and $p > q > 1$. Then M' is either positive on $(0, \mu_*)$, or vanishes at a unique $\mu_c \in (0, \mu_*)$ with*

$$M' \begin{cases} < 0 & \text{on } (0, \mu_c), \\ > 0 & \text{on } (\mu_c, \mu_*). \end{cases} \quad (\text{A.2.24})$$

More precisely:

- *If $q \leq 1 + 4/d$, then $M' > 0$ on $(0, \mu_*)$.*
- *If $d \in \{2, \dots, 6\}$ and $q > 1 + 4/d$, or if $d \geq 7$ and $1 + 4/d < q \leq 1 + 4/(d-2)$, then M' vanishes exactly once.*
- *If $d \geq 7$ and $q > 1 + 4/(d-2)$, there exists a $p_c(q) \geq q$ such that M' vanishes once for $q < p < p_c(q)$ and does not vanish for $p > p_c(q)$.*

The property (A.2.24) is an immediate consequence of Theorems A.2.2 and A.2.3 whenever M' vanishes only once. The conjecture was put forward in [Kil+17; CS20] for the quintic-cubic NLS equation ($p = 5, q = 3$) in dimensions $d \in \{2, 3\}$, and in [Ric18] for $d = 3, p = 7/3, q = 5/3$. These cases have been confirmed by numerical simulations [And71; MI88; Kil+17; Ric18].

In [LR20a] we provide a selection of numerical simulations of the function M in dimensions $d \in \{2, 3, 5, 7\}$ which seem to confirm the conjecture. Although we have run many more simulations and could never disprove the conjecture, we have however not investigated all the possible powers and dimensions in a systematical way.

A.2.3. THE DOUBLE-POWER ENERGY FUNCTIONAL

Since the larger power p is defocusing and always controls the smaller focusing nonlinearity of exponent q , the double-power NLS equation (A.2.1) has a natural variational interpretation in the whole possible range of powers. In particular, consider the energy functional

$$\mathcal{E}(u) = \frac{1}{2} \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx + \frac{1}{p+1} \int_{\mathbb{R}^d} |u(x)|^{p+1} dx - \frac{1}{q+1} \int_{\mathbb{R}^d} |u(x)|^{q+1} dx$$

and the corresponding minimization problem

$$I(\lambda) := \inf_{\substack{u \in H^1(\mathbb{R}^d) \cap L^{p+1}(\mathbb{R}^d) \\ \int_{\mathbb{R}^d} |u|^2 = \lambda}} \mathcal{E}(u) \quad (\text{A.2.25})$$

at fixed mass $\lambda \geq 0$. This problem is well posed for all $p > q > 1$ because we can write

$$\mathcal{E}(u) = \frac{1}{2} \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx - \int_{\mathbb{R}^d} G_{\mu_*}(u(x)) dx - \frac{\mu_* \lambda}{2} \geq -\frac{\mu_* \lambda}{2}.$$

Recall that μ_* in (A.2.4) is precisely the lowest μ for which $G_\mu \leq 0$ on \mathbb{R}_+ . The minimization problem (A.2.25) appears naturally in applications, for instance in condensed matter physics for $d = 3, p = 7/3$ and $q = 5/3$ where it can be obtained from the Thomas-Fermi-von Weisäcker-Dirac functional of atoms, molecules and solids, in a certain limit of a large Dirac term (see [Ric18; GLN20] and references therein).

The existence of minimizers, obtained in [LR20a], follows from rather standard methods of nonlinear analysis.

Theorem A.2.5 (Existence of minimizers for $I(\lambda)$). *Let $d \geq 2$ and $p > q > 1$. The function $\lambda \mapsto I(\lambda)$ is concave non-increasing over $[0, \infty)$. It satisfies*

- $I(\lambda) = 0$ for all $0 \leq \lambda \leq \lambda_c$,
- $\lambda \mapsto I(\lambda)$ is negative and strictly decreasing on (λ_c, ∞) ,

where

$$\lambda_c \begin{cases} = 0 & \text{if } q < 1 + 4/d, \\ = \int_{\mathbb{R}^d} Q^2 & \text{if } q = 1 + 4/d, \\ \in (0, \infty) & \text{if } q > 1 + 4/d, \end{cases}$$

with Q the same NLS function as in Theorem A.2.2. The problem $I(\lambda)$ admits at least one positive radial-decreasing minimizer u for every

$$\lambda \begin{cases} \geq \lambda_c & \text{if } q \neq 1 + 4/d, \\ > \lambda_c & \text{if } q = 1 + 4/d. \end{cases}$$

Any minimizer u solves the Euler-Lagrange equation (A.2.1) for some $\mu \in (0, \mu_*)$, hence must be equal to u_μ . The infimum is not attained for $\lambda < \lambda_c$ or for $\lambda = \lambda_c$ and $q = 1 + 4/d$.

The main difficulty in the proof of Theorem A.2.5 is to deal with the case $\lambda = \lambda_c$ in particular when $q \geq 1 + 4/d$. It is then useful to give a characterization of λ_c in terms of optimizers of the Gagliardo-Nirenberg-type inequality

$$\|u\|_{L^{q+1}(\mathbb{R}^d)}^{q+1} \leq C_{p,q,d} \|u\|_{L^2(\mathbb{R}^d)}^{q-1-\theta(p-1)} \|\nabla u\|_{L^2(\mathbb{R}^d)}^{2(1-\theta)} \|u\|_{L^{p+1}(\mathbb{R}^d)}^{\theta(p+1)} \quad (\text{A.2.26})$$

when $q \geq 1 + 4/d$, with

$$\theta = \frac{q-1-\frac{4}{d}}{p-1-\frac{4}{d}} \in [0, 1).$$

At $q = 1 + 4/d$ we have $\theta = 0$ and obtain the usual Gagliardo-Nirenberg inequality, of which Q is the unique optimizer.

A very natural question is to ask whether minimizers of $I(\lambda)$ are *unique*, up to space translations and multiplication by a phase factor. This does not follow from the uniqueness of u_μ at fixed μ because the minimizers could have different multipliers μ 's. The concavity of I implies that it is differentiable except for countably many values of λ . When the derivative exists and $\lambda > \lambda_c$, it can be seen that the minimizer is unique and given by u_μ with $\mu = -2I'(\lambda)$. Details will be provided later in Theorem A.2.6 where we actually show that the derivative can only have finitely many jumps in (λ_c, ∞) .

Another natural question is to ask whether one solution u_μ could be a candidate for the minimization problem $I(\lambda)$ with $\lambda = M(\mu)$. From the non-degeneracy of u_μ , the answer (see, e.g. [Wei85, App. E]) is that when $M'(\mu) > 0$ the corresponding solution u_μ is a *strict local minimum* of \mathcal{E} at fixed mass $\lambda = M(\mu)$, whereas when $M'(\mu) < 0$, the solution u_μ is a saddle point. In particular, there must always hold $M'(\mu) \geq 0$ for a minimizer u_μ of $I(\lambda)$.

From this discussion, we see that the following would immediately follow from Conjecture 2.

Conjecture 3 (Uniqueness of minimizers). *Let $d \geq 2$ and $p > q > 1$. Then $I(\lambda)$ admits a unique minimizer for all $\lambda \geq \lambda_c$ (resp. $\lambda > \lambda_c$ if $q = 1 + 4/d$).*

In [LR20a], although we were not able to prove this conjecture, we obtain the following uniqueness result.

Theorem A.2.6 (Partial uniqueness of minimizers). *Let $d \geq 2$ and $p > q > 1$. Then $I(\lambda)$ admits a unique positive radial minimizer when*

- λ is large enough;
- $q < 1 + 4/d$ and $\lambda \in [0, \epsilon)$,
- $q \geq 1 + 4/d$ and $\lambda \in (\lambda_c, \lambda_c + \epsilon)$

for some $\epsilon > 0$ small enough. In fact, $I(\lambda)$ has a unique positive radial minimizer for all $\lambda \in [\lambda_c, \infty)$ (resp. $\lambda \in (\lambda_c, \infty)$ when $q = 1 + 4/d$), except possibly at finitely many points in $[\lambda_c, \infty)$. At those values, the number of positive radial minimizers is also finite. For any $\lambda \in (\lambda_c, \infty)$ we have

$$I'(\lambda^-) = -\frac{1}{2} \min \{ \mu : \mathcal{E}(u_\mu) = I(\lambda), M(\mu) = \lambda \},$$

and

$$I'(\lambda^+) = -\frac{1}{2} \max \{ \mu : \mathcal{E}(u_\mu) = I(\lambda), M(\mu) = \lambda \}.$$

In order to better understand the ideas behind the proof of Theorem A.2.6, it is useful to introduce the energy

$$E(\mu) := \mathcal{E}(u_\mu), \quad \mu \in (0, \mu_*)$$

of our branch of solutions u_μ . Note that

$$E'(\mu) = -\frac{\mu}{2}M'(\mu), \quad (\text{A.2.27})$$

that is, the variations of E are exactly opposite to those of M . The following is a simple consequence of Theorems A.2.2 and A.2.3 together with (A.2.27).

Corollary A.2.7 ($E(\mu)$ at 0 and μ_*). *Let $d \geq 2$ and $p > q > 1$.*

- When $\mu \searrow 0$, we have

$$\lim_{\mu \rightarrow 0^+} E(\mu) = \begin{cases} \mathcal{E}(u_0) = \frac{1}{d} \int_{\mathbb{R}^d} |\nabla u_0|^2 & \text{if } d \geq 3 \text{ and } q > 1 + \frac{4}{d-2}, \\ \frac{1}{d} \int_{\mathbb{R}^d} |\nabla S|^2 & \text{if } d \geq 3 \text{ and } q = 1 + \frac{4}{d-2}, \\ 0 & \text{otherwise.} \end{cases}$$

Moreover

$$E(\mu) \begin{cases} < 0 & \text{for } q \leq 1 + 4/d, \\ > 0 & \text{for } q > 1 + 4/d, \end{cases}$$

for μ in a neighborhood of the origin.

- When $\mu \nearrow \mu_*$, we have

$$E(\mu) \underset{\mu \rightarrow \mu_*}{\sim} -\frac{\mu_* \Lambda}{2(\mu_* - \mu)^d}$$

where Λ is the same constant as in Theorem A.2.3.

- $\mu \mapsto E(\mu)$ is real-analytic on $(0, \mu_*)$ and the equation $E(\mu) = e$ always has finitely many solutions for any $e \in (-\infty, \max E]$.

We see that Conjecture 3 would follow if we could prove that

- E is decreasing for $q \leq 1 + 4/d$;
- E has a unique positive zero and is decreasing on the right side of this point, for $q > 1 + 4/d$.

Note that when $q > 1 + 4/d$, Conjecture 3 is really weaker than Conjecture 2 on the mass $M(\mu)$, since the places where $E(\mu) > 0$ do not matter for the minimization problem $I(\lambda)$.

The main difficult part in the proof of Theorem A.2.6 is the fact that there can be at most finitely many λ 's for which uniqueness does not hold. This is done by strongly using the real-analyticity and the behavior of M close to 0 and μ_* from Theorems A.2.2 and A.2.3 (see [LR20a] for more details).

If λ is large or small, the statement follows immediately from Corollary A.2.4 (and the fact that $M'(\mu) \geq 0$ at a minimizer u_μ for $I(\lambda)$ in case there are two solutions to the equation $M(\mu) = \lambda$).

If $q = 1 + 4/d$, we know from Theorems A.2.2 and A.2.5 that $\lambda_c = \int_{\mathbb{R}^d} Q^2 = M(0)$ and we prove in [LR20a] that minimizers for λ close to λ_c necessarily have μ small enough, so that the conclusion follows from the monotonicity of M close to the origin, by Theorem A.2.2.

For every $\lambda > \lambda_c$, the number of μ 's such that $E(\mu) = I(\lambda) < 0$ is finite by Corollary A.2.7. The same holds at λ_c when $q \geq 1 + 4/d$. Hence $I(\lambda)$ always admits finitely many positive radial minimizers.

To conclude it is interesting to remark that from Theorem A.2.3 we find

$$I(\lambda) = -\frac{\mu_* \lambda}{2} + \lambda^{1-\frac{1}{d}} \sqrt{2} \left(\frac{\beta_*^2}{d} \right)^{\frac{1}{d}-1} |\mathbb{S}^{d-1}|^{\frac{1}{d}} \int_0^{\beta_*} |G_{\mu_*}(s)|^{\frac{1}{2}} ds + o\left(\lambda^{1-\frac{1}{d}}\right)_{\lambda \rightarrow \infty} \quad (\text{A.2.28})$$

after inverting the function $\lambda = M(\mu)$ in the neighborhood of μ_* . This can also be derived using a variational argument *à la Modica-Mortola* [MM77; Mod87; KS89]. For instance, letting $v(x) = u(\lambda^{-1/d}x)$ we can rewrite

$$I(\lambda) = -\frac{\mu_* \lambda}{2} + \lambda^{1-\frac{1}{d}} \inf_{\int_{\mathbb{R}^d} |v|^2 = 1} \left\{ \frac{\lambda^{-\frac{1}{d}}}{2} \int_{\mathbb{R}^d} |\nabla v(x)|^2 dx - \lambda^{\frac{1}{d}} \int_{\mathbb{R}^d} G_{\mu_*}(v(x)) dx \right\}$$

and then (A.2.28) follows after adapting [Mod87] to the L^2 constraint. Our analysis in Theorem A.2.3 is however more precise since no scaling of u_μ is needed for the conclusion. It can actually be applied to the general phase transition minimization problems studied in [Mod87], in the case of L^2 constraints.

ORBITAL STABILITY IN HAMILTONIAN PDES WITH SYMMETRY

This chapter is a summary of the articles [DGR15b; DR19b]. It is devoted to the study of the orbital stability of relative equilibria of Hamiltonian dynamical systems on Banach spaces, in the presence of an invariance group for the dynamics.

3.1. INTRODUCTION

The purpose of [DGR15b] was to provide an introduction to the theory of orbital stability of relative equilibria, a notion from the theory of (mostly Hamiltonian) dynamical systems with symmetry that finds its origins in the study of planetary motions [AM78]. In more recent times it has proven important in two new ways at least. It has on the one hand found an elegant reformulation in the modern framework of Hamiltonian mechanics of finite dimensional systems with symmetry in terms of symplectic geometry. It can indeed be phrased and studied in terms of the theory of momentum maps and of symplectic reduction [AM78; LM87]. On the other hand, it also underlies the stability analysis of plane waves, of travelling wave solutions and of solitons in infinite dimensional nonlinear Hamiltonian PDE's, which has received considerable attention over the last forty years or so, and continues to be a very active area of research.

It is clear that in this field nonlinear analysis can be expected to meet geometry in interesting and beautiful ways. It nevertheless appears that in the literature on Hamiltonian PDE's, the simple and elegant geometric ideas underlying the proofs of orbital stability aren't emphasized. The goal of [DGR15b] was to provide a unified formulation of the theory in a sufficiently general but not too abstract framework that allows one to treat finite and infinite dimensional systems on the same footing. In this manner, one may hope to harness the geometric intuition readily gained from treating finite dimensional systems and use it as a guide when dealing with the infinite dimensional ones that are the main focus of our interest, but that demand more sophisticated technical tools from functional analysis and PDE theory.

3.1.1. NOTIONS OF STABILITY

There are many notions of stability for dynamical systems. One may in particular consider stability with respect to perturbations in the vector field generating the dynamics, or stability with respect to a variation in the initial conditions. It is the latter one we shall be considering here.

The simplest possible definition of stability in this context is presumably the following. Let E be a normed vector space, d the corresponding metric on E , and X a vector field on E . Let $u \in E$ and $t \in \mathbb{R} \rightarrow u(t) \in E$ a flow line of X (i.e. $\dot{u}(t) = X(u(t))$, with $u(0) = u$). Let us assume the flow is well-defined globally, with $u(t) = \Phi_t^X(u)$. Then one says that the initial condition u is stable if for all $\epsilon > 0$, there exists a $\delta > 0$ so that, for all $v \in E$,

$$d(v, u) \leq \delta \Rightarrow \sup_{t \in \mathbb{R}} d(v(t), u(t)) \leq \epsilon. \quad (3.1.1)$$

Here $v(t) = \Phi_t^X(v)$. This can be paraphrased as follows: once close, forever not too far. Note that, if u is stable in this sense, then so is $u(t)$ for all $t \in \mathbb{R}$. There exists one situation where proving stability is straightforward. It is the case where $u = u_*$ is a fixed point of the dynamics, meaning $u(t) = u_*$, for all $t \in \mathbb{R}$, and where u_* is a local non-degenerate minimum of a constant of the motion, that is a function $\mathcal{L} : E \rightarrow \mathbb{R}$, referred to as a *Lyapunov function*, satisfying $\mathcal{L}(v(t)) = \mathcal{L}(v)$ for all $t \in \mathbb{R}$, and for all v in a neighborhood of u_* . Let us sketch the argument, which is classic. Supposing $\mathcal{L} \in C^2(E, \mathbb{R})$ and that $D_{u_*}^2 \mathcal{L}$ is positive definite, one obtains from a Taylor expansion of \mathcal{L} about u_* an estimate of the type

$$cd(v, u_*)^2 \leq \mathcal{L}(v) - \mathcal{L}(u_*) \leq Cd(v, u_*)^2, \quad (3.1.2)$$

for all v in a neighborhood of u_* . Then, for v sufficiently close to u_* , one can easily show, using an argument by contradiction, that $v(t)$ stays in this neighborhood and hence, for all t ,

$$cd(v(t), u_*)^2 \leq \mathcal{L}(v(t)) - \mathcal{L}(u_*) = \mathcal{L}(v) - \mathcal{L}(u_*) \leq Cd(v, u_*)^2, \quad (3.1.3)$$

from which (3.1.1) follows immediately. This approach is known as the Lyapunov method for proving stability.¹

In Hamiltonian systems, at least one constant of the motion always exists, namely the Hamiltonian itself. The above argument leads therefore to the perfectly standard result that local minima of the Hamiltonian are stable fixed points of the dynamics. All orbital stability results discussed in [DGR15b; DR19b] are, *in fine*, based on this single argument, appropriately applied and combined with additional geometric properties of (Hamiltonian) systems with symmetry, and, of course, with an appropriate dose of (functional) analysis.

A stronger version of stability than (3.1.1) is an asymptotic one, and goes as follows: there exists a $\delta > 0$ so that, for all $v \in E$,

$$d(v, u) \leq \delta \Rightarrow \lim_{t \rightarrow +\infty} d(v(t), u(t)) = 0.$$

This phenomenon can only occur in dissipative systems. When u is a fixed point of the dynamics, it corresponds to requiring it is attractive. If the flow line issued from u is periodic, one obtains a limit cycle. So in this second definition, the idea is that, if two points start close enough, they end up together. Since our focus here is on Hamiltonian systems, where such behavior cannot occur (because volumes are preserved), we shall not discuss it further. Note, however, that another notion of ‘‘asymptotic stability’’ has been introduced and studied in the context of Hamiltonian nonlinear dispersive PDEs. We shall briefly comment on this later.

There are several cases when definition (3.1.1) is too strong, and a weaker notion is needed, referred to as *orbital stability*. The simplest definition of this notion goes as follows. Suppose $t \in \mathbb{R} \rightarrow u(t) \in E$ is a flow line of the dynamics and consider the dynamical orbit

$$\gamma = \{u(t) \mid t \in \mathbb{R}\}.$$

We say $u = u(0)$ is orbitally stable if the following holds. For all $\epsilon > 0$, there exists $\delta > 0$, so that

$$d(v, u) < \delta \Rightarrow \forall t \in \mathbb{R}, d(v(t), \gamma) \leq \epsilon. \quad (3.1.4)$$

¹Remark that $\mathcal{L}(v(t)) \leq \mathcal{L}(v)$ would suffice in (3.1.3). But in these notes we will exclusively work with constants of the motion.

The point here is that the new dynamical orbit $\tilde{\gamma} = \{v(t) \mid t \in \mathbb{R}\}$ stays close to the initial one, while possibly $v(t)$ can drift away from $u(t)$, for the same value of the time t . As we will see, this can be expected to be the rule since the nearby orbit may no longer be periodic even if the original one was, or have a different period. A simple example that can be understood without computation is this. Think of two satellites on circular orbits around the earth. Imagine the radii are very close. Then the periods of both motions will be close but different. Both satellites will eternally move on their respective circles, which are close, but they will find themselves on opposite sides of the earth after a long enough time, due to the difference in their angular speeds. In addition, a slight perturbation in the initial condition of one of the satellites will change its orbit, which will become elliptical, and again have a different period. But the new orbit will stay close to the original circle. So here the idea is this: if an initial condition v is chosen close to u , then at all later times t , $v(t)$ is close to *some* point on γ , but not necessarily close to $u(t)$, for the same value of t .

3.1.2. SYMMETRIES AND RELATIVE EQUILIBRIA

The definition of orbital stability in (3.1.4) turns out to be too strong still for many applications, in particular in the presence of symmetries of the dynamics. This is notably the case in the study of solitons and standing or travelling wave solutions of nonlinear Hamiltonian differential or partial differential equations. We will therefore present an appropriate generalization of the notion of orbital stability in the presence of symmetries in Section 3.2. For that purpose, we introduce dynamical systems Φ_t^X , $t \in \mathbb{R}$ on Banach spaces E , which admit an invariance group G with an action Φ_g , $g \in G$ on E , i.e. $\Phi_g \Phi_t^X = \Phi_t^X \Phi_g$. We then say $u \in E$ is a *relative equilibrium* if, for all $t \in \mathbb{R}$, $\Phi_t^X(u) \in \mathcal{O}_u$, where $\mathcal{O}_u = \Phi_G(u)$ is the group orbit of u under the action of G . As we will see, solitons, travelling waves and plane waves are relative equilibria. We say a relative equilibrium u is *orbitally stable* if initial conditions $v \in E$ close to u have the property that for all $t \in \mathbb{R}$, $\Phi_t^X(v)$ remains close to \mathcal{O}_u . Note that the larger the symmetry group G is, the weaker is the corresponding notion of stability. As said above, in addition to orbital stability, the stronger property of *asymptotic (orbital) stability* has also been investigated in the context of Hamiltonian nonlinear dispersive PDEs. Roughly speaking, a relative equilibrium u is (orbitally) asymptotically stable if it is orbitally stable and any solutions starting close to its orbit eventually resolves into a “modulation” of the original wave u and a purely dispersive part, solution of the linear version of the governing equation.

The main goal of [DGR15b] was to present a general framework allowing to establish orbital stability of such *relative equilibria* of (both finite and infinite) dynamical systems with symmetry, using an appropriate generalization of the Lyapunov method sketched above. This approach to stability is often referred to as the *energy-momentum method*. In the process, we wished to clearly separate the part of the argument which is abstract and very general, from the part that is model-dependent. We will also indicate for which arguments one needs the dynamics to be Hamiltonian and which ones go through more generally.

The main ingredient in the proof of orbital stability is the existence of a *coercive Lyapunov function* \mathcal{L} , which is a group-invariant constant of the motion satisfying an appropriately generalized coercive estimate. In applications, the proof of orbital stability is thus reduced to the construction of such a function.

It is in this step that the geometry of Hamiltonian dynamical systems with symmetry plays a crucial role. Indeed, the construction of an appropriate Lyapunov function for such systems exploits the special link that exists between their constants of the motion F and their symmetries, as embodied in Noether’s theorem and the theory of the momentum map. This is briefly explained in Section 3.2 below. The crucial observation is then that in Hamiltonian systems, relative equilibria tend to come in families $u_\mu \in E$, indexed by the value μ of the constants of the motion at u_μ . In fact, it turns out that $u_\mu \in E$ is a relative equilibrium of a Hamiltonian system if (and only if) u_μ is a critical point of the restriction of the Hamiltonian to the level surface $\Sigma_\mu = \{u \in E \mid F(u) = \mu\}$ of these constants of the motion (Theorem 3.2.1). This observation at once yields the candidate Lyapunov function \mathcal{L}_μ .

In [DGR15b], we finally explained (see Proposition 3.2.2 below) how the proof of the coercivity of the Lyapunov function can be obtained from a suitable lower bound on its second derivatives $D^2\mathcal{L}_\mu(w, w)$,

with w restricted to an appropriate subspace of E , using familiar arguments from the theory of Lagrange multipliers. This ends the very general, geometric and abstract part of the theory. To prove this *local coercivity* property on $D^2\mathcal{L}_\mu(w, w)$ finally requires an often difficult, problem-dependent, and detailed spectral analysis of the Hessian of the Lyapunov function.

