Solutions of the Dirac-Fock equations without projector

Eric Paturel*
CEREMADE†
Université Paris IX-Dauphine

December 7, 1999

Abstract. In this paper we prove the existence of infinitely many solutions of the Dirac-Fock equations with N electrons turning around a nucleus of atomic charge Z, satisfying $N < Z+1$ and $\alpha \max(Z,N) < \frac{2}{\frac{2}{\pi}+\frac{\pi}{2}}$, where $\alpha \approx \frac{1}{137}$ is the fundamental constant of the electromagnetic interaction. This work is an improvement of an article of Esteban-Séré, where the same result was proved under more restrictive assumptions on N.

1 Introduction

This paper deals with the Dirac-Fock (DF) model in relativistic quantum mechanics. Many atomic or molecular models have been studied from a mathematical point of view, during this last fifty years. The Hartree (H) model, and its more realistic variant, called Hartree-Fock (HF), are among the most famous ones. Many results are known about them, for example the existence of a ground state [12], and infinitely many stationary states [13]. The link between these atomic models and other approximations, like Thomas-Fermi (TF) and Thomas-Fermi-von Weizsäcker (TFW) has been widely studied (cf. the Selecta of E.H. Lieb [14]). The HF model is very useful in computational chemistry, where it yields results on the energy levels of atoms, that agree with experimental data, as long as the atomic charge is not too large.

These models are nevertheless based on a nonrelativistic approximation: the kinetic energy is represented by the stationary Schrödinger operator $-\Delta$. In [16], Swirles introduced the Dirac-Fock energy functional: this functional approximates the relativistic energy of a system of N electrons moving around a static nucleus of large positive charge Z. The approximations are still important: the nucleus is supposed to be fixed (Born-Oppenheimer approximation), the spin

*e-mail: paturel@pi.ceremade.dauphine.fr
†URA CNRS 749, Université Paris IX-Dauphine, place du Maréchal de Lattre de Tassigny, F-75775 Paris cedex 16, France

interactions are neglected, the wave function of N electrons is represented by a Slater determinant, and the only interaction considered (i.e. the electrostatic interaction) is not Lorentz invariant. However, the numerical results obtained with the DF model are in very good agreement with experimental data (see [11], [10], [5]), especially for the inner-shell electrons of heavy atoms. The model also includes the case of molecules, with a distribution of positive charge $Z\mu$, where μ is a probability measure, and Z the total positive charge. Note that it is also possible to take into account non purely electrostatic interaction as perturbations of the electrostatic case. We refer to [9] for a study of a multi-determinant Dirac-Fock model.

In [6], M.J. Esteban and E. Séré proved the existence of infinitely many stationary states for the DF model, provided N and Z satisfy the following conditions:

$$N < Z+1\,,\; \alpha \max(Z, 3N-1) < \frac{2}{\frac{2}{\pi}+\frac{\pi}{2}}\,.$$

Here $\alpha \approx \frac{1}{137}$ stands for the fundamental constant of the electromagnetic interaction. Their method is variational and, after changes in the functional (smoothing the potential and penalizing the constraint), they reduce it thanks to a concavity property: the major advantage is that the new functional is no more strongly indefinite. Once this reduction is made, they build min-max sequences by a linking argument. This result is the first existence result for this model. Unfortunately, as big atoms have many electrons, Esteban-Séré's result does not cover them: the theorem is not valid for neutral atoms with atomic charge greater than 41. The reason is that the concavity argument does not work for $\alpha(3N-1) > \frac{2}{\frac{2}{\pi}+\frac{\pi}{2}}$.

Our aim is to improve this result, so that it becomes true for every N and Z satisfying

$$N < Z+1\,,\; \alpha \max(Z, N) < \frac{2}{\frac{2}{\pi}+\frac{\pi}{2}}\,.$$

Note that the same assumptions assumptions are needed for the existence of a ground state in the Brown-Ravenhall model (see [6]). To set out our result, we first recall the necessary definitions for the DF model. In the whole paper, we use the system of units such that $\hbar = c = 1$, and the mass m_e of the electron is also normalized to 1. The state of a free electron is represented by a wave function $\Psi(t,x)$, with $\Psi(t,.) \in L^2(\mathbb{R}^3, \mathbb{C}^4)$ for any t, which satisfies the free Dirac equation:

$$i\partial_t \Psi = H_0 \Psi, \text{ with } H_0 = -i\sum_{k=1}^{3} \alpha_k \partial_k + \beta\,. \tag{1.1}$$

We denote (X, X') the standard Hermitian product in $\mathbb{C}^4$, and $(\phi,\psi)_{L^2}$ the usual Hermitian product in $L^2(\mathbb{R}^3, \mathbb{C}^4)$. The Dirac equation contains the 4×4

complex matrices α_1, α_2, α_3 and β, whose standard form is

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix},$$

with the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

These matrices satisfy some algebraic conditions which ensure that H_0 is a symmetric operator such that

$$H_0^2 = -\Delta + 1\,. \tag{1.2}$$

The following lemma contains some properties of H_0 and the coulombic potential $V(x) = \frac{1}{|x|}$, whose proof can be found in [2], [19], [18]. This lemma was already stated in [6], we repeat it for the reader's convenience.

Lemma 1.1. *H_0 is a self-adjoint operator on $L^2(\mathbb{R}^3, \mathbb{C}^4)$, with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$. Its spectrum is $(-\infty, -1] \cup [1, +\infty)$. There are two orthogonal projectors on $L^2(\mathbb{R}^3, \mathbb{C}^4)$, Λ^+ and $\Lambda^- = 1_{L^2} - \Lambda^+$, both with infinite rank, and such that*

$$\begin{cases} H_0\Lambda^+ = \Lambda^+ H_0 = \sqrt{1-\Delta}\Lambda^+ = \Lambda^+\sqrt{1-\Delta} \\ H_0\Lambda^- = \Lambda^- H_0 = -\sqrt{1-\Delta}\Lambda^- = -\Lambda^-\sqrt{1-\Delta} \end{cases} \tag{1.3}$$

The coulombic potential $V(x) = \frac{1}{|x|}$ satisfies the following Hardy-type inequalities:

$$(\varphi, V\varphi)_{L^2} \leq \frac{1}{2}\left(\frac{\pi}{2} + \frac{2}{\pi}\right)(\varphi, |H_0|\varphi)_{L^2}\,, \tag{1.4}$$

for all $\varphi \in \Lambda^+(H^{\frac{1}{2}}) \cup \Lambda^-(H^{\frac{1}{2}})$. Moreover,

$$(\varphi, V\varphi)_{L^2} \;\leq\; \frac{\pi}{2}(\varphi, |H_0|\varphi)_{L^2}\,, \forall\varphi \in H^{\frac{1}{2}}\,, \tag{1.5}$$

$$||V\varphi||_{L^2} \;\leq\; 2||\nabla\varphi||_{L^2}\,, \forall\varphi \in H^1\,. \tag{1.6}$$