Nevertheless, one can show that, in the case Hamiltonian systems with a one-dimensional symmetry group, the local coercivity is implied from the so-called *Vakhitov-Kolokolov slope condition* [GSS87b; Stu08; VK73]. Roughly speaking this consists of studying the sign of the variation of the constant of the motion F with respect to μ .

The goal of [DR19b] was to present a natural generalization of this condition to the case where the Hamiltonian system admits a higher dimensional invariance group and to show how to obtain orbital stability from it.

3.2. THE ENERGY-MOMENTUM METHOD

In [DGR15b], we proposed a description of the energy-momentum method which is summarized in this section.

3.2.1. HAMILTONIAN SYSTEMS WITH SYMMETRY

Let E be a Banach space, \mathcal{D} a domain in E (*i.e.* a dense subset of E) and \mathcal{J} a symplector, that is an injective continuous linear map $\mathcal{J} : E \rightarrow E^*$ such that $(\mathcal{J}u)(v) = -(\mathcal{J}v)(u)$. We will refer to $(E, \mathcal{D}, \mathcal{J})$ as a *symplectic Banach triple*. Next, let $H : E \rightarrow \mathbb{R}$ be differentiable on $\mathcal{D} \subset E$. In other words, H is globally defined on E , and differentiable at each point $u \in \mathcal{D}$. We say that the function H has a \mathcal{J} -compatible derivative if, for all $u \in \mathcal{D}$, $D_u H \in \mathcal{R}_{\mathcal{J}}$, where $\mathcal{R}_{\mathcal{J}}$ is the range of \mathcal{J} . In that case we write $H \in \text{Dif}(\mathcal{D}, \mathcal{J})$.

We define a *Hamiltonian flow* for $H \in \text{Dif}(\mathcal{D}, \mathcal{J})$ as a separately continuous map $\Phi^H : \mathbb{R} \times E \rightarrow E$ with the following properties:

- (i) For all $t, s \in \mathbb{R}$, $\Phi_{t+s}^H = \Phi_t^H \circ \Phi_s^H$, $\Phi_0^H = \text{Id}$;
- (ii) For all $t \in \mathbb{R}$, $\Phi_t^H(\mathcal{D}) = \mathcal{D}$;
- (iii) For all $u \in \mathcal{D}$, the curve $t \in \mathbb{R} \rightarrow u(t) := \Phi_t^H(u) \in \mathcal{D} \subset E$ is differentiable and is the unique solution of

$$\mathcal{J}\dot{u}(t) = D_{u(t)}H, \quad u(0) = u. \quad (3.2.1)$$

Note that here and below, $D_u H \in E^*$ is our notation for the derivative of H at u . We refer to (3.2.1) as the Hamiltonian differential equation associated to H and to its solutions as Hamiltonian flow lines.

Next, let G be a Lie group, \mathfrak{g} the Lie algebra of G and $\Phi : (g, x) \in G \times E \rightarrow \Phi_g(x) \in E$, an action of G on E . In what follows we will suppose all Lie groups are connected. We will say Φ is a *globally Hamiltonian action* if the following conditions are satisfied:

- (i) For all $g \in G$, $\Phi_g \in C^1(E, E)$ is symplectic.
- (ii) For all $g \in G$, $\Phi_g(\mathcal{D}) = \mathcal{D}$.
- (iii) For all $\xi \in \mathfrak{g}$, there exists $F_\xi \in C^1(E, \mathbb{R}) \cap \text{Dif}(\mathcal{D}, \mathcal{J})$ such that $\Phi_{\exp(t\xi)} = \Phi_t^{F_\xi}$ is a Hamiltonian flow as defined above and the map $\xi \rightarrow F_\xi$ is linear.

Here and in what follows, we say $\Psi \in C^0(E, E) \cap C^1(\mathcal{D}, E)$ is a symplectic transformation if

$$\forall u \in \mathcal{D}, \forall v, w \in E, (\mathcal{J}D_u\Psi(v))(D_u\Psi(w)) = (\mathcal{J}v)(w). \quad (3.2.2)$$

Note that, in the above definition of globally Hamiltonian action, $\Psi = \Phi_g \in C^1(E, E)$. For further reference, we introduce, for all $u \in \mathcal{D}$ and for all $\xi \in \mathfrak{g}$,

$$X_\xi(u) = \frac{d}{dt} \Phi_{\exp(\xi t)}(u)|_{t=0}. \quad (3.2.3)$$

It follows from the preceding definitions that

$$X_\xi(u) = \mathcal{J}^{-1} D_u F_\xi. \quad (3.2.4)$$

We will always suppose G is a matrix group, in fact, a subgroup of $GL(\mathbb{R}^N)$. We can then think of the Lie algebra \mathfrak{g} as a sub-algebra of the $N \times N$ matrices $\mathcal{M}(N, \mathbb{R})$ and define the adjoint action of G on \mathfrak{g} via

$$\text{Ad}_g \xi = g \xi g^{-1},$$

where in the right-hand side we have a product of matrices. We will write $m = \dim \mathfrak{g} = \dim \mathfrak{g}^*$, where \mathfrak{g}^* designates the vector space dual of the Lie algebra \mathfrak{g} . For details, we refer to Section A.2 of [DGR15b], [AM78] or [LM87]. Note that, for each $u \in E$ fixed, one can think of $\xi \in \mathfrak{g} \rightarrow F_\xi(u) \in \mathbb{R}$ as an element of \mathfrak{g}^* . Hence, if we identify (as we always will) \mathfrak{g} and \mathfrak{g}^* with \mathbb{R}^m and view F as a map $F : E \rightarrow \mathbb{R}^m \simeq \mathfrak{g}^*$, we can write

$$F_\xi = \xi \cdot F,$$

where \cdot refers to the canonical inner product on \mathbb{R}^m . The map F is called the momentum map of the symplectic group action and, in what follows, we will suppose that F is Ad^* -equivariant which means that for all $g \in G$, for all $\xi \in \mathfrak{g}$

$$F_\xi \circ \Phi_g = F_{\text{Ad}_{g^{-1}} \xi},$$

or equivalently, $F \circ \Phi_g = \text{Ad}_g^* F$. Here Ad^* is the co-adjoint action of G on \mathfrak{g}^* .

Now, for all $\mu \in \mathfrak{g}^*$, we define the isotropy group or stabilizer of μ as

$$G_\mu = \{g \in G \mid \text{Ad}_g^* \mu = \mu\};$$

\mathfrak{g}_μ is the Lie algebra of G_μ , and \mathfrak{g}_μ^* its dual. Finally, for all $\mu \in \mathfrak{g}^* \simeq \mathbb{R}^m$, let

$$\Sigma_\mu = \{u \in E \mid F(u) = \mu\}.$$

We will say μ is a *regular value* of F if $\Sigma_\mu \neq \emptyset$ and if, for all $u \in \Sigma_\mu$, $D_u F$ is surjective (maximal rank). Then Σ_μ is a codimension m sub-manifold of E and its tangent space at $u \in \Sigma_\mu$ is

$$T_u \Sigma_\mu = \text{Ker } D_u F. \quad (3.2.5)$$

Finally, since the momentum map is Ad^* -equivariant, it is easy to see $G_\mu = G_{\Sigma_\mu}$, where G_{Σ_μ} is the subgroup of G leaving Σ_μ invariant.

Below, G will be an invariance group of H , in the sense that $H \circ \Phi_g = H$, for all $g \in G$. This implies G is an invariance group for the dynamics generated by H , meaning that for all $g \in G, t \in \mathbb{R}$, $\Phi_g \circ \Phi_t^H = \Phi_t^H \circ \Phi_g$ (See Theorem 3.2.1 (i) below). Noether's Theorem then implies that the components F_i of the moment map are constants of the motion (See Theorem 3.2.1 (ii)) and hence that, for any $\mu \in \mathbb{R}^m \simeq \mathfrak{g}^*$, the level set Σ_μ is invariant under the dynamics Φ_t^H . See [DGR15b; DR19b] and below for examples.

3.2.2. RELATIVE EQUILIBRIA AND ORBITAL STABILITY

Let G be an invariance group for the dynamics Φ_t^H , as above, and let \tilde{G} be a subgroup of G . Let $u \in E$ and let $\mathcal{O}_u^{\tilde{G}} = \Phi_{\tilde{G}}(u)$ be the \tilde{G} -orbit of u . We say u is a relative \tilde{G} -equilibrium of the dynamics if,

for all $t \in \mathbb{R}$, $\Phi_t^H(u) \in \mathcal{O}_u^{\tilde{G}}$. In other words, if the dynamical trajectory through u lies in the group orbit $\mathcal{O}_u^{\tilde{G}}$.

The goal is to investigate under which circumstances these relative equilibria are orbitally stable. A relative \tilde{G} -equilibrium $u \in E$ is orbitally stable if

$$\forall \varepsilon > 0, \exists \delta > 0, \forall v \in E, \left(d(v, u) \leq \delta \Rightarrow \forall t \in \mathbb{R}, d(v(t), \mathcal{O}_u^{\tilde{G}}) \leq \varepsilon \right),$$

with $v(t)$ the solution of the Hamiltonian equation of motion with initial condition $v(0) = v$. Here $d(\cdot, \cdot)$ is the distance function induced by the norm on E . Note that the definitions of relative equilibrium and of orbital stability are increasingly restrictive as the subgroup \tilde{G} is taken smaller. Sharper statements are therefore obtained by choosing smaller subgroups \tilde{G} .

It turns out that, if H is G invariant and the action of G is Ad^* -equivariant, then u is a G -relative equilibrium if and only if u is a G_μ -relative equilibrium, where $\mu = F(u)$ (See Theorem 7 in [DGR15b]). This observation, familiar from the finite dimensional theory (See for instance [AM78; LM87]), explains why it is natural to try to prove G_μ -orbital stability. This is the approach we shall adopt here. It differs from the one in [GSS90b], where orbital stability is studied with respect to an a priori different subgroup, as we will explain in detail in Section 3.7. We will also show there that in many situations of interest, the two subgroups actually coincide.

We will write

$$\mathcal{O}_u = \Phi_{G_\mu}(u), \quad (3.2.6)$$

where $\mu = F(u)$. And, for all $u \in \mathcal{D}$,

$$T_u \mathcal{O}_u = \{X_\xi(u) \mid \xi \in \mathfrak{g}_\mu\} \subset E. \quad (3.2.7)$$

For later reference, we recall the following definitions.

Definition 1. We say F is regular at $u \in E$ if $D_u F$ is of maximal rank. We say μ is a regular value of F , if for all $u \in \Sigma_\mu$, $D_u F$ is of maximal rank. We will refer to relative equilibria u for which $D_u F$ is of maximal rank, as *regular relative equilibria*.

To understand what follows, it is helpful to keep in mind that in practice, the action of the invariance group G is well known explicitly, and typically linear and isometric. The dynamical flow Φ_t^H , on the other hand, is a complex object one tries to better understand using the invariance properties of H .

In [DGR15b], we obtained some results which give a characterization of the relative equilibria of Hamiltonian systems with symmetry and which also yield the candidate Lyapunov function that can be used to study their stability. They are collected in the following theorem.

Theorem 3.2.1. *Let $(E, \mathcal{D}, \mathcal{J})$ be a symplectic Banach triple. Let $H \in C^1(E, \mathbb{R}) \cap \text{Dif}(\mathcal{D}, \mathcal{J})$ and suppose H has a Hamiltonian flow Φ_t^H . Let furthermore G be a Lie group, and Φ a globally Hamiltonian action on E with Ad^* -equivariant momentum map F . Suppose that,*

$$\forall g \in G, \quad H \circ \Phi_g = H. \quad (3.2.8)$$

- (i) *Then G is an invariance group for Φ_t^H .*
- (ii) *For all $t \in \mathbb{R}$, $F \circ \Phi_t^H = F$.*
- (iii) *u is a relative G -equilibrium if and only if u is a relative G_μ -equilibrium.*
- (iv) *Let $u \in \mathcal{D} \subset E$. If there exists $\xi \in \mathfrak{g}$ so that*

$$D_u H - \xi \cdot D_u F = 0, \quad (3.2.9)$$

then u is a relative G_μ -equilibrium. Let $\mu = F(u) \in \mathbb{R}^m \simeq \mathfrak{g}^$; if μ is a regular value of F , then u is a critical point of H_μ on Σ_μ , where $H_\mu = H|_{\Sigma_\mu}$.*

Equation (3.2.9) is referred to as the stationary equation in the PDE literature. The theorem states that its solutions determine relative G - and hence relative G_μ -equilibria.

Note that (i) and (ii) are simply a version of Noether's Theorem in this framework. The proof of (iii) is straightforward and use the fact that F is a constant of the motion which is Ad^* -equivariant.

We now turn to the stability analysis of those relative equilibria. Suppose we are given $\xi \in \mathfrak{g}$ and u_ξ , solution of (3.2.9). We first note that the fact that u_ξ is a critical point of the restriction H_{μ_ξ} of the Hamiltonian H to Σ_{μ_ξ} ($\mu_\xi = F(u_\xi)$) is an immediate consequence of the observation that u_ξ is a critical point of the Lagrange function

$$\mathcal{L}_\xi = H - \xi \cdot F : E \rightarrow \mathbb{R}. \quad (3.2.10)$$

The goal is now to prove that these relative equilibria are orbitally stable. As pointed out in [DGR15b], the basic idea underlying the energy-momentum method is that, modulo technical problems, a relative equilibrium is expected to be stable if it is not only a critical point but actually a local minimum of H_{μ_ξ} . To establish such a result, it is natural to use the second variation of the Lagrange multiplier theory and to establish that the Hessian of \mathcal{L}_ξ is positive definite when restricted to $T_{u_\xi} \Sigma_{\mu_\xi} \cap T_{u_\xi} \mathcal{O}_{u_\xi}^\perp$. The precise statement is given in Proposition 3.2.2 below.

Let $\langle \cdot, \cdot \rangle$ be a scalar product on E , which is continuous in the sense that

$$\forall v, w \in E, \quad |\langle v, w \rangle| \leq \|v\|_E \|w\|_E, \quad (3.2.11)$$

where $\|\cdot\|_E$ is our notation for the Banach norm on E . Note that E is not necessarily a Hilbert space for this inner product. In addition, even if $(E, \|\cdot\|_E)$ is in fact a Hilbert space with the norm $\|\cdot\|_E$ coming from an inner product $\langle \cdot, \cdot \rangle_E$, the second inner product $\langle \cdot, \cdot \rangle$ is not necessarily equal to $\langle \cdot, \cdot \rangle_E$.

Let $\|\cdot\|$ be the norm associated to the scalar product $\langle \cdot, \cdot \rangle$ and define \hat{E} to be the closure of E with respect to the $\|\cdot\|$ -norm, that is

$$\|\cdot\| = \sqrt{\langle \cdot, \cdot \rangle}, \quad \hat{E} = \overline{E}^{\|\cdot\|}. \quad (3.2.12)$$

Note that \hat{E} is a Hilbert space and $E \subset \hat{E}$. As an example, one can think of $E = H^1(\mathbb{R}^n)$ and $\langle \cdot, \cdot \rangle = \langle \cdot, \cdot \rangle_{L^2(\mathbb{R}^n)}$ so that $\hat{E} = L^2(\mathbb{R}^n)$ in that case. This is the typical situation for the nonlinear Schrödinger equation; we refer to [DGR15b] and Section 3.6 for details.

For further reference, we collect our main structural assumptions in the following hypotheses:

Hypothesis A. Let $(E, \mathcal{J}, \mathcal{D}, \langle \cdot, \cdot \rangle, H, G, \Phi, F)$ and suppose:

- (i) $(E, \mathcal{J}, \mathcal{D})$ is a symplectic Banach triple and $\langle \cdot, \cdot \rangle$ a continuous scalar product on $(E, \|\cdot\|_E)$ as in (3.2.11).
- (ii) $H \in C^2(E, \mathbb{R}) \cap \text{Dif}(\mathcal{D}, \mathcal{J})$
- (iii) G is a Lie group, and Φ a globally Hamiltonian G -action on E with Ad^* -equivariant momentum map $F \in C^2(E, \mathbb{R}^m)$.
- (iv) $H \circ \Phi_g = H$ for all $g \in G$.

Hypothesis B. Φ_g is linear and preserves both the structure $\langle \cdot, \cdot \rangle$ and the norm $\|\cdot\|_E$ for all $g \in G$.

One then has:

Proposition 3.2.2. *Suppose Hypotheses A and B hold. Let $\xi \in \mathfrak{g}$ and suppose $u_\xi \in \mathcal{D}$ satisfies (3.2.9), i.e. $D_{u_\xi} \mathcal{L}_\xi = 0$, with $\mathcal{L}_\xi = H - \xi \cdot F$. Let $\mu_\xi = F(u_\xi) \in \mathbb{R}^m \simeq \mathfrak{g}^*$ and suppose μ_ξ is a regular value of F . Suppose in addition that*

$$(i) \quad g \in G_{\mu_\xi} \rightarrow \Phi_g(u_\xi) \in E \text{ is } C^2.$$

$$(ii) \quad \forall j = 1, \dots, m,$$

$$\exists \nabla F_j(u_\xi) \in E \text{ such that } D_{u_\xi} F_j(w) = \langle \nabla F_j(u_\xi), w \rangle \quad \forall w \in E; \quad (3.2.13)$$

(iii) *There exists $C > 0$ so that*

$$\forall w \in E, \quad D_{u_\xi}^2 \mathcal{L}_\xi(w, w) \leq C \|w\|_E^2;$$

(iv) There exists $c > 0$ so that

$$\forall w \in T_{u_\xi} \Sigma_{\mu_\xi} \cap (T_{u_\xi} \mathcal{O}_{u_{\mu_\xi}})^\perp, \quad D_{u_\xi}^2 \mathcal{L}_\xi(w, w) \geq c \|w\|_E^2, \quad (3.2.14)$$

where

$$(T_{u_\xi} \mathcal{O}_{u_\xi})^\perp = \{z \in E \mid \langle z, y \rangle = 0, \forall y \in T_{u_\xi} \mathcal{O}_{u_\xi}\}. \quad (3.2.15)$$

Then there exist $\epsilon > 0, c > 0$ so that

$$\forall u \in \mathcal{O}_{u_\xi}, \forall u' \in \Sigma_{\mu_\xi}, \quad d(u, u') \leq \epsilon \Rightarrow H(u') - H(u) \geq cd^2(u', \mathcal{O}_{u_{\mu_\xi}}). \quad (3.2.16)$$

This result, contained in [DR19b], constitutes a generalization of Proposition 5 in [DGR15b]. In fact, if G_μ is commutative, the latter result applies immediately. If not, the mild regularity condition (i) of the proposition suffices to obtain the result. Note that the proof of Proposition 3.2.2 is based on geometric arguments and does not depend on the model considered.

The basic message of this result is the following. If G is an invariance group for H that has a globally Hamiltonian action on E and if u_ξ satisfies the stationary equation $D_{u_\xi} \mathcal{L}_\xi = 0$ for some $\xi \in \mathfrak{g}$, then, modulo the technical conditions of the proposition, the coercive estimate (3.2.14) on the Hessian of \mathcal{L}_ξ implies that the restriction of the Hamiltonian H to the constraint surface Σ_{μ_ξ} attains a local minimum on the G_{μ_ξ} -orbit \mathcal{O}_{u_ξ} . As explained in Section 8 of [DGR15b], modulo some further technical conditions, (3.2.16) allows one to show that u_ξ is G_{μ_ξ} -orbitally stable by using \mathcal{L}_ξ as a Lyapunov function. (See in particular Theorem 10 and Theorem 11 in [DGR15b]).

The difficulty in proving (3.2.14) comes from the fact that, in general, the bilinear symmetric form $D_{u_\xi}^2 \mathcal{L}_\xi$ is not positive on E , but has instead a non-trivial negative cone

$$\mathcal{C}_- = \{v \in E \mid D_{u_\xi}^2 \mathcal{L}_\xi(v, v) < 0\}.$$

The estimate (3.2.14) implies that $T_{u_\xi} \Sigma_{\mu_\xi}$ does not intersect \mathcal{C}_- . To prove this, we shall show that there exists a maximally negative subspace of E for $D_{u_\xi}^2 \mathcal{L}_\xi$ which is $D_{u_\xi}^2 \mathcal{L}_\xi$ -orthogonal to $T_{u_\xi} \Sigma_{\mu_\xi}$.

The main goal is then to give a condition that implies the local coercivity estimate (3.2.14). When the symmetry group is one-dimensional the condition is known as *Vakhitov-Kolokolov slope condition* (see [DGR15b]). In [DR19b], we generalized the Vakhitov-Kolokolov slope condition to higher dimensional setting (see Theorem 3.3.1 (iv) and Theorem 3.4.2 (iv) below). This condition is in general easier to verify than the coercivity estimate itself and allows one to prove the orbital stability of relative equilibria of general Hamiltonian system. As an example of this method we illustrate in Section 3.6 the applications of the results of [DGR15b; DR19b] to the stability analysis of relative equilibria of the nonlinear Schrödinger equation.

3.3. LOCAL COERCIVITY IN THE HILBERT SPACE SETTING

In this section, we present the main result of [DR19b] (Theorem 3.3.1 below) in the setting where E is a Hilbert space, with inner product $\langle \cdot, \cdot \rangle_E$, and $\|\cdot\|_E = \sqrt{\langle \cdot, \cdot \rangle_E}$. In particular, the inner product $\langle \cdot, \cdot \rangle$ in (3.2.11) and in Hypothesis A is, in this section, equal to $\langle \cdot, \cdot \rangle_E$. The Hilbert space structure will be used mainly to control the Hessian of \mathcal{L}_ξ through the spectral analysis of the associated bounded self-adjoint operator $\nabla^2 \mathcal{L}_\xi$ (see below). This makes for a simpler statement and proof than in the more general setting of Section 3.4, and allows for an easier understanding of the philosophy of the result. We point out that the result we obtain in Theorem 3.3.1 may be of interest also in finite dimensional problems ($\dim E < +\infty$). Indeed, the usual orbital stability results in the literature on finite dimensional Hamiltonian dynamical systems reduce their proof to the coercivity estimate (3.2.14) on the Hessian of \mathcal{L}_ξ , which is of dimension $\dim E$. We reduce the problem here to a control on the Hessian of the function W (see (3.3.3)), which is of dimension $m = \dim G$, typically much lower than $\dim E$, especially when the latter is high-dimensional.

We start with some preliminaries. We will make use of the following hypothesis:

Hypothesis C. There exists an open set $\Omega \subset \mathfrak{g} \simeq \mathbb{R}^m$ and a map $\tilde{u} \in C^1(\Omega \subset \mathfrak{g}, E)$

$$\tilde{u} : \xi \in \Omega \subset \mathfrak{g} \rightarrow u_\xi \in \mathcal{D} \subset E \quad (3.3.1)$$

satisfying, for all $\xi \in \Omega$,

$$D_{u_\xi} H - \xi \cdot D_{u_\xi} F = 0. \quad (3.3.2)$$

As recalled in section 3.2, if u_ξ is a solution to (3.3.2), then u_ξ is G_μ -relative equilibrium with $\mu = \mu_\xi = F(u_\xi)$.