We now introduce the DF model. Although our result can be stated for molecules (see Remark 1.4 below), we restrict ourselves, for the sake of simplicity, to the case of electrons around one nucleus of atomic charge Z. We introduce the functional space of the variational problem associated to the DF model. Let

$$E = H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^4)\,, E^+ = \Lambda^+ E\,, E^- = \Lambda^- E\,.$$

E is a Hilbert space with Hermitian product

$$(\varphi, \psi)_E = \left(\varphi, \sqrt{1-\Delta}\psi\right)_{L^2} = \left(\varphi^+, \psi^+\right)_E + \left(\varphi^-, \psi^-\right)_E\,. \tag{1.7}$$

Now, the DF energy functional, denoted by $\mathcal{E}$, is defined on the space E^N, with

$$\begin{aligned}\mathcal{E}(\Phi) &= \sum_{l=1}^{N}(\varphi_l, H_0\varphi_l)_{L^2} - \alpha Z \sum_{l=1}^{N}(\varphi_l, V\varphi_l)_{L^2} \\ &\quad + \frac{\alpha}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} V(x-y)\left[\rho(x)\rho(y) - \operatorname{tr}\left(R(x,y)R(y,x)\right)\right] d^3x d^3y\,,\end{aligned} \tag{1.8}$$

where α is positive, with physical value $\alpha \approx \frac{1}{137}$, ρ is a scalar and R is a 4×4 complex matrix, given by

$$\rho(x) = \sum_{l=1}^{N}\left(\varphi_l(x), \varphi_l(x)\right)\ ,\ R(x,y) = \sum_{l=1}^{N}\varphi_l(x)\otimes\varphi_l^*(y)\,. \tag{1.9}$$

Physically, ρ is the electronic density, R is the exchange matrix.

We look for critical points of $\mathcal{E}$ under the normalization constraint

$$\Phi \in \Sigma = \{\Phi \in E^N \,|\, \mathrm{Gram}_{L^2}\Phi = \mathbb{1}\}\,. \tag{1.10}$$

The manifold Σ and the DF functional are invariant under the action of the group $\mathcal{U}(N)$ of $N\times N$ self-adjoint complex matrices with determinant of modulus 1. We denote

$$u.\Phi = \left(\sum_l u_{1l}\varphi_l, ..., \sum_l u_{Nl}\varphi_l\right)\ ,\ u\in\mathcal{U}(N)\,,\ \Phi\in E^N\,. \tag{1.11}$$

Thanks to this invariance, we may diagonalize the Lagrange multiplier matrix and write the Euler-Lagrange equations in the following form, called *Dirac-Fock equations*

$$\overline{H}_\Phi\varphi_k = \varepsilon_k\varphi_k\,, \tag{1.12}$$

where

$$\begin{aligned}\overline{H}_\Phi\psi &= H_0\psi - \alpha Z V\psi + \alpha(\rho * V)\psi \\ &\quad -\alpha\int_{\mathbb{R}^3} R(x,y)\psi(y)V(x-y)dy\,.\end{aligned} \tag{1.13}$$

Physically, $\overline{H}_\Phi$ represents the Hamiltonian of an electron in the mean field due to the nuclei and the electrons. The eigenvalues $\varepsilon_1, ..., \varepsilon_N$ are the energies of each electron in this mean field. With the unit convention, the physically interesting states correspond to $0 < \varepsilon_k < 1$: a positive energy less than the rest mass of the electron.

We recall that the result [6] makes use of a concavity argument, more precisely the fact that, under the assumption that $\alpha(3N-1) < \frac{2}{\frac{2}{\pi}+\frac{\pi}{2}}$, the DF-functional is concave in the E^- directions. To get rid of this, we have to handle directly a strongly indefinite functional, which moreover does not satisfy the Palais-Smale property. This is not very comfortable, and we have to do some preliminary work before the usual variational tools can be applied. Our result, which is an extension of [6, Theorem 1.2], is the following:

Theorem 1.2. *Assume that* $\alpha \max(Z, N) < \frac{2}{\frac{2}{\pi}+\frac{\pi}{2}}$, $N < Z+1$, *with* $Z > 0$ *the nuclear charge. Then there exists a sequence* (Φ^n) *of critical points for the DF functional* $\mathcal{E}$ *on* Σ. *The functions* $\varphi_1^n, ..., \varphi_N^n$ *satisfy the normalization constraints* $\mathrm{Gram}_{L^2}\Phi^n = \mathbb{1}$. *They are smooth outside* 0, *decay exponentially as well as their derivatives as* $|x| \to +\infty$, *and are strong solutions, in* $W^{1,\frac{3}{2}}(\mathbb{R}^3, \mathbb{C}^4)$, *of the Dirac-Fock equations*

$$\overline{H}_{\Phi^n}\varphi_k^n = \varepsilon_k^n \varphi_k^n\,,\ 1 \leq k \leq N\,, \tag{1.14}$$

with

$$\forall k\,,\ 0 < \varepsilon_k^n < 1\,. \tag{1.15}$$

Moreover, as n *goes to infinity, the energies* ε_k^n *go to* 1.

Remark 1.3. *The corresponding physical bound for* N *and* Z *is* 124, *with* $N \leq Z$.

Remark 1.4. *As in [6], it is easy to change the formulation of the problem to consider others distributions of positive charge than a punctual nucleus. Theorem 1.2 extends easily to the case of a nuclear charge density* $Z\mu$, *where* $Z > 0$ *is the total nuclear charge and* μ *is a probability measure defined on* $\mathbb{R}^3$. *In this general situation,* Φ^n *is smooth outside Supp(*μ*). In the particular case of* m *point-like nuclei, each one having atomic number* Z_i *at a fixed location* x_i, $Z\mu = \sum_{i=1}^m Z_i\delta_{x_i}$, *and* $Z = \sum_{i=1}^m Z_i$.

The paper is organized as follows: the next section is devoted to a sketch of the proof of Theorem 1.2. Section 3 deals with the reductions of the initial problem to a more comfortable one. We expose in Section 4 a linking procedure. Finally, Section 5 deals with the compactness properties and the limits of the min-max sequences.

2 Sketch of the proof

In order to prove this result, it is hard to use the variational method directly, for many reasons: the corresponding functional is strongly indefinite, there is no compactness property available for this functional, and the coulombic potential is hard to deal with. To avoid successively these obstacles, we are led to consider different stages of approximate problems. Indeed, we use here many approximation tools so that the final variational problem is simpler to handle with. The strategy can be described like this:

(a) In order to get rid of the roughness of the coulombic potential V, we replace it with an approximate one, actually a convolution of V with a normalized gaussian depending on a parameter ν. This gaussian function tends to the Dirac distribution as ν goes to zero. Moreover, as the initial problem is constrained, and the physically interesting states are governed by the Lagrange multipliers given by the constraint, we define instead a problem with penalization of the constraint. The choice of the penalization gives directly a lower bound for the energy of the electrons. This step is exactly the same as in [6].