So our starting point is equation (3.3.2), which in PDE applications is often an elliptic partial differential equation and we suppose we have an m -parameter family of solutions, indexed by ξ . One of the major difficulties to apply the theory is of course to find such families of solutions. In many cases, one has one single such solution for $\xi_* \in \mathfrak{g}$ and one needs to ensure there exists a neighborhood Ω of ξ_* for which such solutions exist. We will come back to this property of ‘‘persistence of relative equilibria’’ in Section 3.5 and present results ensuring Hypothesis C is satisfied. For now, we will suppose this is the case. Next, consider the Lyapunov function \mathcal{L}_ξ defined by (3.2.10) and remark that each u_ξ solution to (3.3.2) is a critical point of \mathcal{L}_ξ . Moreover, define for all $\xi \in \Omega \subset \mathfrak{g}$, the map

$$W : \xi \in \Omega \subset \mathfrak{g} \rightarrow \mathcal{L}_\xi(u_\xi) \in \mathbb{R}. \quad (3.3.3)$$

Note that

$$W(\xi) = H(u_\xi) - \xi \cdot \hat{F}(\xi),$$

where

$$\hat{F} : \xi \in \Omega \subset \mathfrak{g} \rightarrow F(u_\xi) \in \mathfrak{g}^* \simeq \mathbb{R}^m. \quad (3.3.4)$$

For each $\xi \in \Omega$, the Hessian $D_\xi^2 W$ of W is a bilinear form on \mathbb{R}^m . Hence, we can consider the following decomposition

$$\mathbb{R}^m = W_- \oplus W_0 \oplus W_+,$$

where W_0 is the kernel of $D_\xi^2 W$ and where $D_\xi^2 W$ is positive (negative) definite on W_+ (W_-). Let $d_0(D_\xi^2 W), p(D_\xi^2 W), n(D_\xi^2 W)$ be the dimensions of these spaces. Note that the decomposition is not unique, but the respective dimensions are. In other words, W_\pm are maximal positive/negative definite spaces for $D_\xi^2 W$. Also, in order not to burden the notation, we have not made the ξ -dependence of the spaces W_0, W_\pm explicit. Recall that, given a symmetric bilinear form B on a Banach space E , a subspace \mathcal{X} of E is said to be a positive (negative) definite subspace for B on E if $B|_{\mathcal{X} \times \mathcal{X}}$ is positive (negative) definite. A subspace is maximally positive (negative) definite if it is positive (negative) definite and it is not contained in any other positive (negative) definite subspace.

Similarly, the Hessian $D_u^2 \mathcal{L}_\xi$ of \mathcal{L}_ξ is a symmetric bilinear form on E . For each $u \in E$, we define as usual the Morse index $n(D_u^2 \mathcal{L}_\xi)$ of u for \mathcal{L}_ξ as the dimension of a maximally negative definite subspace for $D_u^2 \mathcal{L}_\xi$ in E .

Finally, when E is a Hilbert space, we can define for each $u \in E$ a bounded self-adjoint operator $\nabla^2 \mathcal{L}_\xi(u)$ by

$$\langle v, \nabla^2 \mathcal{L}_\xi(u)w \rangle_E = D_u^2 \mathcal{L}_\xi(v, w). \quad (3.3.5)$$

As a consequence, we can consider the spectral decomposition of E for $\nabla^2 \mathcal{L}_\xi(u_\xi)$

$$E = E_- \oplus E_0 \oplus E_+ \quad (3.3.6)$$

with $E_0 = \text{Ker} \nabla^2 \mathcal{L}_\xi(u_\xi) = \text{Ker} D_{u_\xi}^2 \mathcal{L}_\xi$, and E_\pm the positive and negative spectral subspaces of $\nabla^2 \mathcal{L}_\xi(u)$. Clearly E_\pm are maximally positive/negative subspaces for $\nabla_{u_\xi}^2 \mathcal{L}_\xi$ so that $n(D_{u_\xi}^2 \mathcal{L}_\xi) = \dim E_-$.

The main result of [DR19b] in the Hilbert space setting is the following theorem.

Theorem 3.3.1. *Suppose $(E, \langle \cdot, \cdot \rangle_E)$ is a Hilbert space and that Hypotheses A and C hold. Let $\xi \in \Omega$ and suppose*

- (i) $D_\xi^2 W$ is non-degenerate,
- (ii) $\text{Ker} D_{u_\xi}^2 \mathcal{L}_\xi = T_{u_\xi} \mathcal{O}_{u_\xi}$,
- (iii) $\inf(\sigma(\nabla^2 \mathcal{L}_\xi(u_\xi)) \cap (0, +\infty)) > 0$,
- (iv) $p(D_\xi^2 W) = n(D_{u_\xi}^2 \mathcal{L}_\xi)$.

Then there exists $\delta > 0$ such that

$$\forall v \in T_{u_\xi} \Sigma_{\mu_\xi} \cap (T_{u_\xi} \mathcal{O}_{u_\xi})^\perp, \quad D_{u_\xi}^2 \mathcal{L}_\xi(v, v) \geq \delta \|v\|_E^2. \quad (3.3.7)$$

We will say a relative equilibrium is *non-degenerate* when $D_\xi^2 W$ is non-degenerate. Since (3.3.7) is the same as (3.2.14), one can then use Proposition 3.2.2 together with Theorems 10 and 11 of [DGR15b] to show that u_ξ is orbitally stable. It is the fourth condition of the above theorem that generalizes the Vakhitov-Kolokolov slope condition, as we now explain. Suppose the group G is 1-dimensional, so that $m = 1$. Then W is a scalar function of $\xi \in \mathbb{R} \simeq \mathfrak{g}$. A straightforward calculation gives

$$W''(\xi) = -\hat{F}'(\xi).$$

Hence, the proof of orbital stability for u_ξ reduces to verifying that the spectral conditions on $\nabla_\xi^2 \mathcal{L}_\xi$ are satisfied and notably that $\dim E_- = 1$, and that

$$\hat{F}'(\xi) < 0. \quad (3.3.8)$$

This is the Vakhitov-Kolokolov slope condition. In applications to the Schrödinger equation, where $F(u) = \frac{1}{2} \langle u, u \rangle$, it says that the norm of u_ξ decreases as a function of ξ . In the case $m = 1$, the above result is proven in [GSS87b] (Corollary 3.3.1) and in [Stu08] (Proposition 5.2).

The setup of the Hamiltonian dynamics with higher dimensional symmetry on a Hilbert space we used in this section is similar to the one proposed in [GSS90b] where the decomposition (3.3.6) of the bounded self-adjoint operator $\nabla^2 \mathcal{L}_\xi(u_\xi)$ as well as condition (iii) of Theorem 3.3.1 are also used to obtain a coercivity result of the type (3.3.7). Nevertheless, in [GSS90b] a different constraint surface and orbit are used and some of the arguments provided are incomplete: for a complete comparison between Theorem 3.3.1 and the coercivity results of [GSS90b], we refer to Section 3.7.

We finally note that, when E is infinite dimensional, and the equation under study a PDE, the more general formulation of Section 3.4 is often considerably more pertinent than the simpler Hilbert space formulation proposed here. Indeed, the operator $\nabla^2 \mathcal{L}_\xi(u_\xi)$ introduced in Theorem 3.3.1 is not a partial differential operator (it is bounded) making the analysis of its spectrum generally less convenient than for the operator $\nabla^2 \mathcal{L}_\xi(u_\xi)$ in Theorem 3.4.5, which in applications is a self-adjoint partial differential operator on a suitable auxiliary Hilbert space. We will come back to this point when treating examples in Section 3.6.

One of the key ingredient of the proof of Theorem 3.3.1 is the fact that for all $\eta_1, \eta_2 \in \mathbb{R}^m$,

$$D_{u_\xi}^2 \mathcal{L}_\xi(\eta_1 \cdot \nabla_\xi u_\xi, \eta_2 \cdot \nabla_\xi u_\xi) = -D_\xi^2 W(\eta_1, \eta_2). \quad (3.3.9)$$

To obtain (3.3.9), it is sufficient to take the derivative of the stationary equation (3.3.2) with respect to $\xi \in \mathfrak{g}$ and use that, for all $\eta_1, \eta_2 \in \mathbb{R}^m$,

$$D_\xi^2 W(\eta_1, \eta_2) = -D_{u_\xi} \eta_1 \cdot F(\eta_2 \cdot \nabla_\xi u_\xi). \quad (3.3.10)$$

In other words,

$$D_\xi^2 W = -D_\xi \hat{F}. \quad (3.3.11)$$

This also proves that $D_\xi^2 W$ is non-degenerate if and only if \hat{F} is a local diffeomorphism at ξ .

Now, let $n_- = \dim E_-$ and $\{\eta_1, \dots, \eta_{n_-}\} \subset \mathbb{R}^m$ a family of linearly independent elements of \mathbb{R}^m such that $D_\xi^2 W(\eta, \eta) > 0$ for all $\eta \in \text{span}\{\eta_1, \dots, \eta_{n_-}\}$. As a consequence of (3.3.9),

$$\mathcal{X}_- := \text{span} \{ \eta_1 \cdot \nabla_\xi u_\xi, \dots, \eta_{n_-} \cdot \nabla_\xi u_\xi \}$$

is a negative definite subspace for $D_{u_\xi}^2 \mathcal{L}_\xi$ in E . Moreover, since $\dim \mathcal{X}_- = n_-$, \mathcal{X}_- is a maximally negative definite subspace.

Next, using that \hat{F} is a local diffeomorphism, one can prove that $\mathcal{X}_- \cap T_{u_\xi} \Sigma_{\mu_\xi} = \{0\}$ and conclude that $T_{u_\xi} \Sigma_{\mu_\xi}$ is a positive subspace for $D_{u_\xi}^2 \mathcal{L}_\xi$.

Furthermore, since by hypothesis (ii) of the theorem, $E_0 = \text{Ker } D_{u_\xi}^2 \mathcal{L}_\xi = T_{u_\xi} \mathcal{O}_{u_\xi}$, it follows that

$$\mathcal{Y} := T_{u_\xi} \Sigma_{\mu_\xi} \cap (T_{u_\xi} \mathcal{O}_{u_\xi})^\perp \quad (3.3.12)$$

is a positive definite subspace for $D_{u_\xi}^2 \mathcal{L}_\xi$, meaning that

$$D_{u_\xi}^2 \mathcal{L}_\xi(v, v) > 0, \quad \forall v \in \mathcal{Y} = T_{u_\xi} \Sigma_{\mu_\xi} \cap (T_{u_\xi} \mathcal{O}_{u_\xi})^\perp, v \neq 0. \quad (3.3.13)$$

To obtain the desired coercive bound, we then use the spectral information on $\nabla^2 \mathcal{L}_\xi(u_\xi)$ provided by the hypotheses of the theorem (see [DR19b] for more details).

3.4. LOCAL COERCIVITY IN A MORE GENERAL SETTING

In this section, we present the extension of Theorem 3.3.1 to a more general setting that we now describe. In order to state the main result of [DR19b], we first need to associate to $D_{u_\xi}^2 \mathcal{L}_\xi$ a (typically unbounded) self-adjoint operator on \hat{E} .

Lemma 3.4.1. *Suppose Hypothesis A holds. Let $\xi \in \mathfrak{g}$ and \mathcal{L}_ξ as in (3.2.10) and let $u \in E$. If there exist $\varepsilon, C > 0$ such that*

$$D_u^2 \mathcal{L}_\xi(v, v) \geq \varepsilon \|v\|_E^2 - C \|v\|^2 \quad (3.4.1)$$

for all $v \in E$, then there is a self-adjoint operator $\nabla^2 \mathcal{L}_\xi(u) : \mathcal{D}(\nabla^2 \mathcal{L}_\xi(u)) \subset \hat{E} \rightarrow \hat{E}$ defined by

$$\begin{aligned} \mathcal{D}(\nabla^2 \mathcal{L}_\xi(u)) &= \{z \in E \mid \exists w \in \hat{E} \text{ such that } D_u^2 \mathcal{L}_\xi(z, v) = \langle w, v \rangle \text{ for all } v \in E\}, \\ \nabla^2 \mathcal{L}_\xi(u)z &= w \text{ for all } z \in \mathcal{D}(\nabla^2 \mathcal{L}_\xi(u)). \end{aligned} \quad (3.4.2)$$

Moreover, $\mathcal{D}(\nabla^2 \mathcal{L}_\xi(u_\xi))$ is a form core for $D_u^2 \mathcal{L}_\xi$.

Remark 5. *Note that*

1. E is the form domain of the operator $\nabla^2 \mathcal{L}_\xi(u)$,
2. Since $\mathcal{D}(\nabla^2 \mathcal{L}_\xi(u))$ is a form core for $D_u^2 \mathcal{L}_\xi$ and condition (3.4.1) holds, $\mathcal{D}(\nabla^2 \mathcal{L}_\xi(u))$ is dense in E (see [Kat80, Chapter VI] for details).

The existence and the uniqueness of the operator $\nabla^2 \mathcal{L}_\xi(u)$ is a consequence of the First Representation theorem in Kato [Kat80, Theorem 2.1 and 2.6 in Chapter VI]. Condition (3.4.1) ensures that the hypotheses of the First Representation theorem are satisfied (see [Stu08, Lemma 3.3]). See also [RS80a; Tes09] for more details.

We can now state the main result of [DR19b]. We define $p(D_\xi^2 W)$, $n(D_\xi^2 W)$, W , and $n(D_{u_\xi}^2 \mathcal{L}_\xi)$ as in Section 3.3.

Theorem 3.4.2. *Suppose Hypotheses A,B,C hold. Let $\xi \in \Omega$ and suppose*

$$D_{u_\xi}^2 \mathcal{L}_\xi(v, v) \geq \varepsilon \|v\|_E^2 - C \|v\|^2, \forall v \in E. \quad (3.4.3)$$

Suppose in addition that

- (i) $D_\xi^2 W$ is non-degenerate,
- (ii) $\text{Ker } D_{u_\xi}^2 \mathcal{L}_\xi = T_{u_\xi} \mathcal{O}_{u_\xi}$,
- (iii) $\inf(\sigma(\nabla^2 \mathcal{L}_\xi(u_\xi)) \cap (0, +\infty)) > 0$,
- (iv) $p(D_\xi^2 W) = n(D_{u_\xi}^2 \mathcal{L}_\xi)$,
- (v) for all $u \in \mathcal{O}_{u_\xi}$ and for all $j = 1, \dots, m$, there exists $\nabla F_j(u) \in \mathcal{D}(\nabla^2 \mathcal{L}_\xi(u_\xi)) \subset E$ such that

$$D_u F_j(w) = \langle \nabla F_j(u), w \rangle, \quad \forall w \in E. \quad (3.4.4)$$

Then there exists $\delta > 0$ such that

$$\forall v \in T_{u_\xi} \Sigma_{\mu_\xi} \cap (T_{u_\xi} \mathcal{O}_{u_\xi})^\perp, \quad D_{u_\xi}^2 \mathcal{L}_\xi(v, v) \geq \delta \|v\|_E^2 \quad (3.4.5)$$

with $(T_{u_\xi} \mathcal{O}_{u_\xi})^\perp = \{v \in \hat{E} \mid \langle v, w \rangle = 0 \ \forall w \in T_{u_\xi} \mathcal{O}_{u_\xi}\}$.

Note that here, and in the rest of this section, the orthogonality is with respect to the inner product $\langle \cdot, \cdot \rangle$.

Let us point out that the hypotheses on the bilinear form $D_{u_\xi}^2 \mathcal{L}_\xi$ in Theorem 3.4.2 can be re-expressed in terms of spectral hypotheses on the (unbounded) self-adjoint operator $\nabla^2 \mathcal{L}_\xi(u_\xi)$, as shown in the following lemma. This is important in applications, since it allows one to use the tools of spectral analysis for partial differential operators to establish those conditions.

Lemma 3.4.3. *Under the hypotheses of Lemma 3.4.1, with $u = u_\xi$, $\text{Ker } \nabla^2 \mathcal{L}_\xi(u_\xi) = \text{Ker } D_{u_\xi}^2 \mathcal{L}_\xi$.*

If, in addition $\dim \text{Ker } \nabla^2 \mathcal{L}_\xi(u_\xi) < +\infty$, the negative spectral subspace of $\nabla^2 \mathcal{L}_\xi(u_\xi)$ is finite dimensional, and hypothesis (iii) of Theorem 3.4.2 is satisfied, then the dimension of the negative spectral subspace of $\nabla^2 \mathcal{L}_\xi(u_\xi)$ in \hat{E} is equal to the Morse index $n(D_{u_\xi}^2 \mathcal{L}_\xi)$ of $u_\xi \in E$ for \mathcal{L}_ξ .

This lemma constitutes a slight generalization of [Stu08, Lemma 5.4] and its proof follows along the same lines.

As in the previous section, one can easily show that

$$D_{u_\xi}^2 \mathcal{L}_\xi(v, v) > 0, \quad \forall v \in \mathcal{Y} = T_{u_\xi} \Sigma_{\mu_\xi} \cap (T_{u_\xi} \mathcal{O}_{u_\xi})^\perp, v \neq 0.$$

To obtain the desired coercive bound (3.4.5), some technical lemmas are needed to deal with the fact that unbounded operators are involved and the orthogonality considered is with respect to the inner product $\langle \cdot, \cdot \rangle$ (see [DR19b] for more details).

3.5. PERSISTENCE OF RELATIVE EQUILIBRIA

In this section we come back to the question of persistence of relative equilibria, which is the question of the existence of a family of relative equilibria as in (3.3.1)-(3.3.2). Three situations occur. In some cases, such a family can be explicitly exhibited. In others, its existence can be proven by ad hoc methods adapted to the specific situation at hand. Finally, under suitable conditions, general structural theorems asserting its existence can be proven. We give below a theorem guaranteeing the existence of a family

of relative equilibria as in (3.3.1)-(3.3.2) in the infinite dimensional framework under study here, under a natural condition on the point $\mu_* = F(u_*)$ in \mathfrak{g}^* , which is for example always satisfied when the symmetry group G is commutative and which is satisfied on an open dense subset of \mathfrak{g}^* in all cases.

We will make the following hypothesis throughout this section:

Hypothesis D. E is a Hilbert space with inner product $\langle \cdot, \cdot \rangle_E$ and $\| \cdot \|_E = \sqrt{\langle \cdot, \cdot \rangle_E}$.

With this hypothesis, one can view $\langle \cdot, \cdot \rangle_E$ as a closed form on \hat{E} (defined in (3.2.12)), with form domain E . It follows (Theorem VIII.15 in [RS80a]) that there exists a unique unbounded positive operator T^2 on \hat{E} , with domain $\mathcal{D}(T^2)$, so that, for all $u, v \in \mathcal{D}(T^2)$,

$$\langle u, v \rangle_E = \langle u, T^2 v \rangle,$$

and so that, in addition $E = \mathcal{D}(T)$ and, for all $u, v \in \mathcal{D}(T)$

$$\langle u, v \rangle_E = \langle Tu, Tv \rangle.$$

Here T is the positive square root of T^2 . Note that

$$\langle u, T^2 u \rangle \geq \langle u, u \rangle,$$

so that 0 is in the resolvent set of T^2 and hence T^{-2} is a bounded operator on \hat{E} .

Next, we introduce in the usual manner the scale of spaces $E_\lambda = \overline{\mathcal{D}(T^\lambda)}^{\|\cdot\|_\lambda}$, where $\|u\|_\lambda = \|T^\lambda u\|$ and $\lambda \in \mathbb{R}$. In particular, we have $E = E_1$ and $\hat{E} = E_0$.

Our persistence result stated in [DR19b] then reads as follows:

Theorem 3.5.1. *Let Hypotheses A, B and D hold and suppose there exists $\xi_* \in \mathfrak{g}$ and $u_* \in \mathcal{D} \cap E_2$ so that $D_{u_*} \mathcal{L}_{\xi_*} = 0$. Suppose in addition:*

(a) *There exist $\varepsilon, C > 0$ such that, for all $v \in E$,*

$$D_{u_*}^2 \mathcal{L}_{\xi_*}(v, v) \geq \varepsilon \|v\|_E^2 - C \|v\|^2. \quad (3.5.1)$$

(b) *For all $u \in E_2$ and for all $\xi \in \mathfrak{g}$ there exists $\nabla \mathcal{L}_\xi(u) \in \hat{E}$ such that*

$$D_u \mathcal{L}_\xi(v) = \langle \nabla \mathcal{L}_\xi(u), v \rangle, \quad \forall v \in E. \quad (3.5.2)$$

(c) *The function $(\xi, v) \in \mathfrak{g} \times E_2 \rightarrow \nabla \mathcal{L}_\xi(v) \in \hat{E}$ belongs to $C^1(\mathfrak{g} \times E_2; \hat{E})$.*

(d) *For all $v \in E_2, g \in G \rightarrow \Phi_g(v) \in E$ is C^1 .*

(e) *The function F is regular at u_* .*

(f) *For all μ in a neighbourhood of $\mu_* = F(u_*)$, $\dim \mathfrak{g}_\mu = \dim \mathfrak{g}_{\mu_*}$.*

If in addition,

(i) $\mathcal{D}(\nabla^2 \mathcal{L}_{\xi_*}(u_*)) = \mathcal{D}(T^2)$

(ii) $\text{Ker } D_{u_*}^2 \mathcal{L}_{\xi_*} = T_{u_*} \mathcal{O}_{u_*}$,

(iii) $\inf(\sigma(\nabla^2 \mathcal{L}_{\xi_*}(u_*)) \cap (0, +\infty)) > 0$,

(iv) $n(D_{u_*}^2 \mathcal{L}_{\xi_*}) < +\infty$,

Then there exists a neighborhood Ω of ξ_* in \mathfrak{g} and a C^1 map $\xi \in \Omega \rightarrow u_\xi \in E$ with $u_{\xi_*} = u_*$ so that for all ξ , (3.3.2) holds. The map $\xi \rightarrow u_\xi$ is an injective immersion.

The conditions that are central here are (ii)-(iii)-(iv): they are to be compared to the identically numbered conditions of Theorem 3.4.2. The other conditions, notably (a)-(e), are technical and usually readily verified in applications. They are virtually automatic in finite dimensional problems. Condition (f) is of purely group-theoretic nature. It is known to hold on an open dense set for any Lie group. In fact, on such a set, the orbits all have the same maximal dimension and the Lie algebra \mathfrak{g}_μ of the isotropy group of μ is commutative [DV69].

The proof of this theorem is based on a clever application of the implicit function theorem ([DR19b]).

3.6. EXAMPLE: STABILITY OF SOLITONS FOR THE NONLINEAR SCHRÖDINGER EQUATION

In [DR19b], we used our approach to study several applications of our results to the stability study for relative equilibria of Schrödinger and Manakov equation.

Here we present the well-known example of the stability of solitons for the nonlinear Schrödinger equation. The goal is to illustrate the role of the variation of the mass (the L^2 -norm) of the solution u_ξ with respect to ξ as pointed out in appendix A.2.

We consider the focusing nonlinear Schrödinger equation with a power nonlinearity given by

$$\begin{cases} i\partial_t u(t, x) + \Delta u(t, x) + |u(t, x)|^{p-1}u(t, x) = 0 & \text{in } \mathbb{R}^d \\ u(0, x) = u(x) \end{cases} \quad (3.6.1)$$

with $u(t, x) \in \mathbb{C}$, $1 < p < 1 + \frac{4}{d}$ and $d = 1, 2, 3$. This choice of parameters guarantees the global existence of solution to (3.6.1) in $H^1(\mathbb{R}^d)$ (see [Caz03]).

Equation (3.6.1) is the Hamiltonian differential equation associated to the Hamiltonian

$$H(u) = \frac{1}{2} \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx - \frac{1}{p+1} \int_{\mathbb{R}^d} |u(x)|^{p+1} dx. \quad (3.6.2)$$

Next, let $G = \mathbb{R} \times \mathbb{R}^d$ and define its action on $E = H^1(\mathbb{R}^d, \mathbb{C})$ via

$$\forall u \in H^1(\mathbb{R}^d), \quad (\Phi_{\gamma_1, \gamma_2}(u))(x) = e^{-i\gamma_1} u(x - \gamma_2). \quad (3.6.3)$$

Clearly, $H \circ \Phi_g = H$ and the group G is an invariance group for the dynamics and the quantities

$$F_1(u) = \frac{1}{2} \int_{\mathbb{R}^d} |u(x)|^2 dx \quad (3.6.4)$$

$$F_{1+j}(u) = \frac{1}{2} \int_{\mathbb{R}^d} u^* \left(\frac{1}{i} \partial_{x_j} \right) u dx \quad (3.6.5)$$

for $j = 1, \dots, d$, are the corresponding constants of the motion (see [Caz03]).

The family of solitary waves

$$u_{\omega, c}(x) = e^{i\frac{c}{2} \cdot x} u_\omega(x) \quad (3.6.6)$$

with $c \in \mathbb{R}^d$ and u_ω the unique positive solution (see [Tao06] for more details) to

$$\Delta u_\omega + |u_\omega|^{p-1} u_\omega = -\omega u_\omega \quad (3.6.7)$$

with $\omega \in \mathbb{R}$, $\omega < 0$, are G -relative equilibria of (3.6.1). Indeed, if we define \mathcal{L}_ξ by

$$\mathcal{L}_\xi(u) = H(u) - \xi_1 F_1(u) - \sum_{j=1}^d \xi_{j+1} F_j(u), \quad (3.6.8)$$

we can easily verify that $u_{c,\omega}$ is a solution to the stationary equation $D_u \mathcal{L}_\xi = 0$ with $\xi = (\omega - \frac{|c|^2}{4}, c)$. In other words, for each $\xi \in \Omega = \left\{ (\xi_1, \hat{\xi}) \in \mathbb{R} \times \mathbb{R}^d, \xi_1 + \frac{|\hat{\xi}|^2}{4} < 0 \right\}$,

$$u_\xi(x) = e^{i\frac{\hat{\xi}}{2} \cdot x} u_{\xi_1 + \frac{|\hat{\xi}|^2}{4}}(x)$$

is a G -relative equilibrium of (3.6.1) with $\mu_\xi = F(u_\xi)$. Note that, since G is commutative, $G_{\mu_\xi} = G$. Here, we use the notation $\hat{\xi} = (\xi_2, \dots, \xi_{d+1})$. Note that, if $d = 1$ and $p = 3$, the unique positive solution of (3.6.7) is explicit:

$$u_\omega(x) = \sqrt{-2\omega} \operatorname{sech}(\sqrt{-\omega}x). \quad (3.6.9)$$

The G -orbit of the initial condition $u_\xi(x)$ is given by

$$\mathcal{O}_{u_\xi} = \left\{ e^{-i\gamma_1} u_\xi(x - \hat{\gamma}), (\gamma_1, \hat{\gamma}) \in G_{\mu_\xi} \right\}. \quad (3.6.10)$$

Our goal is to investigate the orbital stability of these relative equilibria and in particular to obtain the coercivity of \mathcal{L}_ξ by means of Theorem 3.4.2. This, together with Proposition 3.2.2 and the results of [DGR15b], leads to the orbital stability. Hypotheses A, B and C are easily seen to be satisfied, with $\mathcal{D} = H^3(\mathbb{R}^d)$. Note in particular that, since $p > 1$, $H \in C^2(E)$. Also, we use for $\langle \cdot, \cdot \rangle$ in Hypothesis B the usual L^2 -scalar product, so that $\hat{E} = L^2(\mathbb{R}^d, \mathbb{C})$ (viewed as a real Hilbert space). To check the further hypotheses of Theorem 3.4.2, we start by computing $D_{u_\xi}^2 \mathcal{L}_\xi(v, w)$. Writing $v(x) = e^{i\frac{\hat{\xi}}{2} \cdot x} \tilde{v}(x)$ and $w(x) = e^{i\frac{\hat{\xi}}{2} \cdot x} \tilde{w}(x)$, we obtain

$$D_{u_\xi}^2 \mathcal{L}_\xi(v, w) = \langle \mathbb{L}\tilde{w}, \tilde{v} \rangle = \langle \nabla^2 \mathcal{L}_\xi(u_\xi)w, v \rangle$$

with

$$\mathbb{L}\tilde{w} = \begin{pmatrix} -\Delta - pu_\omega^{p-1} - \omega & 0 \\ 0 & -\Delta - u_\omega^{p-1} - \omega \end{pmatrix} \begin{pmatrix} \operatorname{Re}(\tilde{w}) \\ \operatorname{Im}(\tilde{w}) \end{pmatrix}. \quad (3.6.11)$$

It then follows that the operator $\nabla^2 \mathcal{L}_\xi(u_\xi)$ introduced in Lemma 3.4.1 is given by

$$\nabla^2 \mathcal{L}_\xi(u_\xi) = U^* \mathbb{L} U \quad \text{with} \quad U = \begin{pmatrix} \cos\left(\frac{c}{2} \cdot x\right) & \sin\left(\frac{c}{2} \cdot x\right) \\ -\sin\left(\frac{c}{2} \cdot x\right) & \cos\left(\frac{c}{2} \cdot x\right) \end{pmatrix}.$$

Clearly, the estimate (3.4.3) is satisfied. Let L_+ and L_- be defined by

$$L_+ = -\Delta - pu_\omega^{p-1} - \omega, \quad L_- = -\Delta - u_\omega^{p-1} - \omega.$$

Since u_ω is the unique positive solution to (3.6.7) and it is non-degenerate, using a decomposition in spherical harmonics and proceeding as in [Wei96, Lemma 4.1], one proves that

$$\operatorname{Ker}(L_+) = \operatorname{span}\{\partial_{x_1} u_\omega, \dots, \partial_{x_n} u_\omega\}$$

and $\operatorname{Ker}(L_-) = \operatorname{span}\{u_\omega\}$. Moreover, since u_ω is strictly positive, one concludes that 0 is the first eigenvalue of L_- . Similarly, one proves L_+ has exactly one negative eigenvalue.

As a consequence, $\operatorname{Ker}(D_{u_\xi}^2 \mathcal{L}_\xi) = T_{u_\xi} \mathcal{O}_{u_\xi}$ and $n(D_{u_\xi}^2 \mathcal{L}_\xi) = 1$.

Next, we have to show that $1 = n(D_{u_\xi}^2 \mathcal{L}_\xi) = p(D_\xi^2 W)$. Since $p(D_\xi^2 W) \leq n(D_{u_\xi}^2 \mathcal{L}_\xi)$, we already know that $D_\xi^2 W$, which is a $(d+1) \times (d+1)$ matrix, has at least d negative eigenvalue $\lambda_1, \dots, \lambda_d$. Let λ_0 the remaining eigenvalue, then

$$(-1)^d \operatorname{sign}(\lambda_0) = \operatorname{sign}(\lambda_0 \lambda_1 \cdots \lambda_d) = \operatorname{sign}(\det(D_\xi^2 W)).$$

A straightforward calculation gives

$$\begin{aligned} W(\xi) &= H(u_\xi) - \xi_1 F_1(u_\xi) - \sum_{j=1}^d \xi_{j+1} F_{j+1}(u_\xi) \\ &= \frac{1}{2} \int_{\mathbb{R}^d} |\nabla u_\omega(x)|^2 dx - \frac{1}{p+1} \int_{\mathbb{R}^d} |u_\omega(x)|^{p+1} dx - \frac{\omega}{2} \int_{\mathbb{R}^d} |u_\omega(x)|^2 dx. \end{aligned} \quad (3.6.12)$$

Therefore, $W(\xi)$ depends only on the single parameter ω which is itself a function of ξ . As a consequence, for each $k = 1, \dots, d+1$,

$$\frac{\partial W}{\partial \xi_k} = \frac{\partial W}{\partial \omega} \frac{\partial \omega}{\partial \xi_k} = \left(-\frac{1}{2} \int_{\mathbb{R}^d} |u_\omega(x)|^2 dx \right) \frac{\partial \omega}{\partial \xi_k}$$

and, writing $f(\omega) = \left(-\frac{1}{2} \int_{\mathbb{R}^d} |u_\omega(x)|^2 dx \right)$,

$$\frac{\partial^2 W}{\partial \xi_\ell \partial \xi_k} = \frac{\partial f}{\partial \omega} \frac{\partial \omega}{\partial \xi_\ell} \frac{\partial \omega}{\partial \xi_k} + f(\omega) \frac{\partial^2 \omega}{\partial \xi_\ell \partial \xi_k}$$

for any $\ell = 1, \dots, d+1$. Recalling $\omega(\xi) = \xi_1 + \frac{|\hat{\xi}|^2}{4}$, this gives

$$\begin{cases} \frac{\partial^2 W}{\partial \xi_1^2} = \frac{\partial f}{\partial \omega} \\ \frac{\partial^2 W}{\partial \xi_1 \partial \xi_k} = \frac{\xi_k}{2} \frac{\partial f}{\partial \omega} & \text{for } k = 2, \dots, d+1 \\ \frac{\partial^2 W}{\partial \xi_\ell \partial \xi_k} = \frac{\xi_\ell \xi_k}{2} \frac{\partial f}{\partial \omega} + \frac{1}{2} \delta_{k\ell} f(\omega) & \text{for } \ell, k = 2, \dots, d+1 \end{cases}$$

and

$$D_\xi^2 W = \begin{pmatrix} \frac{\partial f}{\partial \omega} & & \frac{\hat{\xi}}{2} \frac{\partial f}{\partial \omega} \\ \frac{\hat{\xi}^T}{2} \frac{\partial f}{\partial \omega} & \frac{\hat{\xi}}{2} \frac{\partial f}{\partial \omega} & + \frac{1}{2} f(\omega) \mathbb{I}_{d \times d} \end{pmatrix}.$$

Hence

$$\det(D_\xi^2 W) = \det \begin{pmatrix} \frac{\partial f}{\partial \omega} & \frac{\hat{\xi}}{2} \frac{\partial f}{\partial \omega} \\ 0_{d \times 1} & \frac{1}{2} f(\omega) \mathbb{I}_{d \times d} \end{pmatrix}$$

so that

$$\det(D_\xi^2 W) = \left(\frac{1}{2} f(\omega) \right)^d \frac{\partial f}{\partial \omega} \quad \text{and} \quad \text{sign}(\det(D_\xi^2 W)) = (-1)^d \text{sign} \left(\frac{\partial f}{\partial \omega} \right).$$

As a consequence, $\text{sign} \left(\frac{\partial f}{\partial \omega} \right) = \text{sign}(\lambda_0)$. This implies that $p(D_\xi^2 W) = 1$ if and only if $\frac{\partial f}{\partial \omega} > 0$. Using the definition of $f(\omega)$, we can conclude that $p(D_\xi^2 W) = 1$ if and only if

$$\frac{\partial}{\partial \omega} \int_{\mathbb{R}^d} |u_\omega|^2 dx < 0. \quad (3.6.13)$$

Note that here $\omega = -\mu$ of the appendix A.2.

Condition (3.6.13) can be rewritten as

$$\frac{\partial}{\partial \omega} \int_{\mathbb{R}^d} |u_\omega|^2 dx = 2 \int_{\mathbb{R}^d} u_\omega \frac{\partial u_\omega}{\partial \omega} dx = 2 \int_{\mathbb{R}^d} u_\omega L_+^{-1} u_\omega dx < 0$$

with L_+ defined above. Hence, let S be the scaling operator $S = x \cdot \nabla + \frac{2}{p-1}$. A straightforward calculation gives $L_+ S u_\omega = 2\omega u_\omega$. Indeed, if u_ω is a solution to (3.6.7), then $u_{\omega, \lambda}(x) := u_\omega(\lambda x)$ satisfies

$$\Delta u_{\omega, \lambda} + \lambda^2 |u_{\omega, \lambda}|^{p-1} u_{\omega, \lambda} = -\omega u_{\omega, \lambda}$$

for all $\lambda \in \mathbb{R}_+ \setminus \{0\}$. Hence, by taking the derivative of this equation with respect to λ and choosing $\lambda = 1$, we obtain $L_+ S u_\omega = 2\omega u_\omega$. As a consequence,

$$2 \int_{\mathbb{R}^d} u_\omega L_+^{-1} u_\omega \, dx = \frac{1}{\omega} \int_{\mathbb{R}^d} u_\omega S u_\omega \, dx = \frac{1}{\omega} \int_{\mathbb{R}^d} u_\omega \left(x \cdot \nabla + \frac{2}{p-1} \right) u_\omega \, dx = \frac{1}{\omega} \left(-\frac{d}{2} + \frac{2}{p-1} \right) \int_{\mathbb{R}^d} |u_\omega|^2 \, dx$$

which is strictly negative if and only if $p < 1 + \frac{4}{d}$.

As a consequence, if $1 < p < 1 + \frac{4}{d}$, Theorem 3.4.2 applies and gives the local coercivity of $D_{u_\xi}^2 \mathcal{L}_\xi$. We then have:

Theorem 3.6.1. *Let $d = 1, 2, 3$ and $1 < p < 1 + \frac{4}{d}$. The solitary wave $u_{\omega,c}$, defined as in (3.6.6) is an orbitally stable relative equilibrium.*

When $d = 1$ and $3 \leq p < 5$, this follows from Theorem 3.4.2 together with Proposition 3.2.2 and the results of [DGR15b]. When $d = 1, 2, 3$ and $1 < p < 3$, the nonlinearity is not sufficiently smooth to ensure the ‘‘propagation of the regularity’’ for initial conditions in $\mathcal{D} = H^3(\mathbb{R}^d)$, as required in [DGR15b] (see [Caz03]). Hence, the results of [DGR15b] cannot be directly applied in this case. Nevertheless, to prove the orbital stability once one has the coercivity of \mathcal{L}_ξ , we can use Theorem 10 of [DGR15b] the proof of which can be easily adapted in the case of the Schrödinger equation with a power nonlinearity.

Remark 6.

1. As announced in Section 3.3, $\nabla^2 \mathcal{L}_\xi$ is an unbounded partial differential operator and we are in the setting of Theorem 3.4.2, not of Theorem 3.3.1, nor of Theorem 3.7.1 below, which comes from [GSS90b].
2. A proof of the orbital stability of the soliton of the focusing NLSE for $1 < p < 1 + \frac{4}{d}$, $d = 1, 2, 3$ was given originally using concentration-compactness arguments in [CL82] and with a variational method in [Wei86]. Finally, in [GSS90b], some of the spectral arguments we used to control $\nabla^2 \mathcal{L}_\xi$ are provided.

3.7. ON THE LINK WITH GRILLAKIS-SHATAH-STRAUSS

We will now compare the results described above to [GSS90b]. As we have already pointed out, in [GSS90b] a proof of orbital stability is proposed with respect to an a priori different subgroup of G and under similar but nevertheless different conditions. Both in order to understand the general structure of the theory and with an eye towards further applications, it is important to understand the relations between the two approaches.

Since in [GSS90b] the phase space E on which the dynamics takes place is taken to be a Hilbert space, we place ourselves for this discussion in the Hilbert space setting of Section 3.3 and consider the situation described by (3.3.1)-(3.3.6).

To state the coercivity estimate of [GSS90b] which is the analog of our Theorem 3.3.1, we need some additional notation. We define

$$\tilde{W} : \Omega \cap \mathfrak{g}_\xi \rightarrow \mathcal{L}_\xi(u_\xi) \in \mathbb{R}, \tag{3.7.1}$$

which is the restriction of the W-function (3.3.3) to the sub-Lie-algebra \mathfrak{g}_ξ of \mathfrak{g} , defined as the Lie-algebra of the subgroup

$$G_\xi = \{g \in G \mid \text{Ad}_g \xi = \xi\}. \tag{3.7.2}$$

Also

$$\tilde{\mathcal{O}}_{u_\xi} = \Phi_{G_\xi}(u_\xi), \tag{3.7.3}$$

is the G_ξ orbit through u_ξ . Since a priori G_ξ differs from G_{μ_ξ} , one should not confuse $\tilde{\mathcal{O}}_{u_\xi}$ with \mathcal{O}_{u_ξ} , which is the G_{μ_ξ} -orbit through u_ξ . We introduce furthermore

$$\tilde{\Sigma}_\xi = \{v \in E \mid \eta \cdot F(v) = \eta \cdot \mu_\xi, \forall \eta \in \mathfrak{g}_\xi\}. \tag{3.7.4}$$

In other words, $\tilde{\Sigma}_\xi$ is the constraint surface corresponding to the constants of the motion $\eta \cdot F$ for $\eta \in \mathfrak{g}_\xi$. Note that $\Sigma_{\mu_\xi} \subset \tilde{\Sigma}_\xi$. In fact, when the moment map is regular at μ_ξ , then $\tilde{\Sigma}_\xi$ is a submanifold of E of co-dimension $\dim \mathfrak{g}_\xi$ which contains the submanifold Σ_{μ_ξ} , itself of codimension $\dim \mathfrak{g}$. The following theorem, which is the analog of Theorem 3.3.1 above, can be inferred from the proof of Theorem 4.1 in [GSS90b].

Theorem 3.7.1. *Suppose Hypotheses A and C hold. Let $\xi \in \Omega$ and suppose*

- (i) $D_\xi^2 \tilde{W}$ is non-degenerate, i.e. $\text{Ker}(D_\xi^2 \tilde{W}) = \{0\}$,
- (ii) $\text{Ker} D_{u_\xi}^2 \mathcal{L}_\xi = Z_\xi$, with $Z_\xi = \{X_\eta(u_\xi) \mid \eta \in \mathfrak{g}_\xi\}$,
- (iii) $\inf(\sigma(\nabla^2 \mathcal{L}_\xi(u_\xi)) \cap (0, +\infty)) > 0$,
- (iv) $p(D_\xi^2 \tilde{W}) = n(D_{u_\xi}^2 \mathcal{L}_\xi)$.

Then there exists $\delta > 0$ such that

$$\forall v \in T_{u_\xi} \tilde{\Sigma}_\xi \cap \left(T_{u_\xi} \tilde{\mathcal{O}}_{u_\xi}\right)^\perp, \quad D_{u_\xi}^2 \mathcal{L}_\xi(v, v) \geq \delta \|v\|^2. \quad (3.7.5)$$

It is clear that, when the invariance group G is one-dimensional, i.e. $\dim \mathfrak{g} = 1$, this theorem is identical to Theorem 3.3.1. Indeed, then $G = G_\xi = G_{\mu_\xi}$ and hence $W = \tilde{W}$ so that both the assumptions and the conclusions of both theorems are identical. This is the situation studied in [GSS87b] and [Stu08]. The same conclusions hold true more generally when the group G is abelian, since then again, $G_\xi = G_{\mu_\xi} = G$. In general, however, the groups G_ξ and G_{μ_ξ} may be distinct, and so may therefore be the orbits $\tilde{\mathcal{O}}_{u_\xi}$ and \mathcal{O}_{u_ξ} . Hence, a priori, the two approaches could yield different coercivity estimates and hence different stability results. Their comparison therefore needs to be done with care.

Let us first compare the respective conclusions (3.3.7) and (3.7.5) as follows. Writing

$$\mathcal{C}_- = \{u \in E \mid D_{u_\xi}^2 \mathcal{L}(u, u) < 0\} \quad (3.7.6)$$

for the negative cone of $D_{u_\xi}^2 \mathcal{L}_\xi$, we see that they imply that

$$T_{u_\xi} \Sigma_{\mu_\xi} \cap \mathcal{C}_- = \emptyset, \quad \text{respectively} \quad T_{u_\xi} \tilde{\Sigma}_\xi \cap \mathcal{C}_- = \emptyset, \quad (3.7.7)$$

meaning that $T_{u_\xi} \Sigma$, respectively $T_{u_\xi} \tilde{\Sigma}_\xi$ are positive subspaces of E for $D_{u_\xi}^2 \mathcal{L}$. Since $T_{u_\xi} \Sigma_{\mu_\xi} \subset T_{u_\xi} \tilde{\Sigma}_\xi$ the second of these statements implies the first and should in general be harder to obtain. Indeed, the cone \mathcal{C}_- may avoid $T_{u_\xi} \Sigma_{\mu_\xi}$ but have a non-trivial intersection with $T_{u_\xi} \tilde{\Sigma}_\xi$.

To understand how the stronger conclusion comes about, one may note that condition (iv) of Theorem 3.7.1 has a more limited range of applicability than condition (iv) of Theorem 3.3.1 since in general

$$p(D_\xi^2 \tilde{W}) \leq p(D_\xi^2 W) \leq n(D_{u_\xi}^2 \mathcal{L}_\xi). \quad (3.7.8)$$

In particular, condition (iv) of Theorem 3.7.1 cannot be satisfied when $p(D_\xi^2 \tilde{W}) < p(D_\xi^2 W)$. In [DR19b] we illustrated this phenomenon with a simple finite dimensional example where indeed

$$p(D_\xi^2 \tilde{W}) < p(D_\xi^2 W) = n(D_{u_\xi}^2 \mathcal{L}_\xi),$$

so that Theorem 3.3.1 applies, but Theorem 3.7.1 does not.

The following corollary proved in [DR19b] further clarifies the link between the two results.

Corollary 3.7.2. *Suppose the hypotheses of Theorem 3.7.1 are satisfied. Then*

$$T_{u_\xi} \tilde{\mathcal{O}}_{u_\xi} = T_{u_\xi} \mathcal{O}_{u_\xi}$$

so that there exists $\delta > 0$ such that

$$\forall v \in T_{u_\xi} \tilde{\Sigma}_\xi \cap (T_{u_\xi} \mathcal{O}_{u_\xi})^\perp, \quad D_{u_\xi}^2 \mathcal{L}_\xi(v, v) \geq \delta \|v\|^2. \quad (3.7.9)$$

Moreover, hypotheses (ii), (iii) and (iv) of Theorem 3.3.1 are satisfied. If, in addition, u_ξ is a regular relative equilibrium, then $\mathfrak{g}_{\mu_\xi} = \mathfrak{g}_\xi$.

We can conclude from the previous discussion and the corollary that, under the non-degeneracy hypothesis $\text{Ker}(D_\xi^2 W) = \{0\}$, Theorem 3.3.1 provides the desired coercivity estimate (3.3.7) under weaker conditions than Theorem 3.7.1. As a result, to find a situation where Theorem 3.7.1 does apply, whereas Theorem 3.3.1 does not, one has to suppose $\text{Ker}(D_\xi^2 W) \neq \{0\}$, whereas $\text{Ker}(D_\xi^2 \tilde{W}) = \{0\}$. We did not find an example of such a situation.

To complete our comparative analysis of those two theorems, we further analyse the conditions on the kernel of $D_{u_\xi}^2 \mathcal{L}_\xi$ they impose. Similarly to the non-degeneracy condition (i), those conditions are also not in a clear logical relation, in particular because they refer to two a priori different subgroups of G , namely G_ξ and G_{μ_ξ} . However, if u_ξ is a non-degenerate, and hence regular, relative equilibrium, then the condition on the kernel of $D_{u_\xi}^2 \mathcal{L}_\xi$ of Theorem 3.7.1 implies not only the kernel condition in Theorem 3.3.1, but in addition that $\mathfrak{g}_\xi = \mathfrak{g}_{\mu_\xi}$.

For further details on the link with the results of [GSS90a] see [DR19b].

SCHRÖDINGER EQUATION IN NONLINEAR OPTICS

This chapter is devoted to the study of the propagation of a wave packet in particular optical fibers. The results described here are contained in [Rot+15b; Con+15b; Con+16f; Con+16b; Con+16d].

4.1. INTRODUCTION

The propagation of a wave packet in a nonlinear optical fiber is described by the general nonlinear Schrödinger equation of the form

$$i\frac{\partial u}{\partial z} - \frac{\beta_2(z)}{2}\frac{\partial^2 u}{\partial t^2} + \gamma(z)|u|^2u = 0 \quad (4.1.1)$$

where z and t are the spatial and time coordinates respectively, β_2 is a function that describes the group-velocity dispersion (GVD) and γ is a function that models the intensity of the nonlinear interaction. It is well known that in homogeneous fibers, the GVD depends on the diameter of the fiber for a given transverse structure. One can therefore modulate the GVD by modulating the diameter of the fibers as a function of z .

The interplay between dispersion and nonlinearity can give rise to a physical phenomenon called *modulational instability* (MI). More precisely, the modulational instability refers to a process where a weak periodic perturbation of a solitary wave grows exponentially during the propagation.

This phenomenon occurs for example in dispersion oscillating fibers (DOFs), *i.e.* optical fibers characterized by longitudinal periodic variations of their outer diameter. In DOFs, the occurrence of unstable frequency bands can be explained using the theory of parametric resonance (PR), a well-known instability phenomenon which occurs in linearized systems for which at least one parameter is varied periodically during the evolution [AB12]. Up to now, most experimental investigations carried out in optical fibers have been performed with basic sinusoidal [Dro+12; Dro+13b; Dro+13a; Fin+13; Con+14] or amplitude modulated [Cop+15] modulation formats. Conversely, in [Rot+15b] (see also [Con+15b]), we studied a radically different periodic modulation of the GVD, in the form of a periodic train (or comb) of Dirac delta spikes. This is a fundamental and widespread modulation format, encountered in a variety of physical systems (see the references in [Rot+15b] for more details).

At more fundamental level kicked systems are widely investigated as a paradigm for the emergence of chaos in perturbed Hamiltonian systems, with the delta-kicked rotor being the most renowned example [Chi79]. Its quantum version is described by a Schrödinger equation forced by a Dirac comb and has

been extensively analyzed to study chaos in quantum systems [Cas+79]. Recirculating fiber loops have been used to reproduce the quantum kicked rotor with an optical system, to study chaos and Anderson localization [FRF99; Atk+03], and to illustrate how an optical system can be used to mimic other physical systems that are more difficult to reproduce experimentally. In the same vein, we hope the experimental setup we proposed in [Rot+15b] could be used as an experimental platform to investigate such phenomena in the presence of nonlinearities, a topic of much current interest.