(b) The use of variational tools needs at least some compactness properties. To get this, we change the problem into a *periodic* one, that is, we consider a functional space of periodic functions. We have to change one more time the shape of the potential. The corresponding functional satisfies for example the Palais-Smale compactness property, which is enough to take the limit of min-max sequences.

(c) The last (not the least!) problem is that the functional is still strongly indefinite. To deal with this, we operate a Lyapunov-Schmidt reduction to a finite dimensional problem . This reduction is made possible because of the compactness properties of the functional, once the steps (a) and (b) are fulfilled. Such a tool was used in a famous paper by Conley and Zehnder [3] on Arnold's conjecture.

(d) We develop a linking method in the finite dimensional case. This method is based on the construction of a pseudogradient vector field. The Lyapunov-Schmidt reduction gives then critical points for the periodic problem (b). We have then to translate the estimates on the (Conley-Zehnder) Morse index of the critical points for the finite dimensional problem onto an estimate on the eigenvalues ε_k.

(e) We pass to the limit as the length of the period goes to infinity. There remains to take the limit of the solutions as the penalization parameter p and the smoothness constant ν go respectively to infinity and 0: we will use again the same arguments as in [6].

2.1 First reduction

To begin this program, we will write the variational problems corresponding to its successive steps. We will explain the reasons why we consider these problems and their advantages relatively to the preceding formulations. Recall that the first variational formulation of the problem of finding solutions to the DF equations is

Problem 2.1. *Find critical points for the functional*

$$\begin{aligned}\mathcal{E}(\Phi) &= \sum_{l=1}^{N}(\varphi_l, H_0\varphi_l)_{L^2} - \alpha Z\sum_{l=1}^{N}(\varphi_l, V\varphi_l)_{L^2} \\ &+\frac{\alpha}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} V(x-y)\left[\rho(x)\rho(y) - \mathrm{tr}\,(R(x,y)R(y,x))\right] d^3x d^3y\,,\end{aligned}$$

under the constraint

$$\Phi \in \Sigma = \left\{\Phi \in E^N \,|\mathrm{Gram}_{L^2}\Phi = \mathbb{1}\right\}\,,$$

with the following condition on the matrix of Lagrange multipliers Λ*,*

$$\left\{\begin{array}{l}\exists u \in \mathcal{U}(N)\,,\, u\Lambda u^* = \mathrm{Diag}(\varepsilon_1, ..., \varepsilon_N) \\ \textit{with}\,\forall k,\, 0 < \varepsilon_k < 1\,.\end{array}\right. \tag{2.1}$$

The first transformation of Problem 2.1 into a more practical one was introduced in [6]. We follow the authors and briefly explain the reasons of this transformation to Problem 2.2. We refer to [6] for more details.

As in [6], we have to deal with the fact that the coulombic potential V is not a compact perturbation of H_0. That is why we replace V by the regularized potential, for $\nu > 0$:

$$V_\nu(x) = (g_\nu * V)(x)\,, \tag{2.2}$$

with

$$g_\nu(x) = \frac{1}{(2\pi\nu)^{\frac{3}{2}}} e^{-\frac{|x|^2}{2\nu}}\,.$$

This replacement is made for the attractive potential of the nucleus, as well as for the electronic repulsion and exchange terms. We denote by $\mathcal{E}_\nu$ the corresponding functional, and the associated one-particle Hamiltonian is denoted by $\overline{H}_\Phi^\nu$.

As announced in (a), we also replace the constraint "$\Phi \in \Sigma$" by a penalization term π_p depending on an integer p. We put

$$\pi_p(\Phi) = \mathrm{tr}\left[(\mathrm{Gram}_{L^2}\Phi)^p\,(\mathbb{1} - \mathrm{Gram}_{L^2}\Phi)^{-1}\right]\,, \tag{2.3}$$

and we define the penalized functional

$$\mathcal{F}_{\nu,p} = \mathcal{E}_\nu - \pi_p\,, \tag{2.4}$$

in the domain

$$A = \left\{\Phi \in E^N \,|\, 0 < \mathrm{Gram}_{L^2}\Phi < \mathbb{1}\right\}\,. \tag{2.5}$$

Note that $\mathcal{F}_{\nu,p}$ is invariant under the $\mathcal{U}(N)$ action. Any $\mathcal{U}(N)$ orbit in A contains a point Φ such that $\mathrm{Gram}_{L^2}\Phi$ is diagonal, with eigenvalues in nondecreasing order:

$$\mathrm{Gram}_{L^2}\Phi = \mathrm{Diag}(\sigma_1, ..., \sigma_N),\, 0 < \sigma_1 \leq ... \leq \sigma_N < 1\,. \tag{2.6}$$

We call $\mathcal{O}$ the set of points of A satisfying (2.6). If $\Phi \in \mathcal{O}$, then

$$\frac{\partial \mathcal{F}_{\nu,p}}{\partial \varphi_k}(\Phi) = \overline{H}^{\nu}_{\Phi}\varphi_k - \varepsilon_k \varphi_k\,, \tag{2.7}$$

with

$$\varepsilon_k = e_p(\sigma_k)\,,\, e_p(x) = \frac{d}{dx}\left(\frac{x^p}{1-x}\right) = \frac{px^{p-1}-(p-1)x^p}{(1-x)^2}\,. \tag{2.8}$$

The advantage of this penalization is that e_p is a positive increasing function on $(0,1)$, so that $0 < \varepsilon_1 \le ... \le \varepsilon_N$. Hence, the critical points of $\mathcal{F}_{\nu,p}$ in $\mathcal{O}$ are solutions of a nonlinear eigenvalue problem with *positive* eigenvalues. So we may define the following problem

Problem 2.2. *Find the critical points Φ of the functional $\mathcal{F}_{\nu,p}$ on the domain A, satisfying moreover:*

$$\left\{\begin{array}{l} \exists u \in \mathcal{U}(N)\,|\,\mathrm{Gram}_{L^2}(u.\Phi) = \mathrm{Diag}(\sigma_1, ...\sigma_N)\,, \\ \textit{with, for all}\, k\,,\, \varepsilon_k = e_p(\sigma_k) < 1. \end{array}\right. \tag{2.9}$$

As we see later, we need a control, not only on the critical points for $\mathcal{F}_{\nu,p}$, but also on some of its Palais-Smale sequences. Even if $\mathcal{F}_{\nu,p}$ does not satisfy the Palais-Smale property, we may use a compactness result: [6, Lemma 2.1], which indicates the behaviour some Palais-Smale sequences, and ensures that the solutions of Problem 2.2 we will find actually converge to solutions of Problem 2.1.