The approach that we proposed to analyze MI in the fiber with delta-kicked GVD allows us to enlighten the features of the parametric resonance that are not dependent on the specific format of the modulation.

Finally, while the concept of parametric resonances and modulational instability originates in the linear world, this can impact also the behavior of the system at a *nonlinear* level. In [Con+16d] (see also [Con+16f; Con+16b]), we showed that the parametric resonance and modulational instability give rise to quasi-periodic recurrent evolutions with a remarkably complex (but ordered) underlying phase-plane structure. A byproduct of this structure is the existence of breather-like solutions.

4.2. MODULATIONAL INSTABILITY IN DISPERSION-KICKED OPTICAL FIBERS

As said before, in [Rot+15b] (see also [Con+15b]), we studied, both theoretically and experimentally, modulational instability in optical fibers that have a longitudinal evolution of their dispersion in the form of a Dirac delta comb.

From a mathematical point of view, we provided a simple argument allowing to determine the central frequencies of the unstable sidebands for general periodically modulated fibers. Then, we used Floquet theory to analytically compute the width of the gain bands and as well as their maximum gain in the case of dispersion-kicked fibers.

4.2.1. IDENTIFYING THE GAIN BAND CENTRAL FREQUENCIES

Let us consider the following NLSE

$$i\frac{\partial u}{\partial z} - \frac{\beta_2(z)}{2} \frac{\partial^2 u}{\partial t^2} + \gamma(z)|u|^2 u = 0, \quad (4.2.1)$$

where we assume the z -dependent group-velocity dispersion (GVD) $\beta_2(z)$ and the nonlinear coefficient $\gamma(z)$ to be of the form

$$\beta_2(z) = \beta_{\text{av}} + \beta_m f_Z(z), \quad \gamma(z) = \gamma_{\text{av}} + \gamma_m g_Z(z), \quad (4.2.2)$$

where f_Z and g_Z are periodic functions of period Z such that $\min f_Z = -1 = \min g_Z$, and their mean is vanishing, *i.e.*

$$\int_{-Z/2}^{Z/2} f_Z(z) dz = \int_{-Z/2}^{Z/2} g_Z(z) dz = 0.$$

Our aim is to analyze the stability of the general stationary solution of Eq. (4.2.1) which reads

$$u_0(z) = \sqrt{P} \exp(iP \int_0^z \gamma(z') dz'),$$

where P is the power. We emphasize that in Eq. (4.2.1)-(4.2.2) all the coefficients, as well as distance z and time t , are written in physical units. Hence, all the formulas that we write in the following can be readily interpreted in terms of real-world quantities, thus allowing for a direct comparison with the experimental results. Nonetheless, in order to simplify the graphical illustration of such results, in all the figures of the theoretical sections, we will assume $P = \beta_{\text{av}} = \gamma_{\text{av}} = 1$. This is always possible, without loss of generality, by introducing the normalized distance $z/z_{\text{nl}} \rightarrow z$, time $t/t_0 \rightarrow t$, and field $u/\sqrt{P} \rightarrow u$, where $z_{\text{nl}} = (\gamma_{\text{av}} P)^{-1}$ is the so-called nonlinear length and $t_0 = \sqrt{\beta_{\text{av}} z_{\text{nl}}}$ is a characteristic time. In

this case β_m, γ_m , and Z correspond to the physical quantities measured in units of β_{av}, γ_{av} , and z_{nl} , respectively.

We consider a perturbation of $u_0(z)$ in the form $u(z, t) = [v(z, t) + 1]u_0(z)$, where the perturbation $v(z, t)$ satisfies $|v| \ll 1$. Inserting this expression into Eq. (4.2.1), and retaining only the linear terms, we find

$$i \frac{\partial v}{\partial z} - \frac{\beta_2(z)}{2} \frac{\partial^2 v}{\partial t^2} + \gamma(z)P(v + v^*) = 0. \quad (4.2.3)$$

Writing $v = q + ip$, with q and p real functions, we obtain the following linear system:

$$\begin{cases} \frac{\partial q}{\partial z} - \frac{\beta_2(z)}{2} \frac{\partial^2 p}{\partial t^2} = 0, \\ \frac{\partial p}{\partial z} + \frac{\beta_2(z)}{2} \frac{\partial^2 q}{\partial t^2} - 2\gamma(z)Pq = 0. \end{cases}$$

Finally, taking the Fourier transform of this system in the time variable t , leads to

$$\begin{cases} \frac{\partial \hat{q}}{\partial z} + \frac{\beta_2(z)}{2} \omega^2 \hat{p} = 0, \\ \frac{\partial \hat{p}}{\partial z} - \frac{\beta_2(z)}{2} \omega^2 \hat{q} - 2\gamma(z)P\hat{q} = 0, \end{cases} \quad (4.2.4)$$

where we used the definition $\hat{q}(z, \omega) = \frac{1}{\sqrt{2\pi}} \int q(z, t) e^{-i\omega t} dt$. Note that this is a Hamiltonian dynamical system in a two-dimensional phase plane with canonical coordinates (\hat{q}, \hat{p}) . Analyzing the linear (in)stability of the stationary solution $u_0(z)$ therefore reduces to studying the solutions to (4.2.4) for each ω . Since the coefficients in the equation are z -periodic with period Z , Floquet theory applies. This amounts to study the linearized evolution over one period Z , to obtain the Floquet map Φ_{β_m, γ_m} which in the present situation is the two by two real matrix defined by

$$\Phi_{\beta_m, \gamma_m}^{\text{lin}} \begin{pmatrix} \hat{q}(0) \\ \hat{p}(0) \end{pmatrix} = \begin{pmatrix} \hat{q}(Z) \\ \hat{p}(Z) \end{pmatrix}.$$

As a result

$$\begin{pmatrix} \hat{q}(nZ) \\ \hat{p}(nZ) \end{pmatrix} = \left(\Phi_{\beta_m, \gamma_m}^{\text{lin}} \right)^n \begin{pmatrix} \hat{q}(0) \\ \hat{p}(0) \end{pmatrix}.$$

Note that $\Phi_{\beta_m, \gamma_m}^{\text{lin}}$ necessarily has determinant one, since it is obtained by integrating a Hamiltonian dynamics, of which we know that it preserves phase space volume. As a consequence, if λ is one of its eigenvalues, then so are both its complex conjugate λ^* and its inverse λ^{-1} . This constrains the two eigenvalues of $\Phi_{\beta_m, \gamma_m}^{\text{lin}}$ considerably: they are either both real, or lie both on the unit circle. Now, the dynamics is unstable only if there is one eigenvalue λ satisfying $|\lambda| > 1$, in which case both eigenvalues are real. We will denote as λ_{\pm} the two eigenvalues of $\Phi_{\beta_m, \gamma_m}^{\text{lin}}$. We are interested in studying the gain, that is

$$G(\omega, \beta_m, \gamma_m) = \frac{1}{Z} \ln(\max\{|\lambda_+|, |\lambda_-|\}) \quad (4.2.5)$$

as a function of ω, β_m and γ_m (an example of colormap plot of G in the (ω, β_m) plane is reported in Fig. 4.2, which will be discussed below for the specific case of the delta comb GVD, which is the main subject of this paper). The gain G measures the growth of $(\hat{q}(nZ), \hat{p}(nZ))$. It vanishes if the two eigenvalues lie on the unit circle. The regions where the gain does not vanish are commonly referred to as Arnold tongues. We will explain below that, whereas their precise form depends on the choice of f_Z, g_Z , the position of their tips does not.

Since the system (4.2.4) is not autonomous, it cannot be solved analytically in general. Nevertheless, the above observations will allow us to obtain some information about its (in)stability for small β_m, γ_m , and valid for all perturbations f_Z, g_Z , whatever their specific form.

To see this, we first consider the case $\beta_m = 0 = \gamma_m$. It is then straightforward to integrate the system (4.2.4). The linearized Floquet map is then given by

$$\Phi_{Z,0}^{\text{lin}} = \begin{pmatrix} \cos(kZ) & -\frac{\bar{\beta}_2 \omega^2}{k} \sin(kZ) \\ \frac{k}{\bar{\beta}_2 \omega^2} \sin(kZ) & \cos(kZ) \end{pmatrix} := L, \quad (4.2.6)$$

where

$$k^2 = \frac{\bar{\beta}_2}{2} \omega^2 \left(\frac{\bar{\beta}_2}{2} \omega^2 + 2\gamma_{\text{av}} P \right). \quad (4.2.7)$$

Here $\bar{\beta}_2 = \beta_{\text{av}} > 0$ (normal average dispersion), since we restrict our investigations to the defocusing NLSE. Note that the matrix L has determinant equal to 1, as expected. The eigenvalues of L can be readily computed as

$$\lambda_{\pm}(\omega, \beta_m = 0 = \gamma_m) = \exp(\pm ikZ). \quad (4.2.8)$$

What will happen if we now switch on the interaction terms $f_Z(z)$ and $g_Z(z)$? It is then no longer possible, in general, to give a simple closed form expression of the solution to the system (4.2.4), which is no longer autonomous, and hence of the linearized Floquet map $\Phi_{Z,\beta_m,\gamma_m}^{\text{lin}}$. Nevertheless, we do know that, for small β_m, γ_m , the eigenvalues of $\Phi_{Z,\beta_m,\gamma_m}^{\text{lin}}$ must be close to the eigenvalues $\lambda_{\pm}(\omega, \beta_m = 0 = \gamma_m)$. We then have two cases to consider.

Case 1. $k \neq \frac{\pi \ell}{Z}, \ell \in \mathbb{Z}$. Now $\lambda_{-}(\omega, \beta_m = 0 = \gamma_m) = \lambda_{+}^*(\omega, \beta_m = 0 = \gamma_m)$, they are distinct, and they both lie on the unit circle, away from the real axis. They then must remain on the unit circle under perturbation since, for the reasons explained above, they cannot move into the complex plane away from the unit circle. Consequently, in this case, the stationary solution $u_0(z)$ is linearly stable under a sufficiently small perturbation by $\beta_m f_Z(z)$ and $\gamma_m g_Z(z)$, and this statement does not depend on the precise form of $f_Z(z)$ or of $g_Z(z)$. In fact, with growing β_m and/or γ_m , the two eigenvalues will move along the unit circle until they meet either at -1 or at $+1$ for some critical value of the perturbation parameters. Only for values of the latter above that critical value can the system become unstable. A pictorial description of this situation is shown in the left-hand side of Fig. 4.1.

Case 2. $k = \frac{\pi \ell}{Z}, \ell \in \mathbb{Z}$. Now $\lambda_{+} = \lambda_{-} = \pm 1$ (upper or lower sign holds for ℓ even or odd, respectively) is a doubly degenerate eigenvalue of $\Phi_{Z,0}^{\text{lin}}$. Under a small perturbation, the degeneracy can be lifted and two real eigenvalues can be created, one greater than one, one less than one in absolute value. The system has then become unstable! Of course, it will now depend on the type of perturbation whether the system becomes unstable, remains marginally stable (the two eigenvalues don't move at all, but stay at 1 or -1), or becomes stable (the two eigenvalues move in opposite directions along the unit circle). A pictorial description of this situation is shown in the right-hand side of Fig. 4.1. For the Dirac comb modulation of $\beta_2(z)$, which was our main object of study in [Rot+15b], the details are given in the next subsection.

In conclusion, examining Eq. (4.2.7), one sees that only if $\omega = \omega_{\ell}$, where

$$\omega_{\ell}^2 = \frac{2}{\beta_{\text{av}}} \left(\sqrt{(\gamma_{\text{av}} P)^2 + \left(\frac{\ell \pi}{Z} \right)^2} - \gamma_{\text{av}} P \right), \quad (4.2.9)$$

can an infinitely small Hamiltonian perturbation of $\Phi_{Z,0}^{\text{lin}}$ lead to an unstable linearized dynamics near the fixed points $u_0(z)$ considered. These values of ω therefore correspond to the tips of the Arnold tongues, that is, to the positions of the (centers of) the unstable sidebands of the defocusing NLSE under a general periodic perturbation f_Z, g_Z . This is illustrated for a Dirac comb modulation of the GVD in Fig. 4.2. One also observes in that figure that, for a value of ω close to some ω_{ℓ} , the system becomes unstable only for a small but nonzero critical value of β_m , that we shall compute below for the Dirac delta comb GVD.

Equation (4.2.9) was derived in [AB12] by appealing to the theory of parametric resonance and Poincaré-Lindstedt perturbation theory. Our argument above is elementary and shows in a simple manner

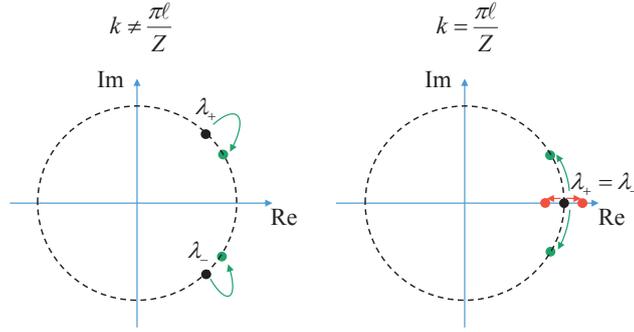


Figure 4.1: Sketch illustrating, in the complex plane, the effect of the interaction terms $f_Z(z)$ and $g_Z(z)$ on the eigenvalues of the linearized Floquet map (4.2.6). Black dots correspond to the unperturbed eigenvalues lying on the unit circle (dashed line). Colored dots show the new position of the eigenvalues after switching on the perturbations, leading to a stable regime when $k \neq \frac{\pi\ell}{Z}$ (left sketch) and an unstable one when $k = \frac{\pi\ell}{Z}$ (right sketch).

that the resonant frequencies ω_ℓ do not at all depend on the form of f_Z or g_Z . Note that, if $f_Z(z) = 0$ and $g_Z(z) = \sin(\frac{2\pi}{Z}z)$, the system (4.2.4) is equivalent to the equation of a harmonic oscillator of (spatial) frequency k , sinusoidally modulated with period Z . In that case the system leads to a Mathieu equation for which it is known that resonance occurs when the period of the modulation is a integer multiple of the half (spatial) period of the oscillator, which is $2\pi/k$.

Additional physical insight can be obtained by expanding Eq. (4.2.9) for small power, i.e. assuming $\gamma_{av}P \ll |\ell|\pi/Z$. At zero order we recover the well known quasi-phase-matching relation [SD96; Dro+12; Mat+93]

$$\beta_{av}\omega_\ell^2 + 2\gamma_{av}P = \frac{2\pi\ell}{Z}. \quad (4.2.10)$$

4.2.2. CALCULATION OF THE MODULATIONAL INSTABILITY GAIN BANDS: DIRAC COMB

We now turn our attention to the computation of the gain $G(\omega)$, in particular for values of ω close to the resonant frequencies. We concentrate on the special case where the GVD is a Dirac delta comb:

$$f_Z(z) = \left[\sum_{n \in \mathbb{Z}} \delta(z/Z - n) \right] - 1, \quad \gamma_m = 0. \quad (4.2.11)$$

Since in the rest of this paper, $\gamma_m = 0$, we will drop it from the notation (the case of periodic nonlinearities can be considered along similar lines). To compute the gain, we need to compute the linearized dynamics $\Phi_{\beta_m}^{\text{lin}}$ and determine the behavior of its eigenvalues $\lambda_\pm(\beta_m, \omega)$ in the neighborhood of $\beta_m = 0$ and $\omega = \omega_\ell$ in the (ω, β_m) -plane.

In this case the linearized Floquet map is easily seen to be explicitly given by

$$\Phi_{\beta_m}^{\text{lin}} = LK \quad (4.2.12)$$

where L is defined by Eq. (4.2.6), but now with $\bar{\beta}_2 = [\beta_{av} - \beta_m]$, and

$$K = \begin{pmatrix} \cos\left(\beta_m \frac{\omega^2}{2} Z\right) & -\sin\left(\beta_m \frac{\omega^2}{2} Z\right) \\ \sin\left(\beta_m \frac{\omega^2}{2} Z\right) & \cos\left(\beta_m \frac{\omega^2}{2} Z\right) \end{pmatrix}. \quad (4.2.13)$$

The characteristic polynomial of LK is given by

$$\lambda^2 - 2\rho(\omega, \beta_m)\lambda + 1 = 0,$$

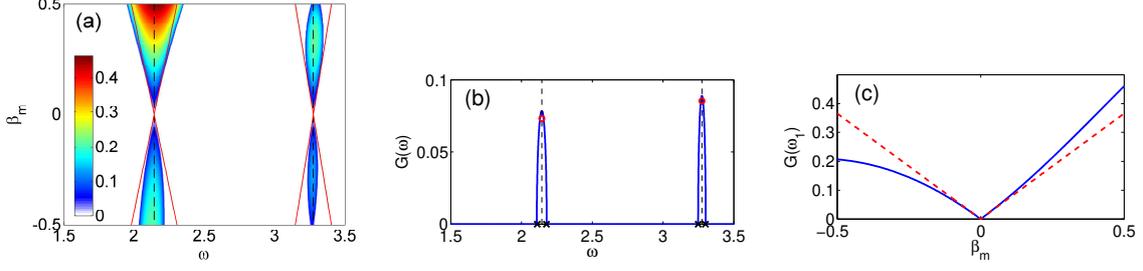


Figure 4.2: (a) Color level plot of the gain $G(\omega, \beta_m) = \ln(\max\{|\lambda_+|, |\lambda_-|\})/Z$ in the (ω, β_m) plane, for $\beta_{av} = 1$, $Z = 1$, $\gamma_{av} = 1$ and $P = 1$. The dashed black lines corresponds to the tips of the Arnold tongues (4.2.9) at $\omega = \omega_1 = 2.1433$ and $\omega_2 = 3.2748$. The solid red lines corresponds to the gain bandwidth, which can be computed from Eq. (4.2.19). (b) MI gain for $\beta_m = 0.1$; Red circles, estimates of maximum gain from Eq. (4.2.18); Black crosses, estimates of the bandwidth (4.2.19). (c) Solid blue curve, MI gain for $\omega = \omega_1$; Dashed red curve, approximation of maximum gain from Eq. (4.2.18).

so that the eigenvalues of (4.2.12) can be computed explicitly as:

$$\lambda_{\pm}(\omega, \beta_m) = \rho(\omega, \beta_m) \pm \sqrt{\rho(\omega, \beta_m)^2 - 1}, \quad (4.2.14)$$

with $\rho = \rho(\omega, \beta_m)$ reading as

$$\rho = \cos(kZ) \cos(\theta) - \frac{\bar{\beta}_2 \omega^2 + \gamma_{av} P}{k} \sin(kZ) \sin(\theta),$$

and $\theta = \beta_m \frac{\omega^2}{2} Z$.

A Taylor expansion of $\rho(\omega, \beta_m)$ about $(\omega_\ell, 0)$ yields

$$\rho(\Omega, \beta_m) \simeq (-1)^\ell [1 + C_\ell \beta_m^2 - D_\ell (\omega - \omega_\ell)^2], \quad (4.2.15)$$

where $\Omega = \omega - \omega_\ell$ and

$$C_\ell = Z^2 \left(\frac{\omega_\ell^2}{2}\right)^2 \left(\frac{Z}{\pi\ell}\right)^2 (\gamma_{av} P)^2, \quad (4.2.16)$$

$$D_\ell = \beta_{av}^2 Z^2 \omega_\ell^2 \left[\left(\frac{Z}{\pi\ell}\right)^2 (\gamma_{av} P)^2 + 1 \right]. \quad (4.2.17)$$

The dependence in β_m^2 (not in β_m) entails that the sign of the kick has no incidence in this regime, i.e. assuming $|\beta_m| \ll 1$.

Formula (4.2.15) shows that $(\omega_\ell, 0)$ is a saddle point for $\rho(\omega, \beta_m)$. If ℓ is even, $\lambda_+(\omega, \beta_m) > 1$ occurs close to $(\omega_\ell, 0)$, and if ℓ is odd, $\lambda_-(\omega, \beta_m) < -1$ close to $(\omega_\ell, 0)$. More precisely,

$$\max(|\lambda_+|, |\lambda_-|) = 1 + \sqrt{C_\ell \beta_m^2 - D_\ell (\omega - \omega_\ell)^2}$$

from which we obtain the following estimate of the gain amplitude $G(\omega_\ell, \beta_m)$ and of the bandwidth $B(\omega_\ell, \beta_m)$ near the tips of the tongue at ω_ℓ :

$$G(\omega_\ell, \beta_m) \approx |\beta_m| \frac{\omega_\ell^2}{2} \frac{Z}{\pi\ell} \gamma_{av} P, \quad (4.2.18)$$

$$B(\omega_\ell, \beta_m) = \frac{|\beta_m| \omega_\ell}{\beta_{av}} \frac{\gamma_{av} P}{2 \sqrt{\left(\frac{\pi\ell}{Z}\right)^2 + (\gamma_{av} P)^2}}. \quad (4.2.19)$$

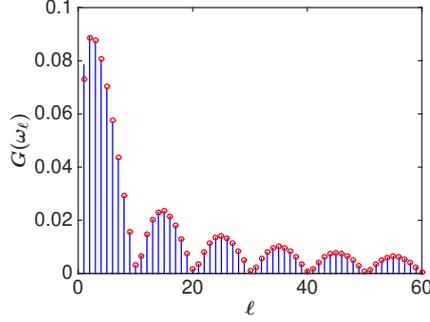


Figure 4.3: (Color online) MI gain for $\omega = \omega_\ell$ as a function of ℓ ; Red circles, estimated gain given by (4.2.20). Parameter values are $\beta_{\text{av}} = 1$, $Z = 1$, $\gamma_{\text{av}} = 1$, $P = 1$, $\beta_m = 0.1$.

Note that the threshold value for β_m above which instability occurs can be read off from the above by setting $|\rho(\beta_m, \omega)| = 1$ which corresponds to

$$|\beta_m| \geq \sqrt{\frac{D_\ell}{C_\ell}} |\omega - \omega_\ell|.$$

This confirms again, as expected, that an arbitrary small β_m will generate instability right at $\omega = \omega_\ell$.

In Fig. 4.2(a) we show an example of the analytically computed MI gain, showing the first two Arnold tongues. As can be seen, for a small enough strength of perturbation, let's say $|\beta_m| \leq 0.1$, the approximation (4.2.19) gives a good estimate of the width of the parametric resonance (see red curves). This situation is detailed further in Figs. 4.2(b,c), showing a section for $\beta_m = 0.1$ and $\omega = \omega_1$, respectively.

Finally, a straightforward calculation gives the asymptotic behavior of the gain G at ω_ℓ for ℓ large and β_m fixed, that is

$$G(\omega_\ell, \beta_m) \approx \frac{\sqrt{4\beta_{\text{av}}^2 \sin^2(\alpha(\ell))(\gamma_{\text{av}}P)^2 - \beta_m^2(\gamma_{\text{av}}P)^4 Z^2}}{2|\beta_m| \pi \ell} \quad (4.2.20)$$

with $\alpha(\ell) = \frac{\beta_m}{\beta_{\text{av}}}(\pi\ell - \gamma_{\text{av}}PZ)$ whenever $4\beta_{\text{av}}^2 \sin^2(\alpha(\ell)) - \beta_m^2(\gamma_{\text{av}}P)^2 Z^2 > 0$, and $G(\omega_\ell) \approx 0$ otherwise.

In Fig. 4.3, we show an example of the analytically computed MI gain at ω_ℓ as a function of ℓ . We compare it to the approximation (4.2.20), which is very accurate, even for small ℓ (see red circles). Note in particular that the oscillating behavior of the gain is well captured by Eq. (4.2.20) which, for ℓ large enough and β_m small, can be approximated by

$$G(\omega_\ell, \beta_m) \simeq |\beta_m| \left| \frac{\sin \left[\frac{\beta_m}{\beta_{\text{av}}} (\pi\ell - \gamma_{\text{av}}PZ) \right]}{\frac{\beta_m}{\beta_{\text{av}}} \pi \ell} \right|.$$

Summing up. It is clear from the above discussion that, precisely at the values ω_ℓ , which only depend on Z and on $\gamma_{\text{av}}P$, but not on the precise form of f_Z , any small perturbation can create an instability and hence a gain. At frequencies ω near these particular values, a minimal threshold strength of β_m is needed to create an instability. This minimal value, and even the fact that an instability is indeed generated, does depend on the precise form of f_Z . For the Dirac comb the explicit expression for the gain in this regime can be read off from Eq. (4.2.20).

4.2.3. EXPERIMENTAL RESULTS

In [Rot+15b; Con+15b], we experimentally reported multiple modulational instability lobes at the output of well-constructed dispersion-kicked optical fibers. In particular, we exploited the fact that the

Dirac delta comb can be well approximated by a series of short Gaussian pulses in order to perform an experimental investigation using microstructured optical fibers.

For more details on experimental results see [Rot+15b; Con+15b].

4.3. NONLINEAR STAGE OF MODULATIONAL INSTABILITY

In [Con+16d] (see also [Con+16f; Con+16b]), we investigated the nonlinear stage of the modulational instability in the defocusing nonlinear Schrödinger equation describing optical fibers with periodic dispersion.

As before, we consider the periodic NLSE

$$i\frac{\partial\psi}{\partial z} - \frac{\beta(z)}{2}\frac{\partial^2\psi}{\partial t^2} + |\psi|^2\psi = 0, \quad (4.3.1)$$

referring, without loss of generality, to the notation used in optical fibers in suitable scaled units. The dispersion is $\beta(z) = \beta_{av} + \beta_m f_\Lambda(z)$, with positive average $\beta_{av} > 0$ (equivalent to the defocusing regime); $f_\Lambda(z)$ has period $\Lambda = 2\pi/k_g$, zero mean and minimum -1 . The method can be easily extended to deal also with periodic nonlinearities. We are interested in the nonlinear evolution of perturbations of the stationary background solution $\psi_0 = \sqrt{P}\exp(iPz)$ with power $P = |\psi_0|^2$.

As we have seen in the previous section, any arbitrarily small perturbation $\beta_m \neq 0$ induces, regardless of its shape $f_\Lambda(z)$, instability at multiple frequencies ($p = 1, 2, \dots$)

$$\omega_p = \sqrt{\frac{2}{\beta_{av}} \left(\sqrt{P^2 + \left(\frac{p\pi}{\Lambda}\right)^2} - P \right)}. \quad (4.3.2)$$

The Floquet analysis gives rise to instability islands, or Arnold tongues, in the plane (ω, β_m) , with ω_p representing the tip of the tongues, as shown in Fig. 4.4(a), taking as an example $f_\Lambda(z) = \cos(k_g z)$ and $p = 1, 2$. Figure 4.4(b) shows the instability gain spectrum $g_F(\omega)$ at $\beta_m = 0.5$, which accurately predicts the spontaneous growth of MI bands obtained from NLSE numerical integration [inset in Fig. 4.4(b)].

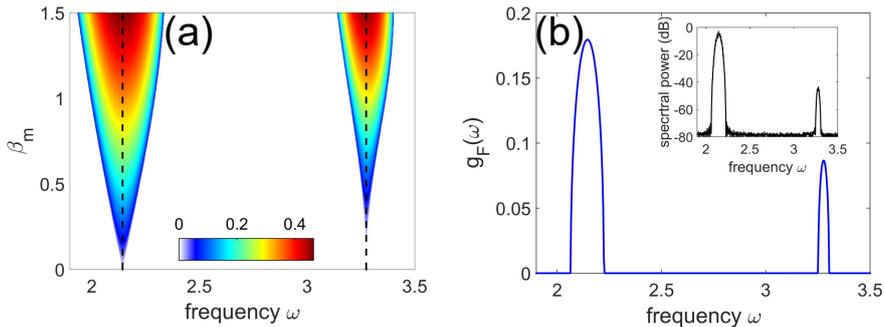


Figure 4.4: Results of the linear Floquet analysis for $f_\Lambda(z) = \cos(k_g z)$, $\Lambda = 1$, $P = 1$: (a) false color plot showing first two MI tongues in the plane (ω, β_m) [dashed vertical lines stand for ω_p , $p = 1, 2$, from Eq. (4.3.2)]; (b) section at $\beta_m = 0.5$ showing gain curves $g_F(\omega)$; Inset: spectral output from NLSE (4.3.1) numerical integration.

Two aspects of this kind of instability are of crucial importance: (i) it exhibits narrowband features around the tongue tip frequencies ω_p ; (ii) different ω_p are generally incommensurate, which greatly reduces the possibility that the harmonics of a probed frequency experience exponential amplification due to higher-order bands. Under such circumstances, three-mode truncations constitute a suitable approach to describe the underlying structure of the dynamics [Whi74; Bis+90; TW91; Mil+98].

Moreover, in order to unveil the dynamics, we need to combine the mode truncation approach with suitable phase transformations and averaging [CBK97]. We start by substituting in Eq. (4.3.1) the field $\psi = A_0(z) + a_1(z) \exp(-i\omega t) + a_{-1}(z) \exp(i\omega t)$ and group all nonlinear terms vibrating at frequencies $0, \pm\omega$, neglecting higher-order harmonic generation. For sake of simplicity we consider henceforth the case of symmetric sidebands $a_1 = a_{-1} \equiv A_1/\sqrt{2}$, though our analysis and conclusions straightforwardly extend to the case $a_1 \neq a_{-1}$. We obtain the following non-autonomous Hamiltonian system of ODEs (dot stands for d/dz)

$$-i\dot{A}_0 = (|A_0|^2 + 2|A_1|^2)A_0 + A_1^2 A_0^*, \quad (4.3.3)$$

$$-i\dot{A}_1 = \left[\frac{\beta(z)\omega^2}{2} + \left(\frac{3|A_1|^2}{2} + 2|A_0|^2 \right) \right] A_1 + A_0^2 A_1^*, \quad (4.3.4)$$

where the only conserved quantity, i.e. $P = |A_0|^2 + |A_1|^2$, is not sufficient to guarantee integrability. In order to describe the mode mixing in the p -th unstable band beyond the linearized stage, we transform to new phase-shifted variables $u(z), w(z)$, defined as

$$A_0(z) = u(z); \quad A_1(z) = w(z) e^{i\left(p\frac{k_g}{2}z + \frac{\delta k(z)}{2}\right)}, \quad (4.3.5)$$

where $\delta k(z) = \beta_m \omega^2 \int_0^z f_\Lambda(z') dz'$ physically accounts for the oscillating wavenumber mismatch of the three-wave interaction. Then, we exploit the general Fourier expansion $\exp[i\delta k(z)] = \sum_n c_n \exp(-ink_g z)$, which allows us to cast Eqs. (4.3.3-4.3.4) in the form

$$-i\dot{u} = (P + |w|^2)u + [c_p + F_\Lambda(z)] w^2 u^*, \quad (4.3.6)$$

$$-i\dot{w} = \left(\frac{\kappa}{2} + \frac{|w|^2}{2} + |u|^2 \right) w + [c_p^* + F_\Lambda^*(z)] u^2 w^*, \quad (4.3.7)$$

where $F_\Lambda(z) \equiv \sum_{n \neq p} c_n \exp[-i(n-p)k_g z]$, and $\kappa \equiv \beta_{av} \omega^2 - pk_g + 2P$ measures the mismatch from optimal linearized amplification (at least at zero order). Indeed, $\kappa = 0$ is equivalent to the quasi-phase-matching condition $\beta_{av} \omega^2 + 2P = pk_g$, where the quasi-momentum pk_g associated to the forcing compensates for the average nonlinear wavenumber mismatch of the three-wave interaction. In the quasi-matched regime ($|\kappa| \ll 1$), the dominant mixing terms $c_p w^2 u^*$ and $c_p^* u^2 w^*$ in Eqs. (4.3.6-4.3.7) are responsible for the growth of sidebands associated with the instability in the p -th band. However, additional contributions to the mixing arise from the mismatched terms contained in the Λ -periodic function $F_\Lambda(z)$. In order to evaluate their impact we generalize the approach of Ref. [CBK97] developed for quadratic media. We assume $1/k_g$ to be small and expand u, w as

$$u(z) = \sum_n u_n(z) e^{inpk_g z} \quad \text{and} \quad w(z) = \sum_n w_n(z) e^{inpk_g z}$$

$u(z) = \sum_n u_n(z) e^{inpk_g z}$, $w(z) = \sum_n w_n(z) e^{inpk_g z}$ where w_n, u_n are assumed to vary slowly with respect to $\exp(ik_g z)$. Moreover, we assume that the harmonics are of order $1/k_g$ (or smaller) compared to leading order or spatial average u_0, w_0 . Hence, taking into account only the lowest order terms in the equations for the harmonics, we are able to express w_n, u_n through the relations

$$u_n = \frac{1}{pk_g} \frac{c_{p(1-n)}}{n} w_0^2 u_0^* \quad \text{and} \quad w_n = \frac{1}{pk_g} \frac{c_{p(1+n)}^*}{n} u_0^2 w_0^*.$$

This allows us to obtain a self-consistent system for $u_0(z), w_0(z)$

$$-i\dot{u}_0 = (P + |w_0|^2)u_0 + c_p w_0^2 u_0^* + \alpha (|w_0|^4 - 2|w_0 u_0|^2) u_0, \quad (4.3.8)$$

$$-i\dot{w}_0 = \left(\frac{\kappa}{2} + \frac{|w_0|^2}{2} + |u_0|^2 \right) w_0 + c_p^* u_0^2 w_0^* - \alpha (|u_0|^4 - 2|w_0 u_0|^2) w_0, \quad (4.3.9)$$

which shows that the mismatched terms result into an effective quintic correction weighted by the (small) coefficient $\alpha = \frac{1}{pk_g} \sum_{n \neq 0} \frac{|c_p(1-n)|^2}{n}$. Equations (4.3.8-4.3.9) can be cast in Hamiltonian form

$$\begin{aligned} \dot{\eta} &= -\frac{\partial H_p}{\partial \phi}; \quad \dot{\phi} = \frac{\partial H_p}{\partial \eta}, \\ H_p &= |c_p| \eta(1-\eta) \cos 2\phi + \frac{\kappa}{2} \eta - \frac{3}{4} \eta^2 - \alpha \eta (1-3\eta+2\eta^2), \end{aligned} \quad (4.3.10)$$

in terms of fractional sideband power $\eta = |w_0|^2 \approx |A_1|^2$ and overall phase $\phi = \text{Arg}[w_0(z)] - \text{Arg}[u_0(z)] + \phi_p/2$, $\phi_p = \text{Arg}[c_p]$.

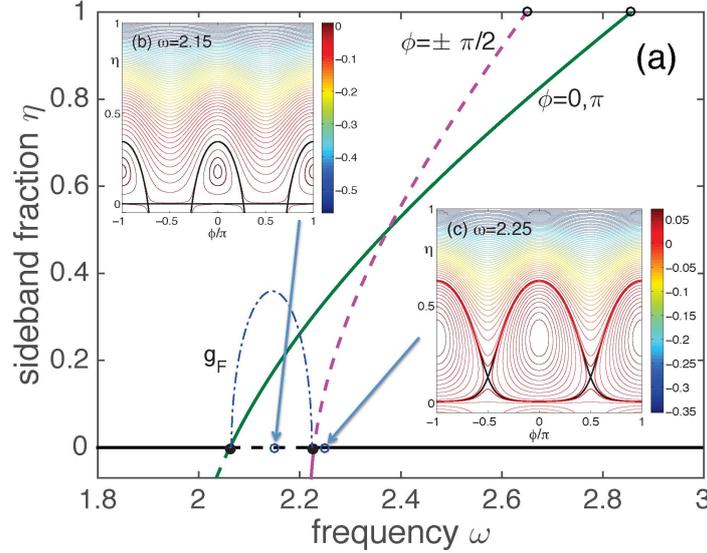


Figure 4.5: (a) Bifurcation diagram from Eqs. (4.3.10): sideband fraction η of unstable (dashed red) and stable (solid green) branches vs. ω . The instability range of the pump mode $\eta = 0$ coincides with the bandwidth calculated from Floquet analysis (gain g_F , dot-dashed line). Insets (b,c): phase-plane pictures for (b) $\omega = 2.15$ inside gain bandwidth; (c) $\omega = 2.25$, outside gain bandwidth, where the topology is affected by saddle eigenmodulations with $\eta \neq 0$. Here $p = 1$, $\beta_m = 0.5$, $\Lambda = 1$, $P = 1$.

Equations (4.3.10) constitute an averaged integrable description of the fully nonlinear stage of the instability, which holds valid regardless of the choice of order p and the specific function $f_\Lambda(z)$. Among the different tests that we have performed, in the following we present the results obtained for the harmonic case $f_\Lambda(z) = \cos(k_g z)$ already considered in Fig. 4.4.

Explicit solutions of Eqs. (4.3.10) can be written in terms of hyperelliptic functions. However, their phase-plane representation (level set of H_p) along with the bifurcation analysis are sufficient to gain a full physical insight. Figure 4.5 shows the bifurcation diagram, i.e. the value η of the stationary points (solutions of $\dot{\eta} = \dot{\phi} = 0$) versus frequency ω . The instability of the pump mode $\eta = 0$ reflects the modulational instability of order p . Indeed $\eta = 0$, $\phi^\pm = \pm \frac{1}{2} \cos^{-1}[(\alpha - \kappa/2)/|c_p|]$ turn out to be saddle points of the Hamiltonian H_p in the range of frequencies implicitly determined by the condition $-|c_p(\omega)| \leq \alpha(\omega) - \kappa(\omega)/2 \leq |c_p(\omega)|$, which agree with the bandwidth from linear Floquet analysis [see the comparison in Fig. 4.5 for $p = 1$]. Within such range of frequencies, the accessible portion of the phase plane ($\eta \geq 0$) is characterized by a heteroclinic separatrix which connects such saddles, dividing the phase plane into regions of inner and outer orbits which are similar to those describing librations and rotations of a standard pendulum, respectively [see Fig. 4.5(b)]. At the edges of such frequency span, the pump mode bifurcates and new phase-locked eigenmodulation branches appear with modulation depth $\eta = \eta_s \neq 0$ variable with frequency, and phase locked either to $\phi = 0, \pi$ (stable, centers) or $\phi = \pm\pi/2$ (unstable, saddles). New heteroclinic connections emanate from the latter, dividing the accessible phase plane into three different domains [see Fig. 4.5(c)].

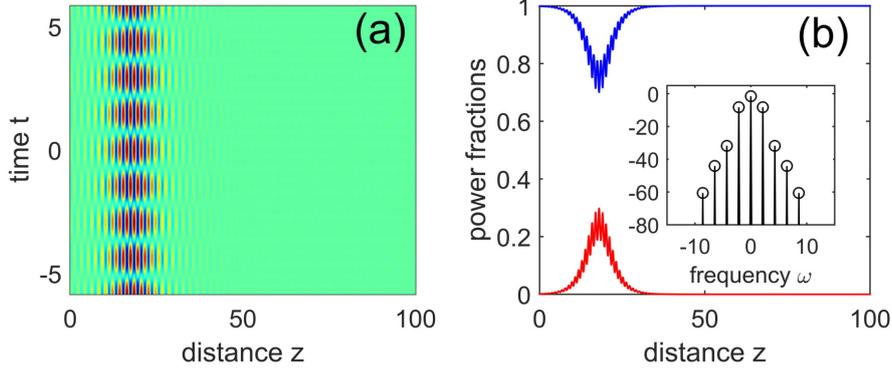


Figure 4.6: PR breather excitation from numerical integration of NLSE (4.3.1): (a) color level plot of $|\psi|^2$; (b) fractions $|A_0|^2$, $|A_1|^2$ of Fourier modes vs. z . Inset: log scale spectrum at the point of maximum depletion, $z = 18$. Here $\beta_m = 0.5$, $\omega = 2.15$, $\Lambda = 1$, $P = 1$, and initial condition $\eta_0 = 0.001$, $\phi_0 = 0.24162\pi$ corresponds to the separatrix in Fig. 2(b).

The structure illustrated in Fig. 4.5 has deep implications for the long-term evolution of the modulationally unstable states in the full NLSE (4.3.1). In order to show this we numerically integrated Eq. (4.3.1) with initial value representing a weakly modulated background:

$$\psi_0(t) = \sqrt{1 - \eta_0} + \sqrt{2\eta_0} \exp(i\theta_0) \cos(\omega t), \quad \eta_0 \ll 1,$$

where θ_0 is linked to the overall initial phase $\phi_0 = \phi(0)$ as $\phi_0 = \theta_0 + \phi_p/2$.

Considering first frequencies within an unstable band, we show in Fig. 4.6 the excitation of the infinite-dimensional analog of the heteroclinic separatrix shown in the left inset in Fig. 4.5, obtained from a very weak modulation ($\eta_0 = 0.001$) with suitable phase. This entails a single cycle of amplification connecting the background to itself with opposite phases, i.e. the analog of the well known Akhmediev breather of the integrable *focusing* NLSE. This type of solutions of the periodic NLSE (4.3.1), which we term as parametric resonance breathers (PR breathers), are characterized by a main breathing occurring on top of the short Λ -scale breathing. PR breathers can be excited for all frequencies inside the unstable bandwidth.

A PR breather divides the phase-plane into two types of dynamical behaviors which exhibit cyclic amplification and de-amplification of the modulation over scales much longer than the Λ -scale of small oscillations. One of such recurrent regimes is displayed in Fig. 4.7(a,b), obtained for $\eta_0 = 0.02$, $\phi_0 = 0$. When we flip the initial phase to $\phi_0 = \pi/2$ we observe a very similar behavior (not shown). However, the projection of the NLSE evolutions onto the phase-space (η, ϕ) reveals very different behaviors for the two initial phases. While in both cases we observe quasi-periodic evolutions, in one case ($\phi_0 = 0$) the recurrence occurs around the libration-type of orbit of the averaged system [Fig. 4.7(c)], whereas the recurrent dynamics for $\phi_0 = \pi/2$ follows rotation-type of dynamics with the phase spanning continuously the full range $(-\pi, \pi)$ [Fig. 4.7(d)]. This is the clear signature of the hidden heteroclinic structure of the modulational instability in the periodic NLSE.

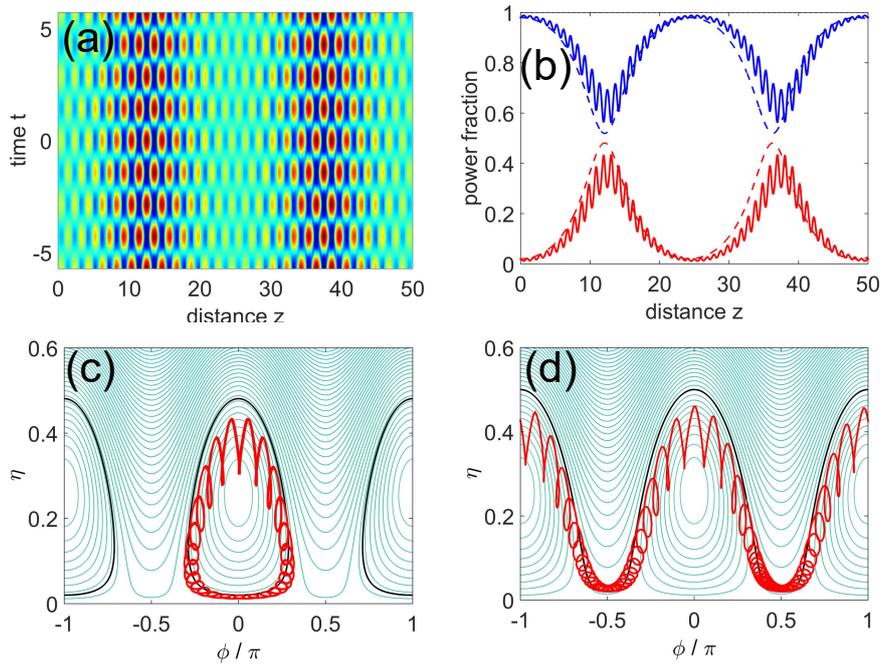


Figure 4.7: Quasi-periodic recurrent evolution from full NLSE numerical integration with $\eta_0 = 0.02$: (a) colormap of $|\psi|^2$; (b) evolution of extracted pump and sideband power fractions for $\phi_0 = 0$ (solid lines), compared with those from the average model (dashed lines), Eq. (4.3.10). (c-d) projections of the NLSE numerical evolutions over the phase plane of the averaged system for $\phi_0 = 0$ (c) and $\phi_0 = \pi/2$ (d). Here $\beta_m = 0.5$, $\omega = 2.2$, $\Lambda = 1$, $P = 1$.

MICROSCOPIC DESCRIPTION OF MINIMIZERS FOR COULOMB AND RIESZ GASES

This chapter is devoted to study of the behavior of minimizers of Coulomb and Riesz gases in any dimension $d \geq 1$. It describes the results contained in [RS15b; PR18b].

The description of the problem and of the known results is based on the Serfaty's lecture notes [Ser15].

Let us remark that the results contained in this chapter concerning the Coulomb gases have been recently improved by Armstrong and Serfaty in [AS20]. It seems therefore interesting to continue the study of this kind of questions in the case of Riesz gases.

5.1. INTRODUCTION

A long-standing question and direction of research at the intersection of mathematics and physics is to ask how solving the minimization problem of sums of two-body interactions between a large number of particles, or more simply between a large number of points, can lead to “collective behavior” of the minimizers, in which some better order structure is seen to emerge. A type of emergent phenomenon, in which a more rigid structure for minimizers tends to diminish the overall complexity of the configurations and is observed empirically in a large number of situations, is usually termed “crystallization”. This name refers in the most restrictive meaning to the appearance of periodic structures for minimizers (see the recent review [BL15]).

The particular model which we considered in [RS15b; PR18b] comes from the theory of Coulomb and Riesz gases already studied in [SS12; SS15b; SS15a; RS16; PS16]. In [PR18b], we highlighted and rigorously proved a *rigidity phenomenon* at zero temperature which is a weak version of crystallization. More precisely, we showed that, after blow-up at the scale corresponding to the interparticle distance, the value of the energy in any large enough set is completely determined by the macroscopic density of points (see Theorem 5.3.2 and Theorem 5.4.2 below). A corollary of our results is that minimizers of the Coulomb gases are very uniform configurations (see Theorem 5.3.3 below). This extends the result [RS15b] valid for the 2-dimensional Coulomb gases to the case of general dimension d and of Riesz gases with power-law interactions with power $s \in [\min\{0, d-2\}, d]$, using the strategies for localizing the energy available in [PS16], and inspired by [CS07].

Moreover, the result in [PR18b] completes the parallel between the work of Rota Nodari and Serfaty [RS15b] and the one of Alberti, Choksi and Otto [ACO09] to general dimensions, for the case $s = d - 2$. In [ACO09], the authors proved such results for the minimizers, which are expected to be periodic, of a

similar energy arising in the context of the Ohta-Kawasaki type model. A consequence of this parallel and of our result is the conjecture that [ACO09] might have extensions to nonlocal interactions corresponding to Green functions for the fractional Laplacian.

Crystallization problems have up to now been solved only for specific short range interaction potentials (see [The06; BPT14; HR80; Süt05; Rad81] and references therein) that do not cover Coulomb forces, or in 1D systems [BL02; Kun74; SS15a]. In particular, Sandier and Serfaty proved in [SS15a] that in the case of the 1-dimensional logarithmic interaction the minimum is achieved at the lattice configuration \mathbb{Z} . As a positive result in higher dimension, in [SS12; PS16] it was shown that in dimension 2 and for the above range of exponents s , if the minimizer is a lattice, then it has to be the triangular one. This, together with simulations and experimental evidences, leads to the so-called *Abrikosov conjecture* [SS12; PS16] valid in dimension 2 and in the range of exponents s considered above, *i.e.* the energy (suitably renormalized as we will see below) is in fact minimized by a suitably rescaled copy of the triangular lattice $\mathbb{Z} + e^{i\pi/3}\mathbb{Z}$. An analogous conjecture holds for the minimizers of the Ohta-Kawasaki type model of [ACO09]. However, it is believed that in high enough dimension the lattice structure is not characteristic of minimizing configurations (see for example [BL15, Sec. 2.3] and the references therein).