Lemma 2.3 ([6]-Lemma 2.1). *Assume that $\alpha \max(Z,N) < \frac{2}{\frac{\pi}{2}+\frac{2}{\pi}}$.*

(a) Let (ν_n) be a sequence of real numbers in $(0,1)$, (p_n) a sequence of positive integers, and (Φ_n) a sequence in $\mathcal{O}$, i.e. such that

$$\mathrm{Gram}_{L^2}\Phi_n = \mathrm{Diag}(\sigma_{1,n}, ..., \sigma_{N,n}),\ 0 < \sigma_{1,n} \le ... \le \sigma_{N,n} < 1\,.$$

We denote $\varepsilon_{k,n} = e_{p_n}(\sigma_{k,n})$. We assume that

$$\mathcal{F}'_{\nu_n,p_n}(\Phi_n) \xrightarrow{n\to\infty} 0\,, \tag{2.10}$$

for the strong topology of $\left[H^{-\frac{1}{2}}(\mathbb{R}^3,\mathbb{C}^4)\right]^N = \left(E^N\right)^*$. We also assume that

$$\liminf_{n\to\infty} \sigma_{1,n} > 0\,. \tag{2.11}$$

Then,

$$\liminf_{n\to\infty} \sigma_{1,n} \ge h_0\,, \tag{2.12}$$

where $h_0 \in (0,1)$ is a constant which depends only on αZ, αN.

(b) If moreover,

$$\limsup_{n\to\infty} \sigma_{N,n} < 1 \,, \tag{2.13}$$

then, after extraction of a subsequence, the functions $\varphi_{k,n}$ converge to N functions $\varphi_k \in E \cap \bigcap_{1\le q\le \frac{3}{2}} W^{1,q}(\mathbb{R}^3, \mathbb{C}^4)$, for the strong $H^{\frac{1}{2}}$ topology.

(b.1) In the case $\nu_n \to \nu \in (0,1)$, and $p_n = p$ for n large, $\Phi = (\varphi_1, ..., \varphi_N)$ is a critical point of $\mathcal{F}_{\nu,p}$ in $\mathcal{O}$. Moreover, $\mathcal{F}_{\nu,p} = \lim_{n\to\infty} \mathcal{F}_{\nu_n,p_n}(\Phi_n)$.

(b.2) In the case $\nu_n \to 0$, and $p_n \to +\infty$, $\varphi_1, ..., \varphi_N$ satisfy the orthonormality constraints $(\varphi_l, \varphi_k)_{L^2} = \delta_{kl}$. They are strong solutions, in $\Sigma \cap \bigcap_{1\le q\le\frac{3}{2}} W^{1,q}(\mathbb{R}^3, \mathbb{C}^4)$, of the DF-equations

$$\overline{H}_\Phi \varphi_k = \varepsilon_k \varphi_k \,,\; \varepsilon_k = \lim_{n\to\infty} \varepsilon_{k,n} \in [h_0, 1) \,, \tag{2.14}$$

and the DF-energy is

$$\mathcal{E}(\Phi) = \lim_{n\to\infty} \mathcal{F}_{\nu_n,p_n}(\Phi_n) \,. \tag{2.15}$$

2.2 Reduction to the periodic setting

From now on, we consider fixed $\nu \in (0,1)$ and $p > 3$. It is possible to proceed to another transformation of the variational problem, as announced in (b). Let $L \in \mathbb{R}$, $L > 0$ and $\omega = \frac{2\pi}{L}$,

$$E_\omega = H^{\frac{1}{2}}_{per}((-\frac{L}{2}, \frac{L}{2})^3, \mathbb{C}^4) \,,$$

defined as functions with the following Fourier series,

$$\psi(x) = \sum_{p\in\mathbb{Z}^3} a_{\omega p} e^{i\omega p.x}$$

where the Fourier coefficients $a_{\omega p} \in \mathbb{C}^4$ satisfy

$$\sum_{p\in\mathbb{Z}^3} \left(1 + |\omega p|^2\right)^{\frac{1}{2}} |a_{\omega p}|^2 < \infty \,.$$

We may define the periodic free Dirac operator acting on $L^2_{per}((-\frac{L}{2}, \frac{L}{2})^3, \mathbb{C}^4)$ with domain E_ω with the same formula (1.1). Since $H_0^2 = -\Delta + 1$, the spectrum of this operator is contained in $(-\infty, -1] \cup [1, +\infty)$. This allows to define two orthogonal projectors on $L^2_{per}((-\frac{L}{2}, \frac{L}{2})^3, \mathbb{C}^4)$, still denoted by Λ^+ and Λ^-, having the same properties (1.3) as their equivalent in the non-periodic case.

In order to define a DF-functional on E_ω, we have to define a periodic potential corresponding to the coulombic potential. Let $G_{\nu,\omega}$ be the periodic potential defined by its Fourier series

$$G_{\nu,\omega}(x) = \frac{\omega}{4\pi} \sum_{p\in\mathbb{Z}^3, p\neq 0} \frac{g_\nu(p) e^{i\omega p.x}}{|p|^2} \,.$$

Remark that the coefficients are, for $p \neq 0$,

$$c_{\omega p} = \frac{\omega g_\nu(p)}{4\pi |p|^2} = \widehat{V_\nu}(p)\,.$$

Unlike the coulombic potential, this periodic potential is no more positive, but we get the following property: there exists a positive constant C_0 independent of ω such that

$$G_{\nu,\omega} \geq -\omega C_0\,. \tag{2.16}$$

This causes a little change in the computations, relatively to the non-periodic case, but, as we will see, the essential properties are preserved, as ω is close enough to 0. We may see $G_{\nu,\omega}$ as a function looking like V_ν in a neighborhood of 0 and the other points of the form Lp, with $p \in \mathbb{Z}^3$. Note that

$$\frac{1}{\omega} G_{\nu,\omega}\left(\frac{x}{\omega}\right) = G_1(x)\,,$$

where G_1 satisfies $-\Delta G_1 = \sum_{\lambda \in 2\pi\mathbb{Z}^3} V_\nu(. - \lambda) - 1$.

Thanks to the Fourier series computation, we are able to translate in the periodic case the results of Lemma 1.1: we express these inequalities using the Fourier transform and pass to the limit from a regular transform to a sum of Dirac distributions, corresponding to a Fourier series. The details of the computations are left to the reader.