The main tool used in [RS15b; PR18b] to tackle this problem is the so-called *jellium energy* which is the interaction energy of an infinite configuration of points in the whole space in a constant neutralizing background. As we will see below, this appears naturally in the control of the next-order term in the expansion of the Hamiltonian for Coulomb and Riesz gases and leads to the definition of the renormalized energy \mathcal{W} . In [RS15b; PR18b], we proved that \mathcal{W} is equidistributed at the microscopic scale in any arbitrary hypercube.

The proof of this equidistribution result is based on a *screening procedure* and on a *bootstrap argument*.

The screening procedure consists in modifying the (possibly infinite) configuration of points near the boundary of an hypercube to make the normal component of the associated (electric) field vanish on the boundary while keeping the points well-separated. This modification is done by adding a negligible energy cost. The vanishing normal component makes in particular the configurations “boundary compatible” with each other, which allows to copy and paste them together. This screening procedure is however possible only on hypercube with “good boundary”. Selecting a “good boundary” is done by using an a priori bound on the energy of field and, as briefly explained below, is the main difficulty in the generalization of our result to Riesz gases.

The bootstrap argument is done on the size of the hypercube. An *a priori* bound at the macroscopic scale is used to find a hypercube with a “good boundary” in which we can apply the screening procedure to obtain the expected bound on the renormalized energy for this hypercube. This is only possible if the size of the hypercube is not too small compared to the macroscopic scale. Then we bootstrap the argument to go down to desired size of the hypercube.

5.2. GENERAL FRAMEWORK OF THE PROBLEM

We now proceed to the precise description of our problem. We study the equilibrium properties of a system of n points in the full space of dimension $d \geq 1$, interacting via repulsive Riesz kernel interactions and confined by an “external field” or potential V . More precisely, we consider energies of the form

$$H_n(x_1, \dots, x_n) = \sum_{i \neq j} g(x_i - x_j) + n \sum_{i=1}^n V(x_i) \quad (5.2.1)$$

where x_1, \dots, x_n are n points in \mathbb{R}^d and the interaction kernel is given by either

$$g(x) = \frac{1}{|x|^s} \quad \max(0, d-2) \leq s < d, \quad (5.2.2)$$

or

$$g(x) = -\log|x| \quad \text{in dimension } d = 1, \quad (5.2.3)$$

or

$$g(x) = -\log|x| \quad \text{in dimension } d = 2. \quad (5.2.4)$$

In the mean-field setting, the factor n multiplying the one-body potential term has the role of giving equal influence to this term as compared to the two-body interaction term. If V has some particular homogeneity, then often we can reduce to an energy of this form by an appropriate scaling. The case of $s \in [d-2, d], s < 0$, which is not treated here, can happen only for $d = 1$ and this seems to be a more tractable situation. Note that, in what follows, we will take the convention that $s = 0$ when $g(x) = -\log|x|$, *i.e.* in the cases (5.2.3) and (5.2.4).

The reason why systems of particles with Coulomb and Riesz interactions are interesting in *statistical physics* is that they represent the most basic model containing the long-range interaction potentials typical of the electrostatic potential. See [Ser15] for a review on studies in the Coulomb case. The possibility of changing the exponent s allows to “turn on” or “off” the locality of the PDEs associated to the interactions. The case $s \geq d$ (also called *hypersingular* case [SK97; BHS12]) corresponds to interaction potentials of more local nature. In [SS12], the precise energy of our form is linked to the study of vortex systems, that appear in classical and quantum fluids [Cag+92; CY08; CRY11]. 2-dimensional β ensembles featuring Coulomb interactions are also relevant to fractional quantum Hall physics [Gir05; RSY13; RSY14].

Our interaction energy is also appearing in the theory of *random matrix ensembles*, such as Ginibre and symmetric matrix ensembles, relevant $d = 2, s = 0$ and Gaussian orthogonal ensemble or Gaussian unitary ensemble for $d = 1, s = 0$, (see [Gin65; Wig58; Dys62; AGZ10; For10]).

Another direction of study in which this type of energy appears is related to Smale’s 7th problem [Sma98], which asks to find fast algorithms for minimizing our energy up to a very small error. Studies of this question are related to the optimal conditioning for interpolation points and to the theory of quadrature (see [SS93; SK97; ST97] and the references therein).

5.2.1. MACROSCOPIC BEHAVIOR OF MINIMIZERS

In this kind of systems, if V grows fast enough at infinity, the leading order behavior of minimizers of H_n is known: there holds

$$\frac{1}{n} \sum_{i=1}^n \delta_{x_i} \rightharpoonup \mu_V,$$

where the convergence is the weak convergence of probability measures, and μ_V is the equilibrium measure, *i.e.* the minimizer of the energy

$$I(\mu) := \int \int_{\mathbb{R}^d \times \mathbb{R}^d} g(x-y) d\mu(x) d\mu(y) + \int_{\mathbb{R}^d} V(x) d\mu(x). \quad (5.2.5)$$

More precisely, we have the following proposition which is a collection of known results described for example in [Ser15] (see also the references therein).

Proposition 5.2.1. *Let $\mathcal{P}(\mathbb{R}^d)$ the space of Borel probability measures on \mathbb{R}^d endowed with the topology of weak convergence. For any $\mu \in \mathcal{P}(\mathbb{R}^d)$, we let H_n be*

$$H_n(\mu) = \begin{cases} H_n(x_1, \dots, x_n) & \text{if } \mu \text{ is of the form } \frac{1}{n} \sum_{i=1}^n \delta_{x_i} \\ +\infty & \text{otherwise} \end{cases}. \quad (5.2.6)$$

- (Γ -convergence of $\frac{1}{n^2} H_n$) Assume V is continuous and bounded below. The sequence $\{\frac{1}{n^2} H_n\}_n$ of functions defined on $\mathcal{P}(\mathbb{R}^d)$ as above Γ -converges as $n \rightarrow +\infty$, with respect to the weak convergence of probability measures, to the function $I : \mathcal{P}(\mathbb{R}^d) \rightarrow (-\infty, +\infty]$ defined by (5.2.5).

- (Frostman [Fro35] existence and characterization of the equilibrium measure) Assume V satisfies the following assumptions:

$$V \text{ is l.s.c. and bounded below,} \quad (5.2.7)$$

$$\lim_{|x| \rightarrow \infty} V(x) = +\infty, \quad \text{resp.} \quad \lim_{|x| \rightarrow \infty} \frac{V(x)}{2} - \log|x| = +\infty \text{ in cases (5.2.3) – (5.2.4),} \quad (5.2.8)$$

$$\{x : V(x) < \infty\} \text{ has positive } g\text{-capacity,} \quad (5.2.9)$$

then the minimum of I over $\mathcal{P}(\mathbb{R}^d)$ exists, is finite and is achieved by a unique equilibrium measure μ_V , which has a compact support Σ of positive g -capacity¹. In addition, μ_V is uniquely characterized by the fact that²

$$\begin{cases} h^{\mu_V} + \frac{V}{2} \geq c & \text{q.e.} \\ h^{\mu_V} + \frac{V}{2} = c & \text{q.e. on } \Sigma \end{cases}$$

where $h^{\mu_V}(x) := \int g(x-y)d\mu_V(y)$ is the electrostatic potential generated by μ_V and $c := I(\mu_V) - \int \frac{V}{2}d\mu_V$.

As a consequence, we may conclude with the following result, which goes back to Choquet [Cho59].

Theorem 5.2.2 (Convergence of minimizers and minima of H_n). *Assume that V is continuous, finite and satisfies (5.2.8).³ Assume that for each n , $\{(x_1, \dots, x_n)\}_n$ is a minimizer of H_n . Then,*

$$\frac{1}{n} \sum_{i=1}^n \delta_{x_i} \rightharpoonup \mu_V \text{ in the weak sense of probability measures,}$$

where μ_V is the unique minimizer of I , and

$$\lim_{n \rightarrow +\infty} \frac{H_n(x_1, \dots, x_n)}{n^2} = I(\mu_V).$$

This gives the *macroscopic* behavior of minimizers of H_n . Indeed, as the length scale of $\text{supp}\mu_V$ is of order 1 (it is independent of n), we will call this the *macroscopic scale*. Since the typical interparticle distance is of order $n^{-1/d}$, we will call it the *microscopic scale*, or *microscale*. Intermediate length scales are called *mesoscales*.

In what follows, we will write

$$\zeta := h^{\mu_V} + \frac{V}{2} - c \geq 0. \quad (5.2.10)$$

Finally, in [RS15b; PR18b], like in [SS15b; RS16; PS16], it is assumed that μ_V is absolutely continuous with respect to the Lebesgue measure, with density also denoted by m_V , and in order to make the explicit constructions easier, we need to assume that this density is bounded and sufficiently regular on its support. More precisely, we make the following technical, and certainly not optimal, assumptions:

$$\partial\Sigma \text{ is } C^1 \quad (5.2.11)$$

$$\mu_V \text{ has a density which is } C^{0,\beta} \text{ in } \Sigma, \quad (5.2.12)$$

$$\exists c_1, c_2, \bar{m} > 0 \text{ s.t. } c_1 \text{dist}(x, \partial\Sigma)^\alpha \leq m_V(x) \leq \min(c_2 \text{dist}(x, \partial\Sigma)^\alpha, \bar{m}) < \infty \text{ in } \Sigma,$$

with the conditions

$$0 < \beta \leq 1, \quad 0 \leq \alpha \leq \frac{2\beta d}{2d-s}. \quad (5.2.13)$$

Of course if $\alpha < 1$ one should take $\beta = \alpha$, and if $\alpha \geq 1$, one should take $\beta = 1$ and $\alpha \leq \frac{2d}{d-s}$.

¹Recall that the g -capacity of a compact set $K \subset \mathbb{R}^d$ is defined by $\text{cap}(K) := \Phi(\inf_{\mu \in \mathcal{P}(K)} \iint_{\mathbb{R}^d} g(x-y)d\mu(x)d\mu(y))$ with $\Phi(t) = e^{-t}$ if $d = 1, 2$ and $\Phi(t) = t^{-1}$ if $d \geq 3$, and where $\mathcal{P}(K)$ denotes the set of probability measures supported in K

²Recall that using the usual notation of potential theory [Lan72], here “quasi everywhere”, abbreviated “q.e.”, means “up to sets of zero g -capacity”.

³This is enough to have also (5.2.7) and (5.2.9)

5.2.2. NEXT-ORDER BEHAVIOR OF MINIMIZERS

Once the leading order behavior of the Hamiltonian H_n has been determined, the following questions arise naturally :

1. What lies beyond the term $n^2 I(\mu_V)$ in the asymptotic expansion of $\min H_n$ as $n \rightarrow +\infty$? Is the next term of order n ?
2. What is the optimal microscopic distribution of the points?

To study these questions, one has to zoom or blow-up the configurations by the factor $n^{1/d}$ (the inverse of the typical distance between two points), so that the points are well-separated (typically with distance $O(1)$), and find a way of expanding the Hamiltonian to next order.

As first observed in [SS15b], [SS15a] via methods later extended in [RS16] and [PS16] to our general setting, if μ_V is the minimizer of I , then H_n can be split into two contributions corresponding to a constant leading order term and a typically next order term as follows:

$$H_n(x_1, \dots, x_n) = n^2 I(\mu_V) + 2n \sum_{i=1}^n \zeta(x_i) + n^{1+s/d} w_n(x_1, \dots, x_n) \quad (5.2.14)$$

in the case (5.2.2) and respectively

$$H_n(x_1, \dots, x_n) = n^2 I(\mu_V) - \frac{n}{d} \log n + 2n \sum_{i=1}^n \zeta(x_i) + n w_n(x_1, \dots, x_n) \quad (5.2.15)$$

in the cases (5.2.3) or (5.2.4), where w_n will be made explicit in Proposition 5.2.4 and ζ is an “effective potential” (defined above in (5.2.10)) depending only on V , which is nonnegative and vanishes on $\text{supp}(\mu_V) := \Sigma$.

The starting point to obtain this “splitting” of the Hamiltonian is the following : given a configuration of points $(x_1, \dots, x_n) \in (\mathbb{R}^d)^n$, let us set $\nu_n = \sum_{i=1}^n \delta_{x_i}$. Since we expect $\frac{1}{n} \nu_n$ to converge to μ_V , let us expand ν_n as

$$\nu_n = n\mu_V + (\nu_n - n\mu_V)$$

The first term in the right-hand side gives the leading order, and the second one describes the fluctuation of ν_n around it. Note that in contrast to the equilibrium measure μ_V assumed to be a nice measure with a bounded density, the fluctuation $\nu_n - n\mu_V$ is still singular, with an atom at each point of the configuration.

Inserting this splitting in the definition of the Hamiltonian H_n , one finds

$$\begin{aligned} H_n(x_1, \dots, x_n) &= \iint_{\Delta^c} g(x-y) d\nu_n(x) d\nu_n(y) + n \int V(x) d\nu_n(x) \\ &= n^2 \iint_{\Delta^c} g(x-y) d\mu_V(x) d\mu_V(y) + n^2 \int V(x) d\mu_V(x) + 2n \iint_{\Delta^c} g(x-y) d\mu_V(x) d(\nu_n - n\mu_V)(y) \\ &\quad + n \int V(x) d(\nu_n - n\mu_V)(x) + \iint_{\Delta^c} g(x-y) d(\nu_n - n\mu_V)(x) d(\nu_n - n\mu_V)(y). \end{aligned}$$

Next, we recall that ζ is defined in (5.2.10) by

$$\zeta(x) = h^{\mu_V}(x) + \frac{V(x)}{2} - c = \int g(x-y) d\mu_V(y) + \frac{V(x)}{2} - c$$

and that $\zeta = 0$ in Σ . Hence, we obtain

$$\begin{aligned} &2n \iint_{\Delta^c} g(x-y) d\mu_V(x) d(\nu_n - n\mu_V)(y) + n \int V(x) d(\nu_n - n\mu_V)(x) \\ &= 2n \int \left(h^{\mu_V}(x) + \frac{V(x)}{2} \right) d(\nu_n - n\mu_V)(x) = 2n \int (\zeta(x) + c) d(\nu_n - n\mu_V)(x) \\ &= 2n \int \zeta(x) d\nu_n(x). \end{aligned}$$

The last equality is due to the facts that $\zeta \equiv 0$ on the support of μ_V and that ν_n and $n\mu_V$ have the same mass n . We also have to notice that, since μ_V has an L^∞ density with respect to the Lebesgue measure, it does not charge the diagonal of $\mathbb{R}^d \times \mathbb{R}^d$ (whose Lebesgue measure is zero), and we can include it back in the domain of integration. By that same argument, one may recognize that

$$n^2 \iint_{\Delta^c} g(x-y) d\mu_V(x) d\mu_V(y) + n^2 \int V(x) d\mu_V(x) = n^2 I(\mu_V).$$

As a consequence,

$$H_n(x_1, \dots, x_n) = n^2 I(\mu_V) + 2n \sum_{i=1}^n \zeta(x_i) + \iint_{\Delta^c} g(x-y) d(\nu_n - n\mu_V)(x) d(\nu_n - n\mu_V)(y)$$

Note that this is an exact relation, valid for any configuration of points. The first term in the right-hand side gives the leading order, *i.e.* the energy of the equilibrium measure. In the second term, ζ plays the role of an effective confining potential, which is active only outside Σ . The last term in the right-hand side is the most interesting, it measures the discrepancy between the diffuse equilibrium measure μ_V and the discrete empirical measure $\frac{1}{n}\nu_n$. It is an electrostatic interaction between a “negatively charged background” $-n\mu_V$ and the n positive discrete charges at the points x_1, \dots, x_n .

To go further, we note that in cases (5.2.2) for $s > 0$ or (5.2.3) and (5.2.4) for $s = 0$, the function g is the fundamental solution for the operator $(-\Delta)^{\frac{d-s}{2}}$ on \mathbb{R}^d . In cases (5.2.2) for $s = d-2 > 0$ and in case (5.2.4) this is the Laplacian, which is a local operator, while in the remaining cases $d-2 < s < d$, it is a fractional Laplacian, which is a nonlocal operator. It turns out however that, as originally noticed in [CS07], if $d-2 < s < d$ then this fractional Laplacian operator can be transformed into a local but inhomogeneous operator of the form $\operatorname{div}(|y|^\gamma \nabla \cdot)$ by adding one space variable $y \in \mathbb{R}$ to the space \mathbb{R}^d . The number γ is chosen such that

$$\gamma = s - d + 2 - k \tag{5.2.16}$$

where k will denote the dimension extension. We will take $k = 0$ in all the Coulomb cases, *i.e.* $s = d-2$ and $d \geq 3$ or (5.2.4). In all other cases, we will need to take $k = 1$. In the particular case of $s = d-1$ then $\gamma = 0$, and this corresponds to using a harmonic extension (see [CS07; SS15a; PS16] for more details). Points in the space \mathbb{R}^d will be denoted by x , and points in the extended space \mathbb{R}^{d+k} by X , with $X = (x, y)$, $x \in \mathbb{R}^d$ and $y \in \mathbb{R}^k$. In \mathbb{R}^{d+k} , the potential generated by the configuration (x_1, \dots, x_n) is then defined by

$$h_n(X) = g * \left(\sum_{i=1}^n \delta_{(x_i, 0)} - nm_V \delta_{\mathbb{R}^d} \right) (X). \tag{5.2.17}$$

This is equivalent to

$$-\operatorname{div}(|y|^\gamma \nabla h_n) = c_{s,d} \left(\sum_{i=1}^n \delta_{(x_i, 0)} - nm_V \delta_{\mathbb{R}^d} \right) \text{ in } \mathbb{R}^{d+k}. \tag{5.2.18}$$

Hence, at least formally, using Green’s formula and the decay of h_n (see [PS16] for more details), we can write

$$\iint_{\Delta^c} g(x-y) d(\nu_n - n\mu_V)(x) d(\nu_n - n\mu_V)(y) \sim \frac{1}{c_{d,s}} \int_{\mathbb{R}^{d+k}} |y|^\gamma |\nabla h_n|^2$$

Such a computation allows to replace the sum of pairwise interactions of all the charges and the background by an integral quantity which is easier to handle. However, this does not make sense because $\int_{\mathbb{R}^{d+k}} |y|^\gamma |\nabla h_n|^2$ is not finite due to the presence of Dirac masses. This is why we need a *truncation procedure*.

More precisely, we need to truncate and regularize the Riesz (or logarithmic) kernel. In [PR18b], we defined the truncated kernel as in [PS16]. For $1 > \eta > 0$ and $X \in \mathbb{R}^{d+k}$, let

$$f_\eta(X) = (g(X) - g(\eta))_+. \tag{5.2.19}$$

We note that the function f_η vanishes outside $B(0, \eta)$ and satisfies that

$$\delta_0^{(\eta)} := \frac{1}{c_{s,d}} \operatorname{div}(|y|^\gamma \nabla f_\eta) + \delta_0 \quad (5.2.20)$$

is a positive measure of mass 1 supported on $\partial B(0, \eta)$, and which is such that for any test-function φ ,

$$\int \varphi \delta_0^{(\eta)} = \frac{1}{c_{s,d}} \int_{\partial B(0, \eta)} \varphi(X) |y|^\gamma g'(\eta).$$

We may write

$$-\operatorname{div}(|y|^\gamma \nabla f_\eta) = c_{s,d}(\delta_0 - \delta_0^{(\eta)}) \quad \text{in } \mathbb{R}^{d+k}. \quad (5.2.21)$$

We will also denote by $\delta_p^{(\eta)}$ the measure $\delta_0^{(\eta)}(X - p)$, for $p \in \mathbb{R}^d \times \{0\}$. In the Coulomb cases, *i.e.* when $k = 0$, then $\delta_0^{(\eta)}$ is the same as in [RS16]. If h can be written in the form (5.2.17), then we will also denote

$$h_\eta := h - \sum_{i=1}^n f_\eta(x - x_i). \quad (5.2.22)$$

In view of (5.2.21), $h_{n,\eta}$ defined from h_n via (5.2.22), satisfy

$$-\operatorname{div}(|y|^\gamma \nabla h_{n,\eta}) = c_{s,d} \left(\sum_{i=1}^n \delta_{x_i}^{(\eta)} - n m_V \delta_{\mathbb{R}^d} \right) \quad \text{in } \mathbb{R}^{d+k} \quad (5.2.23)$$

with the usual embedding of \mathbb{R}^d into \mathbb{R}^{d+k} . This way, the truncation of the potential is simply equivalent to “smearing out” each Dirac charge uniformly onto the sphere of radius η centered at the charge.

We then have the following lemma from [PS16].

Lemma 5.2.3. *For any n , any configuration of distinct points $(x_1, \dots, x_n) \in \mathbb{R}^d \times \{0\}$, letting h_n be as in (5.2.17) and $h_{n,\eta}$ deduced from it via (5.2.22), we have*

$$\iint_{\Delta^c} g(x - y) d(\nu_n - n\mu_V)(x) d(\nu_n - n\mu_V)(y) = \lim_{\eta \rightarrow 0} \left(\frac{1}{c_{s,d}} \int_{\mathbb{R}^{d+k}} |y|^\gamma |\nabla h_{n,\eta}|^2 - n g(\eta) \right). \quad (5.2.24)$$

The quantity appearing in the right-hand side of (5.2.24) provides a way of computing $\int_{\mathbb{R}^{d+k}} |y|^\gamma |\nabla h|^2$ in a *renormalized* fashion, by truncating the divergent parts of ∇h and substrating off from $\int_{\mathbb{R}^{d+k}} |y|^\gamma |\nabla h|^2$ the expected divergence $c_{s,d} g(\eta)$ corresponding to each point. This can be seen as precursor of the renormalized energy defined in subsection 5.2.3.

Finally, to obtain (5.2.14) and (5.2.15), we have to blow-up at a scale where the points are well-separated. The convergence of the empirical measure of the n points to a fixed compactly supported measure suggests that there are typically n points in a bounded domain, so that the distance between two points should be of order $n^{-1/d}$. To get a $O(1)$ distance, one thus has to change the scale by a factor $n^{1/d}$.

For the blown-up quantities we will use the following notation (with the convention $s = 0$ in the cases (5.2.3) or (5.2.4)):

$$x' = n^{1/d} x \quad X' = n^{1/d} X \quad x'_i = n^{1/d} x_i \quad (5.2.25)$$

$$m'_V(x') = m_V(x) \quad (5.2.26)$$

$$h'_n(X') = n^{-\frac{s}{d}} h_n(X). \quad (5.2.27)$$

In particular if $\Sigma = \operatorname{supp}(m_V)$, $\Sigma' = \operatorname{supp}(m'_V)$ then there holds

$$\Sigma' = n^{\frac{1}{d}} \Sigma. \quad (5.2.28)$$

Moreover, h'_n satisfies

$$-\operatorname{div}(|y|^\gamma \nabla h'_n) = c_{s,d} \left(\sum_{i=1}^n \delta_{x'_i} - m'_V \delta_{\mathbb{R}^d} \right) \quad \text{in } \mathbb{R}^{d+k}, \quad (5.2.29)$$

and $h'_{n,\eta}$ defined via (5.2.22) is such that

$$-\operatorname{div}(|y|^\gamma \nabla h'_{n,\eta}) = c_{s,d} \left(\sum_{i=1}^n \delta_{x'_i}^{(\eta)} - m'_V \delta_{\mathbb{R}^d} \right) \quad \text{in } \mathbb{R}^{d+k}. \quad (5.2.30)$$

Finally, using the relation $\gamma = s + 2 - d - k$ and a change of variables, we obtain

$$\int_{\mathbb{R}^{d+k}} |y|^\gamma |\nabla h_{n,\eta n^{-1/d}}|^2 = n^{\frac{s}{d}} \int_{\mathbb{R}^{d+k}} |y|^\gamma |\nabla h'_{n,\eta}|^2.$$

This, together with the definition of g , gives the following splitting formula from [PS16].

Proposition 5.2.4 (Splitting formula). *For any n , any x_1, \dots, x_n distinct points in $\mathbb{R}^d \times \{0\}$, letting h_n be as in (5.2.17) and $h_{n,\eta}$ deduced from it via (5.2.22), we have in the case (5.2.2)*

$$H_n(x_1, \dots, x_n) = n^2 I(\mu_V) + 2n \sum_{i=1}^n \zeta(x_i) + n^{1+\frac{s}{d}} \lim_{\eta \rightarrow 0} \frac{1}{c_{s,d}} \left(\frac{1}{n} \int_{\mathbb{R}^{d+k}} |y|^\gamma |\nabla h'_{n,\eta}|^2 - c_{s,d} g(\eta) \right), \quad (5.2.31)$$

respectively in the cases (5.2.3)–(5.2.4)

$$H_n(x_1, \dots, x_n) = n^2 I(\mu_V) + 2n \sum_{i=1}^n \zeta(x_i) - \frac{n}{d} \log n + n \lim_{\eta \rightarrow 0} \frac{1}{c_{s,d}} \left(\frac{1}{n} \int_{\mathbb{R}^{d+k}} |y|^\gamma |\nabla h'_{n,\eta}|^2 - c_{s,d} g(\eta) \right). \quad (5.2.32)$$

One expects the repelling points x_i to organise in a very uniform way, and thus that the interpoint distance asymptotically decreases like $n^{-1/d}$. The following is proven in [PS16], by potential-theoretic methods [Lan72; BDS14] and using the maximum principle.

Proposition 5.2.5 (Point separation, [PS16, Thm. 5]). *Let (x_1, \dots, x_n) minimize H_n . Then for each $i \in [1, n]$, $x_i \in \Sigma$, and for each $i \neq j$, it holds*

$$|x_i - x_j| \geq \frac{r}{(n \max_x |m_V(x)|)^{1/d}},$$

where r is some positive constant depending only on s and d .

As already remarked above, the scale $\sim n^{-1/d}$ is then termed the *microscopic scale* of our gases, and the two-scale reformulation of the energy H_n as done in [SS15b; RS16; PS16] involves separating the energy contributions from the macroscale and from this microscopic scale. In particular the distribution of points at the microscopic scale is governed by the last term in the splitting formula and by the so-called the renormalized energy \mathcal{W} to be introduced below.

5.2.3. THE RENORMALIZED ENERGY

As shown in [SS15b; SS15a; RS16; PS16], the renormalized energy appears as a limit of w_n from (5.2.14) or (5.2.15) after a blow-up is performed, at the inverse of the typical nearest neighbor distance between the points, *i.e.* $n^{1/d}$.

More precisely, consider the formulas appearing in Proposition 5.2.4. Since ζ plays no other role than confining the points to Σ (the support of μ_V), this formulas show that it suffices to analyze the behavior of

$$\lim_{\eta \rightarrow 0} \left(\int_{\mathbb{R}^{d+k}} |y|^\gamma |\nabla h'_{n,\eta}|^2 - c_{s,d} n g(\eta) \right)$$

as n goes to infinity. This last term produces the next-order term of the energy and the ultimate goal is to find the asymptotic limit of this lower order term as $n \rightarrow +\infty$. The limiting object that will appear is the so-called *renormalized energy*. This justifies the definition of the renormalized energy \mathcal{W} as the interaction energy of an infinite configuration of points in the whole space in a constant neutralizing background. Such a system is called in physics a *jellium*.

The reason why we need to consider such systems is that in the previous subsections we dealt with function h'_n that solved a linear equation of the type

$$-\operatorname{div}(|y|^\gamma \nabla h'_n) = c_{s,d} \left(\sum_{i=1}^n \delta_{x'_i} - m'_V \delta_{\mathbb{R}^d} \right) \quad \text{in } \mathbb{R}^{d+k}, \quad (5.2.33)$$

in which it is easy, at least formally, to pass to the limit $n \rightarrow +\infty$. Previously, we had chosen to center the blow-up at the origin $0 \in \mathbb{R}^{d+k}$. In that case, the density $m'_V(x') = m_V(x' n^{-1/d})$ converges pointwise to the constant $m_V(0)$ as $n \rightarrow +\infty$ (at least if m_V is sufficiently regular). If we had chosen to blow up around a different point, say $(x_0, 0) \in \mathbb{R}^{d+k}$, then we would obtain instead the constant $m_V(x_0)$ as the limit. In all case, this constant is the local density of the neutralizing background charge. As $n \rightarrow +\infty$, the number of points becomes infinite and they fill up the whole space, so that if we blow-up around the origin, which lies in the support of μ_V , we obtain as a, at least formal, limit as $n \rightarrow +\infty$ of (5.2.33) an equation of the form

$$-\operatorname{div}(|y|^\gamma \nabla h) = c_{s,d} \left(\sum_{p \in \Lambda} N_p \delta_p - m \delta_{\mathbb{R}^d} \right) \quad \text{in } \mathbb{R}^{d+k}, \quad (5.2.34)$$

where Λ is a discrete set of points in \mathbb{R}^d , N_p are positive integers (the multiplicities of the points), and $m = m_V(0)$ is a positive constant.

It is sometimes convenient to denote the gradient of h by E , standing for “electric field”, in analogy with the Coulomb case. Then E will solve a relation of the form

$$-\operatorname{div}(|y|^\gamma E) = c_{d,s} \left(\sum_{p \in \Lambda} \delta_p - m(x) \delta_{\mathbb{R}^d} \right) \quad \text{in } \mathbb{R}^{d+k} \quad (5.2.35)$$

where Λ is some discrete set in $\mathbb{R}^d \times \{0\}$ (identified with \mathbb{R}^d). On the one hand, due to the fact that (as recalled in Proposition 5.2.5) the minimizers of our energy have separated charges, in [PR18b], we restrict ourselves to fields E corresponding to multiplicity-one charges, as opposed to general positive integer multiplicity case considered in [RS16; PS16]. On the other hand, we take into account the possibility of a varying background given by a nonnegative density function $m : \mathbb{R}^d \rightarrow \mathbb{R}^+$.

For any such E (defined over \mathbb{R}^{d+k} or over subsets of it), we define, by a formula generalizing (5.2.22),

$$E_\eta := E - \sum_{p \in \Lambda} \nabla f_\eta(X - p). \quad (5.2.36)$$

We will write Φ_η for the map that sends E to E_η , and note that it is a bijection from the set of vector fields satisfying a relation of the form (5.2.35) to those satisfying a relation of the form

$$-\operatorname{div}(|y|^\gamma E_\eta) = c_{d,s} \left(\sum_{p \in \Lambda} \delta_p^{(\eta)} - m(x) \delta_{\mathbb{R}^d} \right) \quad \text{in } \mathbb{R}^{d+k}. \quad (5.2.37)$$

The class of vector fields on which we are going to concentrate is thus the following:

Definition 2 (Admissible vector fields). Given a non-negative density function $m : \mathbb{R}^d \rightarrow \mathbb{R}^+$, we define the class \mathcal{A}_m to be the class of gradient vector fields $E = \nabla h$ that satisfy

$$-\operatorname{div}(|y|^\gamma E) = c_{s,d} \left(\sum_{p \in \Lambda} \delta_p - m(x) \delta_{\mathbb{R}^d} \right) \quad \text{in } \mathbb{R}^{d+k} \quad (5.2.38)$$

where Λ is a discrete set of points in $\mathbb{R}^d \times \{0\}$.

In case $m \in L_{loc}^\infty$, vector fields as above blow up exactly in $1/|X|^{s+1}$ near each $p \in \Lambda$ (with the convention $s = 0$ for the cases (5.2.3)–(5.2.4)); such vector fields naturally belong to the space $L_{loc}^p(\mathbb{R}^{d+k}, \mathbb{R}^{d+k})$ for $p < \frac{d+k}{s+1}$.

We are now in a position to define the renormalized energy for blow-up configurations like in [RS16; PS16]. In the definition, we let K_R denote the hypercubes $[-R/2, R/2]^d$.

Definition 3 (Renormalized energy). Let $E \in \mathcal{A}_m$ satisfy (5.2.35) and $f : \mathbb{R}^{d+k} \rightarrow \mathbb{R}^+$ be a measurable function. Then for $0 < \eta < 1$ we define

$$\mathcal{W}_\eta(E, f) = \int_{\mathbb{R}^{d+k}} |y|^\gamma f |E_\eta|^2 - c_{d,s} g(\eta) \int_{\mathbb{R}^{d+k}} f \sum_{p \in \Lambda} \delta_p^{(\eta)}. \quad (5.2.39)$$

For $A \subset \mathbb{R}^d$ a Borel set we define $\mathcal{W}_\eta(E, A) := \mathcal{W}_\eta(E, 1_{A \times \mathbb{R}^k})$ where 1_S is the characteristic function which equals 1 on a set S and 0 outside S . We then define

$$\mathcal{W}(E, A) = \lim_{\eta \rightarrow 0} \mathcal{W}_\eta(E, A), \quad \mathcal{W}(E) = \lim_{\eta \rightarrow 0} \limsup_{R \rightarrow \infty} \frac{\mathcal{W}_\eta(E, K_R)}{R^d}. \quad (5.2.40)$$

Remark 7. Note that if $\chi_{A,\epsilon}(x, y) = 1_A * \rho_\epsilon^{(d)}(x) 1_{[-R_\epsilon, R_\epsilon]^k} * \rho_\epsilon^{(k)}(y)$ are C_c^∞ functions approximating $1_{A \times \mathbb{R}^k}$ where $R_\epsilon \rightarrow \infty$ as $\epsilon \rightarrow 0$ and $\rho_\epsilon^{(n)}(z) = \epsilon^{-n} \rho^{(n)}(z/\epsilon)$ denotes mollifiers based on a smooth radial probability density $\rho^{(n)}$ supported on the unit ball of \mathbb{R}^n , then we have $\mathcal{W}_\eta(E, A) = \lim_{\epsilon \rightarrow 0} \mathcal{W}_\eta(E, \chi_{A,\epsilon})$, by monotone convergence in (5.2.39).

The name renormalized energy, originating in Bethuel-Brezis-Hélein [BBH94] in the context of two-dimensional Ginzburg-Landau vortices, reflects the fact that $\int |y|^\gamma |\nabla h|^2$ which is infinite, is computed in a renormalized way by first changing h into h_η and then removing the appropriate divergent terms $c_{s,d} g(\eta)$ corresponding to all points as presented above.

The above is a generalized version of the renormalized energy defined in [PS16], and fits in the framework of the study of “jellium energies”, for which we refer to [BL15] and to the references therein. As in [RS16; PS16] the next-order functional \mathcal{W} differs from the one defined in previous works by Sandier-Serfaty [SS12; SS15a] for the one and two-dimensional logarithmic interaction, essentially in the fact that the order of the limits $R \rightarrow \infty$ and $\eta \rightarrow 0$ is reversed. We refer to [RS16] for a further discussion of the comparison between the two.

In the case of constant m , by scaling we may always reduce to studying the class \mathcal{A}_1 , indeed, if $E \in \mathcal{A}_m$ and A is Borel, then $\hat{E} = m^{-\frac{s+1}{d}} E(c_{s,d} \cdot m^{-1/d}) \in \mathcal{A}_1$ and

$$\mathcal{W}_\eta(E, A) = m^{1+s/d} \mathcal{W}_{\eta m^{1/d}}(\hat{E}, m^{1/d} A) \quad \mathcal{W}(E) = m^{1+s/d} \mathcal{W}(\hat{E}) \quad (5.2.41)$$

in the case (5.2.2), and respectively

$$\mathcal{W}_\eta(E, A) = m \left(\mathcal{W}_{m\eta}(\hat{E}, m^{1/d} A) - \frac{2\pi}{d} \log m \right) \quad \mathcal{W}(E) = m \left(\mathcal{W}(\hat{E}) - \frac{2\pi}{d} \log m \right) \quad (5.2.42)$$

in the cases (5.2.3)–(5.2.4).

⁴with the convention $s = 0$ in cases (5.2.3) and (5.2.4)

The goal is then to understand the behavior of minimizers of \mathcal{W} . While we know how to prove the existence of minimizers of \mathcal{W} , the identification of its minimum remains widely open. The exceptions are the case of the one-dimensional logarithmic interaction, for which the minimum is proven in [SS15a] to be achieved at the perfect lattice configuration \mathbb{Z} , and the case of the two-dimensional Coulomb and Riesz gases in [SS12; PS16], where it is shown that, within the class of configurations of points that are forming a perfect lattice, the minimizer is the Abrikosov triangular lattice.

As mentioned above, it is a hard mathematical conjecture corroborated by simulations and experimental evidences (the so-called ‘‘Abrikosov conjecture’’ in 2-dimensions being the most celebrated case), that in low dimensions the minimum of \mathcal{W} is achieved at simple crystalline configurations, *i.e.* minimizers of \mathcal{W} are expected to resemble perfect lattices. In [SS15b; SS15a; RS16; PS16] the analysis of the microscopic behavior of minimizers of H_n was thus connected to the behavior of minimizers of \mathcal{W} by allowing to rigorously formulate the crystallization conjecture in terms of \mathcal{W} .

5.3. MAIN RESULTS FOR COULOMB GASES

We now state the main results of [PR18b] in the case of Coulomb gases, *i.e.* $s = d - 2$ and $d \geq 3$ in (5.2.2) or (5.2.4). These results are the generalization of the result of [RS15b] for the 2-dimensional Coulomb gases to the case of general dimension d . More precisely, we prove that the renormalized energy \mathcal{W} is equidistributed at the microscopic scale in an arbitrary square provided that the square is chosen sufficiently far away from $\partial\Sigma$. Moreover, we improve the result of [PS16, Thm. 4], where it was established that almost minimizers of H_n tend to minimize \mathcal{W} after blow-up at scale $n^{1/d}$ around *almost every* point in Σ . Here we show that if we deal with a minimizer of H_n this holds after blow-up around *any* point sufficiently far from the boundary of Σ .

Theorem 5.3.1. *Let (x_1, \dots, x_n) be a minimizer of H_n with g as in (5.2.2), for $s = d - 2$ and $d \geq 3$, or as in (5.2.4). Let $\mu_V = m_V(x)dx$, $\mu'_V = m'_V(x')dx'$ be respectively the equilibrium measure and its blow-up at scale $n^{1/d}$. Let Σ be the support of μ_V and Σ' be the support of μ'_V . Suppose that $m_V \in C^{0,\alpha}(\Sigma)$ for some $\alpha \in]0, 1[$ and that there exist constants $\underline{m}, \overline{m} > 0$ such that $\underline{m} \leq m_V(x) \leq \overline{m}$ for all $x \in \Sigma$.*

Let $E'_n = \nabla h'_n$ be the vector fields expressed as the gradient of the potentials of blow-up configurations corresponding to these minimizers, as in (5.2.29) above.

There exists $q \in]0, 1[$ such that for $a_n \in \Sigma'$, if $K_\ell(a_n) = a_n + [-\ell/2, \ell/2]^d \subset \mathbb{R}^d$ and in the regime where $\text{dist}(K_\ell(a_n), \partial\Sigma') \geq n^{q/d}$, we have

$$\lim_{\eta \rightarrow 0} \limsup_{\ell \rightarrow \infty} \limsup_{n \rightarrow \infty} \left| \frac{\mathcal{W}_\eta(E'_n, K_\ell(a_n))}{|K_\ell|} - \frac{1}{|K_\ell|} \int_{K_\ell(a_n)} \min_{\mathcal{A}_{m'_V(x')}} \mathcal{W} dx' \right| = 0, \quad (5.3.1)$$

where $\mathcal{A}_{m'_V(x')}$ is the class of admissible vector fields defined in Definition 2.

In the above result it is natural to ask under which conditions we can interchange the renormalization limit $\eta \rightarrow 0$ with the other ones, obtaining a result valid for \mathcal{W} rather than for the family \mathcal{W}_η .

Our proof strategy for the above result is to select ‘‘good boundaries’’, and then use a screening procedure like in [PS16], in order to compare different boundary conditions for the minimizers. In this case the requirement for a ‘‘good boundary’’ is that the field E_η should not have a large concentration of energy on such boundaries.

Unfortunately the purely energetic considerations which we apply in our proof make it impossible to control whether or not the locations of the supports $\partial B(p, \eta)$, $p \in \Lambda$ of the smeared charges $\delta_p^{(\eta)}$ appearing in the second term in (5.2.39) ‘‘follow’’ the energy concentration of E_η locally near such good boundaries, and governed by the first term in (5.2.39). In this sense the definition (5.2.39) of our energy is really just a global one, and it may happen that large discrepancies between the behaviors $\mathcal{W}_\eta(K_\ell(a))$ and $\int_{K_\ell(a) \times \mathbb{R}^k} |y|^\gamma |E_\eta|^2$ occur for exceptional choices of $K_\ell(a)$. This lack of control prevents the exchange of the $\eta \rightarrow 0$ limit with the $n, \ell \rightarrow \infty$ limit without further assumptions on $K_\ell(a)$.

However, if we allow ourselves to slightly perturb the cubes and if we use the charge separation result of Proposition 5.2.5, stated below, we can perform the desired interchange of limits for the perturbed hyperrectangles, and we obtain the following:

Theorem 5.3.2. *Under the same hypotheses as in Theorem 5.3.1, assume that $E'_n = \nabla h'_n$ are a sequence of blown-up vector fields associated to minimizers of H_n .*

In the regime linking a_n, ℓ, n like in Theorem 5.3.1, there exists sets Γ_n which can be expressed as bi-Lipschitz deformations $f_n : K_\ell(a_n) \rightarrow \Gamma_n$ such that $\|f_n - id\|_{L^\infty} \leq 1$ and such that we have

$$\limsup_{\ell \rightarrow \infty} \limsup_{n \rightarrow \infty} \left| \frac{\mathcal{W}(E'_n, \Gamma_n)}{|\Gamma_n|} - \frac{1}{|\Gamma_n|} \int_{\Gamma_n} \min_{\mathcal{A}'_{m'_V(x')}} \mathcal{W} dx' \right| = 0, \quad (5.3.2)$$

where $\mathcal{A}'_{m'_V(x')}$ is the class of admissible vector fields defined in Definition 2. Moreover, we may assume that Γ_n is a hyperrectangle.

5.3.1. BOUND ON CHARGE DISCREPANCY FOR COULOMB GASES

As a consequence of Theorem 5.3.1, we deduce a decay of discrepancies, valid for Coulomb gases in dimension $d \geq 2$, and which precisely shows that minimizers of the Coulomb jellium energy have a controlled charge discrepancy in all dimensions:

Theorem 5.3.3 (Discrepancy bound of jellium minimizers). *Under the same hypotheses as in Theorem 5.3.1, assume that $E'_n = \nabla h'_n$ are vector fields associated to minimizers of H_n and consider a regime in which (5.3.1) holds. Then letting*

$$\nu'_n := \sum_{i=1}^n \delta_{x'_i}$$

we have a finite asymptotic bound of the discrepancy of the ν'_n with respect to μ'_V as follows:

$$\limsup_{\ell \rightarrow \infty} \limsup_{n \rightarrow \infty} \frac{1}{\ell^{d-1}} \left| \nu'_n(K_\ell(a)) - \int_{K_\ell(a)} m'_V(x) dx \right| < \infty. \quad (5.3.3)$$

We note that for the $d = 2$ case the above result is already present in [RS15b]. A weaker version in which, still for $d = 2$, the decay of the absolute value term in (5.3.3) is shown to be $o(\ell^d)$ rather than $O(\ell^{d-1})$ like here, was also proved via Beurling-Landau densities, in [AO12]. Note that this result has been recently improved by Armstrong-Serfaty in [AS20].

5.4. RESULTS FOR RIESZ GASES

We now state the results of [PR18b] in the case of Riesz gases with power-law interaction, *i.e.* $\max(0, d - 2) < s < d$ and $d \geq 2$ in (5.2.2). Theorem 5.4.1 and Theorem 5.4.2 below are the analogue of Theorem 5.3.1 and Theorem 5.3.2 described above. As before, we prove that the renormalized energy \mathcal{W} is equidistributed at the microscopic scale in an arbitrary square provided that the square is chosen large enough and sufficiently far away from $\partial\Sigma$. However, note that for the Riesz case, our results are substantially weaker. Indeed, we require the strong extra condition (5.4.1). We conjecture that this hypothesis is automatically verified for sequences of minimizing configurations, but it seems to be out of reach of the present methods. We expect that fundamentally new methods and ideas will be needed for proving this conjecture.

Theorem 5.4.1. *Let (x_1, \dots, x_n) be a minimizer of H_n with g as in (5.2.2), for $\max(0, d - 2) < s < d$ and $d \geq 2$. Let $\mu_V = m_V(x) dx$, $\mu'_V = m'_V(x') dx'$ be respectively the equilibrium measure and its blow-up*

at scale $n^{1/d}$. Let Σ be the support of μ_V and Σ' be the support of μ'_V . Suppose that $m_V \in C^{0,\alpha}(\Sigma)$ for some $\alpha \in]0, 1]$ and that there exist constants $\underline{m}, \bar{m} > 0$ such that $\underline{m} \leq m_V(x) \leq \bar{m}$ for all $x \in \Sigma$.

Let $E'_n = \nabla h'_n$ be the vector fields expressed as the gradient of the potentials of blow-up configurations corresponding to these minimizers, as in (5.2.29) above. Assume that, if $K_R \subset \mathbb{R}^d$ are hypercubes of size R , then

$$\lim_{t \rightarrow \infty} \lim_{R \rightarrow \infty} \lim_{n \rightarrow \infty} \frac{1}{|K_R|} \int_{K_R \times (\mathbb{R} \setminus [-t, t])} |y|^\gamma |E'_n|^2 = 0 \quad (5.4.1)$$

uniformly with respect to the choice of the centers of the hypercubes K_R . For every $\varepsilon_0 > 0$ there exists a convergence regime for $\ell \rightarrow \infty$ depending on (5.4.1) and compatible with the condition $\text{dist}(K_\ell(a_n), \partial\Sigma') \geq \varepsilon_0 n^{1/d}$ for $a_n \in \Sigma' \times \{0\}$ such that (5.3.1) holds, that is

$$\lim_{\eta \rightarrow 0} \limsup_{\ell \rightarrow \infty} \limsup_{n \rightarrow \infty} \left| \frac{\mathcal{W}_\eta(E'_n, K_\ell(a_n))}{|K_\ell|} - \frac{1}{|K_\ell|} \int_{K_\ell(a_n)} \min_{\mathcal{A}_{m'_V(x')}} \mathcal{W} dx' \right| = 0,$$

where $\mathcal{A}_{m'_V(x')}$ is the class of admissible vector fields defined in Definition 2.

Theorem 5.4.2. Under the same hypotheses as in Theorem 5.4.1, assume that $E'_n = \nabla h'_n$ are a sequence of blown-up vector fields associated to minimizers of H_n . Further assume that (5.4.1) holds uniformly with respect to the choice of the centers of the hypercubes K_R .

In the regime linking a_n, ℓ, n like in Theorem 5.4.1 there exists sets Γ_n which can be expressed as bi-Lipschitz deformations $f_n : K_\ell(a_n) \rightarrow \Gamma_n$ such that $\|f_n - \text{id}\|_{L^\infty} \leq 1$ and such that (5.3.2) holds, that is

$$\limsup_{\ell \rightarrow \infty} \limsup_{n \rightarrow \infty} \left| \frac{\mathcal{W}(E'_n, \Gamma_n)}{|\Gamma_n|} - \frac{1}{|\Gamma_n|} \int_{\Gamma_n} \min_{\mathcal{A}_{m'_V(x')}} \mathcal{W} dx' \right| = 0,$$

where $\mathcal{A}_{m'_V(x')}$ is the class of admissible vector fields defined in Definition 2. Moreover, we may assume that Γ_n is a hyperrectangle.

Remark that in both theorems, even with the strong hypothesis (5.4.1), the result is slightly weaker in the case of Riesz gases. In particular, ℓ and n must be large enough depending on the decay rate in (5.4.1). The decay in the extra dimension y of the energy vector fields E'_n corresponding to minimizing configurations of points is in general not known. This is why we need hypothesis (5.4.1). If we were able to prove that the l.h.s. of (5.4.1) decays to zero as a negative power of t , then (5.3.1) and (5.3.2) would hold in the regime where $\text{dist}(K_\ell(a_n), \partial\Sigma') \geq n^{q/d}$ for some $q \in]0, 1[$ as for the Coulomb gases. Note that such decay is not true for general configurations for which $\mathcal{W}(E) < +\infty$, and it seems to be equivalent to a uniformity condition on the field-generating configuration. For example, condition (5.4.1) holds in the case of lattice-like configurations. See [PR18b] for a more detailed discussion on this.

Moreover, because of this lack of knowledge on the decay rate in the extra dimension, a discrepancy result as in Theorem 5.3.3 cannot be obtained directly from Theorem 5.4.1.

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