Lemma 2.4. *The periodic potential $G_{\nu,\omega}$ satisfies the following Hardy-type inequalities, uniformly in $\nu \in (0,1)$:*

$$(\phi, G_{\nu,\omega}\phi)_{L^2_{per}} \leq \frac{1}{2}\left(\frac{\pi}{2} + \frac{2}{\pi}\right)(\phi, |H_0|\phi)_{L^2_{per}}\,, \tag{2.17}$$

for all $\phi \in \Lambda^+(E_\omega) \cup \Lambda^-(E_\omega)$. Moreover,

$$(\phi, G_{\nu,\omega}\phi)_{L^2_{per}} \leq \frac{\pi}{2}(\phi, |H_0|\phi)_{L^2_{per}}\,,\ \forall \phi \in E_\omega, \tag{2.18}$$

$$||G_{\nu,\omega}\phi||_{L^2_{per}} \leq 2||\nabla\phi||_{L^2_{per}}\,,\ \forall \phi \in H^1_{per}\,. \tag{2.19}$$

We may define the periodic DF-functional, depending on the parameters ν, p (fixed) and ω:

$$\mathcal{P}_\omega(\Phi) = \mathcal{E}_{\nu,\omega}(\Phi) - \pi_{p,\omega}(\Phi)\,, \tag{2.20}$$

that is,

$$\begin{aligned}
\mathcal{P}_\omega(\Phi) \;=\; & \sum_{k=1}^N (\varphi_k, H_0\varphi_k)_{L^2_{per}} - \alpha Z \sum_{k=1}^N (\varphi_k, G_{\nu,\omega}\varphi_k)_{L^2_{per}} \\
& + \frac{\alpha}{2}\iint_{(-\frac{L}{2},\frac{L}{2})^3 \times (-\frac{L}{2},\frac{L}{2})^3} G_{\nu,\omega}(x-y)\,[\rho(x)\rho(y) - \mathrm{tr}(R(x,y)R(y,x))]\,dxdy \\
& - \mathrm{tr}\left[(\mathrm{Gram}_{L^2_{per}}\Phi)^p(\mathbb{1} - \mathrm{Gram}_{L^2_{per}}\Phi)^{-1}\right]\,.
\end{aligned} \tag{2.21}$$

This functional is defined in the space

$$A_\omega = \left\{ \Phi \in E_\omega^N \,|\, 0 < \mathrm{Gram}_{L^2_{per}} \Phi < \mathbb{1} \right\} . \tag{2.22}$$

We write the Euler-Lagrange equations related to the Problem 2.7:

$$\overline{\Pi}_\Phi^\omega \varphi_k = \frac{\partial \pi_{p,\omega}}{\partial \varphi_k} , \tag{2.23}$$

where $\overline{\Pi}_\Phi^\omega$ is the one-particle Hamiltonian associated to the periodic problem, i.e.

$$\begin{aligned} \overline{\Pi}_\Phi^\omega \psi &= H_0\psi - \alpha Z G_{\nu,\omega}\psi + \alpha(\rho * G_{\nu,\omega})\psi \\ & \quad -\alpha \int_{(0,L)^3} R(x,y)\psi(y) G_{\nu,\omega}(x-y)dy . \end{aligned} \tag{2.24}$$

The most interesting properties of the new functional are the two following lemmas.

Lemma 2.5. *Assume that $\alpha(N-1) < \frac{2}{\frac{\pi}{2}+\frac{2}{\pi}}$, and let $\nu \in (0,1)$, $p \geq 3$ be fixed, and $M > 0$. Then, there exists $\varepsilon_0 > 0$, and two constants $\bar{K}(M,\nu) > 0$ and $\bar{\sigma}(M,\nu,p) < 1$ such that, given any sequence $(\Phi_n)_{n\geq 0} \in A_\omega$ verifying, for n large enough*

$$\begin{cases} |\mathcal{P}_\omega(\Phi_n)| & \leq M , \\ ||\mathcal{P}'_\omega(\Phi_n)||_{H^{-\frac{1}{2}}_{per}} & \leq \varepsilon_0 , \end{cases}$$

we get the following estimates, for n large enough

$$\left(\sum_k ||\varphi_{k,n}||^2_{E_\omega} \right)^2 \leq \bar{K}(M,\nu) , \tag{2.25}$$

and

$$\sigma_{N,n} \leq \bar{\sigma}(M,\nu,p) . \tag{2.26}$$

In other words, Palais-Smale sequences for $\mathcal{P}_\omega$ stay in a closed ball of E_ω^N. This allows to prove the Palais-Smale property for $\mathcal{P}_\omega$.

Lemma 2.6. *Given $\delta \in (0, \frac{1}{2})$, the functional $\mathcal{P}_\omega$ satisfies the Palais-Smale condition in $B_{\delta,\omega} = \{\Phi \in E_\omega^N \,|\, \delta \mathbb{1} \leq \mathrm{Gram}_{L^2_{per}} \Phi < \mathbb{1}\}$, i.e. any Palais-Smale sequence in $B_{\delta,\omega}$ is bounded and, up to a subsequence, converges to a critical point for $\mathcal{P}_\omega$.*

Note that, as in the non-periodic case, this functional is invariant by the action of $\mathcal{U}(N)$. We may define the periodic variational problem:

Problem 2.7. *Find critical points Ψ of the functional $\mathcal{P}_\omega$ in the space A_ω, with the following property*

$$\begin{cases} \exists u \in \mathcal{U}(N) \,|\, \mathrm{Gram}_{L^2_{per}}(u.\Psi) = \mathrm{Diag}(\sigma_1, ...\sigma_N) , \\ \exists b_0 \, , \forall k \, , \varepsilon_k = e_p(\sigma_k) \leq b_0 < 1. \end{cases} \tag{2.27}$$

The resolution of this variational framework will give solutions of Problem 2.2 provided we get a convergence lemma, which achieves the point (b) of the program:

Lemma 2.8. *Let (ω_n) be a sequence of positive real numbers such that* $\lim_{n\to\infty}\omega_n = 0$ *and (Φ_n) a sequence of critical points of $\mathcal{P}_{\omega_n}$ in A_{ω_n} satisfying:*

$$\exists u_n \in \mathcal{U}(N) \,|\, \mathrm{Gram}_{L^2_{per}}(u_n.\Phi_n) = \mathrm{Diag}(\sigma_{1,n}, ..., \sigma_{N,n})\,, \tag{2.28}$$

and

$$\exists b_0 \in (0,1) \,|\, \lim_{n\to\infty} \max_k e_p(\sigma_{k,n}) \le b_0\,. \tag{2.29}$$

Then, after extraction of a subsequence, the sequence (Φ_n) converges, in E, to a critical point Φ for $\mathcal{F}_{\nu,p}$, with

$$h_0 \mathbb{1} \le \mathrm{Gram}_{L^2_{per}}\Phi < \mathbb{1}\,,$$

where h_0 is the constant of Lemma 2.3.

2.3 Lyapunov-Schmidt reduction

So we are led to find critical points for the functional $\mathcal{P}_\omega$ corresponding to the periodic problem. Unfortunately, this functional is still strongly indefinite. One way to deal with this problem is to reduce the functional space to a finite dimensional space, thanks to a *Lyapunov-Schmidt* method.

This reduction is based on the fact that we may split any wave function Φ into two components: a "high frequency" component Φ_U and a "low frequency" one Φ_D, where frequency is meant to be the eigenvalue for the free Dirac operator H_0. Thanks to a contraction property of H_0^{-1}, we solve, using a fixed point theorem, the part of the DF-equations related to the high frequency part: this solution depends of course of the low frequency component.

Let $\tilde\lambda > 1$. We consider the projection Λ_U (resp. Λ_D) on the eigenspaces for H_0 corresponding to eigenvalues λ with $|\lambda| > \tilde\lambda$ (resp. $|\lambda| \le \tilde\lambda$). We get of course $H_0\Lambda_U = \Lambda_U H_0$, and $H_0\Lambda_D = \Lambda_D H_0$. We put $\Phi_U = \Lambda_U\Phi$, and $\Phi_D = \Lambda_D\Phi$.

Using the projectors Λ_U and Λ_D on (2.23), together with the commutation properties, we get the following system:

$$\left\{\begin{array}{rl} (\varphi_k)_D = & H_0^{-1}\left(\Lambda_D\left[M_\rho\varphi_k + N_R\varphi_k + \frac{\partial\pi_{p,\omega}}{\partial\varphi_k}\right]\right) \\ (\varphi_k)_U = & H_0^{-1}\left(\Lambda_U\left[M_\rho\varphi_k + N_R\varphi_k + \frac{\partial\pi_{p,\omega}}{\partial\varphi_k}\right]\right) \end{array}\right.\,, \tag{2.30}$$

where $M_\rho = \alpha Z G_{\nu,\omega} - \alpha(\rho * G_{\nu,\omega})$ and N_R is the operator

$$N_R(\psi) = \int_{(-\frac{L}{2},\frac{L}{2})^3} R(x,y)\psi(y)G_{\nu,\omega}(x-y)dy\,.$$

We observe that, given $\bar{\Phi} = (\bar{\varphi}_k) \in \Lambda_D E_\omega$ for every k, a solution to the second equation of (2.23) may be written as $\Xi = (\xi_k)_{1\leq k\leq N}$, with $\xi_k \in \Lambda_U E_\omega$ for all k, and Ξ is a fixed point of the operator $\mathcal{I}_{\bar{\Phi}}$ mapping $(\Lambda_U E_\omega)^N$ into itself, given by

$$\Xi \xrightarrow{\mathcal{I}_{\bar{\Phi}}} \left(H_0^{-1} \left[\Lambda_U \left(M_{\rho(\bar{\Phi}+\Xi)} \xi_k + N_{R(\bar{\Phi}+\Xi)} \xi_k + \frac{\partial \pi_{p,\omega}}{\partial \varphi_k}(\bar{\Phi}+\Xi) \right) \right] \right)_{1\leq k\leq N} .$$

The next lemma shows that we may apply the Banach fixed point theorem to find an unique $\bar{\Xi}$ associated to $\bar{\Phi}$. The following estimate will depend on ν, and we have to check that the considered $\bar{\Phi}+\bar{\Xi}$ is not too close to the boundary $\{\Phi \,|\, \mathrm{Gram}_{L^2_{per}} \Phi = \mathbb{1}\}$.

Lemma 2.9. *Let $\mu \in (0,1)$. Recall that we have fixed $\nu \in (0,1)$ and $p > 3$. There exists $\tilde{\lambda} > 0$ such that, given any $\lambda \geq \tilde{\lambda}$ and $\bar{\Phi} \in (\Lambda_D E_\omega)^N$ satisfying $0 < \mathrm{Gram}_{L^2_{per}} \Phi < (1-\mu)\mathbb{1}$, (where the projections Λ_D and Λ_U are defined with λ), the application $\mathcal{I}_{\bar{\Phi}}$ defined above, restricted to a ball of radius $\frac{\mu}{2}$ around 0, is contracting , i.e. there exists $k(\tilde{\lambda}) < 1$ such that for every Ξ_1, Ξ_2 in $(\Lambda_U(E_\omega))^N \cap B_{(L^2_{per})^N}(0, \frac{\mu}{2})$,*

$$||\mathcal{I}(\Xi_1) - \mathcal{I}(\Xi_2)||_{L^2_{per}} \leq k(\tilde{\lambda}) ||\Xi_1 - \Xi_2||_{L^2_{per}} .$$

Moreover, taking $\tilde{\lambda}$ large enough, the ball $(\Lambda_U(E_\omega))^N \cap B_{(L^2_{per})^N}(0, \frac{\mu}{2})$ is globally invariant relatively to the action of $\mathcal{I}_{\bar{\Phi}}$.

Then the application of the Banach fixed point theorem gives a fixed point for $\mathcal{I}_{\bar{\Phi}}$ in the ball $(\Lambda_U(E_\omega))^N \cap B_{(L^2_{per})^N}(0, \frac{\mu}{2})$. Thus we may define the map $h_{\tilde{\lambda}}$ from $(\Lambda_D E_\omega)^N$ to $(\Lambda_U E_\omega)^N \cap B_{(L^2_{per})^N}(0, \frac{\mu}{2})$, associating to every $\bar{\Phi}$ the unique fixed point of $\mathcal{I}_{\bar{\Phi}}$ in the ball. We put $\bar{\Xi} = h_{\tilde{\lambda}}(\bar{\Phi})$.

Thanks to this property, we can reduce our problem to a finite dimensional one: if we put, for $\Phi \in (\Lambda_D E_\omega)^N$

$$\mathcal{Q}_\omega(\Phi) = \mathcal{P}_\omega\left(\Phi + h_{\tilde{\lambda}}(\Phi)\right) , \tag{2.31}$$

then Problem 2.7 is solved when the following problem is solved:

Problem 2.10. *Find critical points $\Phi \in (\Lambda_D E_\omega)^N$ of the functional $\mathcal{Q}_\omega$, such that $\Psi = \Phi + h_{\tilde{\lambda}}(\Phi)$ satisfies condition (2.27).*

2.4 End of the proof

Once this reduction is done, we may use variational tools on the function $\mathcal{Q}_\omega$ acting on the finite dimensional space $(\Lambda_D E_\omega)^N$. Briefly speaking, we build a min-max using a linking property. In particular, we have to avoid critical points corresponding to solutions with N' electrons, for $N' < N$, i.e. critical points Φ with a null determinant Gram matrix. For more details, see Section 4. The result of this construction is the following lemma.

Lemma 2.11. *Let N and Z satisfy $\alpha \max(N,Z) < \frac{2}{\frac{\pi}{2}+\frac{2}{\pi}}$, and recall that ν and p are fixed. Given $\omega > 0$ small, there exists $J(\omega) \in \mathbb{N}$, and a sequence $(\Psi^j_\omega)_{0\le j\le J(\omega)}$, of critical points of $\mathcal{P}_\omega$. These critical points satisfy*

$$0 < \mathrm{Gram}_{L^2_{per}} \Psi^j_\omega < \mathbb{1}\,,$$

and there exists a positive sequence $\underline{c}_j$ such that, for any $j \ge 0$, we have $0 < \underline{c}_j < N$, $\lim_{j\to\infty} \underline{c}_j = N$, with

$$N > \mathcal{P}_\omega(\Psi^j_\omega) \ge \underline{c}_j\,. \tag{2.32}$$

Moreover, each Ψ^j_ω is of the form

$$\Psi^j_\omega = \Phi^j_\omega + h_{\hat\lambda}(\Phi^j_\omega)\,, \tag{2.33}$$

for some $\hat\lambda(\omega,\nu,p)$. The function Φ^j_ω is a critical point of $\mathcal{Q}_\omega$, i.e. the reduced functional associated to ω and $\hat\lambda$, and its Morse index $i_{\omega,j}$ satisfies

$$i_{\omega,j}(\Phi^j_\omega) \le Nm(\tilde\lambda,\omega) + N^2 + 2Nj\,, \tag{2.34}$$

where $2Nm(\tilde\lambda,\omega)$ is the (real) dimension of $(\Lambda_D E_\omega)^N$.

We remark that, for the construction of linkings of higher order, the functional space needs to have a sufficiently large dimension. Then, the Lyapunov-Schmidt reduction gives a critical point for $\mathcal{P}_\omega$ if a critical point for $\mathcal{Q}_\omega$ is found. We take advantage of the Morse-type information (2.34), as we see in the next lemma, to find an upper bound for the eigenvalues ε_k strictly lower than 1.

Lemma 2.12. *Let ν, p fixed. With the preceding notations, there exists two nondecreasing sequences $a(j)$ and $b(j) \in (0,1)$, independent of ω small, such that*

$$\overline{\Pi}^\omega_\Psi \psi^j_{k,\omega} = \varepsilon^j_{k,\omega}\psi^j_{k,\omega}\,, \tag{2.35}$$

with

$$0 < a(j) \le \varepsilon^j_1 \le \ldots \le \varepsilon^j_N \le b(j) < 1\,. \tag{2.36}$$

Now, it is possible, thanks to Lemma 2.8, to pass to the limit as the pulsation ω goes to 0: we obtain then a sequence $\tilde\Psi^j$ of critical points for the functional $\mathcal{F}_{\nu,p}$, with eigenvalues $\tilde\varepsilon^j_k$.

Finally, the use of Lemma 2.3 allows to pass to the limit as the parameters ν and p go respectively to 0 and ∞.

Remark 2.13. *One may probably get rid of the last reduction (Lyapunov-Schmidt reduction) by the use of the work of Abbondandolo [1], where a new Conley-Zehnder index is presented, allowing to handle directly strongly indefinite functionals.*

The end of this paper is organized as follows: Section 3 is devoted to the proof of Lemmas 2.5, 2.6, 2.8, 2.9. Section 4 is devoted to the linking procedure in the finite dimensional setting, i.e. the proof of Lemma 2.11. Section 5 deals with the estimates on the eigenvalues related to the Morse index, i.e. the proof of 2.12.

3 Convergence of approximate problems

3.1 Preliminary results

We are going to prove some results that will be used in the following proofs. They deal with the "periodic one-electron Hamiltonian" $\overline{\Pi}^{\omega}_{\Phi}$. These results are the analogues of [6, Lemma 3.1] in the periodic case. The main difference is the appearance of a term, which vanishes as ω goes to 0.

Lemma 3.1. *Assume* $\alpha \max(Z,N) < \frac{2}{\frac{2}{\pi}+\frac{\pi}{2}}$.

(i) There exists two constants $h_0 > 0$ *and* $\omega_0 > 0$*, such that, for any* $\nu \in [0,1]$, $0 < \omega < \omega_0$ *and* $\Phi \in E_\omega^N$ *such that* $\mathrm{Gram}_{L^2_{per}}\Phi \leq \mathbb{1}$*, and* $\psi \in E_\omega$*,*

$$h_0 ||\psi||_{H^{\frac{1}{2}}_{per}} \leq ||\overline{\Pi}^{\omega}_{\Phi}\psi||_{H^{-\frac{1}{2}}_{per}} . \tag{3.1}$$

In other words, for ω *small enough,* $\overline{\Pi}^{\omega}_{\Phi}$ *is a self-adjoint isomorphism between* $H^{\frac{1}{2}}_{per}$ *and its dual* $H^{-\frac{1}{2}}_{per}$*, whose inverse is bounded independently of* Φ*,* ν*.*

(ii) Fix $\nu \in (0,1]$ *and* $p \geq 3$*. Let* $\omega_n > 0$ *and* $\Phi_n \in E^N_{\omega_n}$*, with* $\mathrm{Gram}_{L^2_{per}}\Phi_n \leq \mathbb{1}$*. We assume that* $||\varphi_{k,n}||_{E_{\omega_n}}$ *is a bounded sequence. Let* $\psi_n \in E_{\omega_n}$ *be such that the sequence* $||\overline{\Pi}^{\omega_n}_{\Phi_n}\psi_n||_{L^2_{per}}$ *is bounded. then* ψ_n *is precompact in* $H^{\frac{1}{2}}_{loc}(\mathbb{R}^3,\mathbb{C}^4)$*.*

Proof. (i) We only point out the differences with [6, Lemma 3.1]. Let $\psi^\pm = \Lambda^\pm\psi$. From inequalities (2.17) and (2.16), we have

$$\begin{aligned}(\psi^+,\overline{\Pi}^{\omega}_{\Phi}\psi^+)_{E_\omega\times E^*_\omega} - (\psi^-,\overline{\Pi}^{\omega}_{\Phi}\psi^-)_{E_\omega\times E^*_\omega} \;\geq\;& \left(1-\frac{(\frac{\pi}{2}+\frac{2}{\pi})\alpha Z}{2} - \omega N C_1\right)||\psi^+||^2_{E_\omega}\\ &+ \left(1-\frac{(\frac{\pi}{2}+\frac{2}{\pi})\alpha N}{2} - \omega Z C_2\right)||\psi^-||^2_{E_\omega} ,\end{aligned}$$

where C_1,C_2 are constants coming from (2.16). With the assumption on N and Z, there exists $\omega_0 > 0$ such that, given any $\omega \in (0,\omega_0)$, the two factors are positive. Let us choose $h_0 = 1 - \frac{(\frac{\pi}{2}+\frac{2}{\pi})\alpha\max(N,Z)}{2} - \omega_0\max(C_1N, C_2Z)$. We get, for $\omega \leq \omega_0$,

$$\begin{aligned}||\psi||_{E_\omega}||\overline{\Pi}^{\omega}_{\Phi}\psi||_{E^*_\omega} &\geq Re(\psi^+ - \psi^-, \overline{\Pi}^{\omega}_{\Phi}\psi)_{E_\omega\times E^*_\omega} &(3.2)\\ &= (\psi^+,\overline{\Pi}^{\omega}_{\Phi}\psi^+)_{E_\omega\times E^*_\omega} - (\psi^-,\overline{\Pi}^{\omega}_{\Phi}\psi^-)_{E_\omega\times E^*_\omega} &(3.3)\\ &\geq h_0||\psi||^2_{E_\omega} , &(3.4)\end{aligned}$$

and (3.1) is proved.

(ii) From (i), a bound on $||\overline{\Pi}^{\omega_n}_{\Phi_n}\psi_n||_{L^2_{per}}$ implies a bound on $||\psi_n||_{E_{\omega_n}}$, hence a bound of the norm of ψ_n in $L^r((-\frac{\pi}{\omega_n},\frac{\pi}{\omega_n})^3,\mathbb{C}^4)$, for any $2\le r<3$. Moreover, the potential G_{ν,ω_n} is in the Marcinkiewicz space $\mathcal{M}^3((-\frac{\pi}{\omega_n},\frac{\pi}{\omega_n})^3,\mathbb{C}^4)$, and its norm in this space is bounded independently of ω_n. So $G_{\nu,\omega_n}\psi_n$ is bounded in any $L^q_{loc}(\mathbb{R}^3,\mathbb{C}^4)$, with $1\le q<\frac{3}{2}$, and $(\rho_{\Phi_n}*G_{\nu,\omega_n})\psi_n-\int G_{\nu,\omega_n}(x-y)R_{\Phi_n}(x,y)\psi_n(y)dy$ is in any $L^{q'}_{loc}(\mathbb{R}^3,\mathbb{C}^4)$, with $1\le q'<3$. As a consequence, using (i),

$$\psi_n=H_0^{-1}\left(\alpha ZG_{\nu,\omega_n}\psi_n-\alpha(\rho_{\Phi_n}*G_{\nu,\omega_n})\psi_n+\alpha\int G_{\nu,\omega_n}(x-y)R_{\Phi_n}(x,y)\psi_n(y)dy+\overline{\Pi}^{\omega}_{\Phi_n}\psi_n\right)$$

is precompact in $H^{\frac{1}{2}}_{loc}(\mathbb{R}^3,\mathbb{C}^4)$.$\diamond$

3.2 Proof of Lemmas 2.5 and 2.6

Consider a sequence $(\Phi_n)\in A_\omega$ satisfying

$$\left\{\begin{array}{ll}|\mathcal{P}_\omega(\Phi_n)| & \le M\,,\\ ||\mathcal{P}'_\omega(\Phi_n)|| & \le\varepsilon_0\,,\end{array}\right. \tag{3.5}$$

with

$$\mathrm{Gram}_{L^2_{per}}\Phi=\mathrm{Diag}(\sigma_{1,n},...,\sigma_{N,n}),\;0<\sigma_{1,n}\le...\le\sigma_{N,n}<1\,.$$

We have to prove that such a sequence is bounded in E^N_ω, if ε_0 is close enough to 0. For $\nu>0$ fixed, there is a constant $\mathcal{K}_1(\nu)>0$ such that, for any $\Phi\in A_\omega$,

$$\mathcal{E}'_{\nu,\omega}(\Phi).\Phi\le 2\mathcal{E}_{\nu,\omega}(\Phi)+\mathcal{K}_1(\nu)\,. \tag{3.6}$$

From (3.5), with the notations $\theta_p(t)=\frac{t^p}{1-t}$, $\theta'_p(t)=e_p(t)$, we infer

$$\mathcal{E}_{\nu,\omega}(\Phi_n)\le M+\sum_k\theta_p(\sigma_{k,n})\,, \tag{3.7}$$

and

$$\mathcal{E}'_{\nu,\omega}(\Phi_n).\Phi_n\ge\sum_k e_p(\sigma_{k,n})\sigma_{k,n}-\varepsilon_0\left(\left[\sum_k||\varphi_{k,n}||^2_{E_\omega}\right]^{\frac{1}{2}}\right)\,. \tag{3.8}$$

Combining (3.5), (3.6), (3.7) and (3.8), we get

$$\begin{aligned}\sum_k e_p(\sigma_{k,n})\sigma_{k,n}-2\theta_p(\sigma_{k,n}) &\le \mathcal{E}'_{\nu,\omega}(\Phi_n).\Phi_n-2\mathcal{E}_{\nu,\omega}(\Phi_n)+2M\\ &\quad+\varepsilon_0\left[\sum_k||\varphi_{k,n}||^2_{E_\omega}\right]^{\frac{1}{2}},\\ &\le \mathcal{K}_2(\nu,M)+\varepsilon_0\left[\sum_k||\varphi_{k,n}||^2_{E_\omega}\right]^{\frac{1}{2}}.\end{aligned}$$

Since $\frac{e_p(t)t}{\theta_p(t)} = \frac{\sum_{n\geq p} nt^n}{\sum_{n\geq p} t^n} \geq p$, the assumption $p \geq 3$ leads to

$$\sum_k e_p(\sigma_{k,n})\sigma_{k,n} \leq \mathcal{K}_3(\nu, M) + \varepsilon_0 \left[\sum_k ||\varphi_{k,n}||^2_{E_\omega}\right]^{\frac{1}{2}} . \tag{3.9}$$

On the other side, consider the product of $\mathcal{P}'_\omega(\Phi_n)$ with $\Phi_n^+ - \Phi_n^-$. We recall the notation $\Phi^\pm = (\Lambda^\pm\varphi_1, ..., \Lambda^\pm\varphi_N)$. We get

$$\begin{aligned} \mathcal{P}'_\omega(\Phi_n).(\Phi_n^+ - \Phi_n^-) &= \mathcal{E}'_{\nu,\omega}(\Phi_n).(\Phi_n^+ - \Phi_n^-) - \pi_{p,\omega}(\Phi_n).(\Phi_n^+ - \Phi_n^-) \\ &\geq \left(1 - \frac{(\frac{\pi}{2} + \frac{2}{\pi})\alpha \max(Z, N)}{2}\right) \left[\sum_k ||\varphi_{k,n}||^2_{E_\omega}\right]^{\frac{1}{2}} \\ &\qquad - \sum_k e_p(\sigma_{k,n})\sigma_{k,n} + 2\pi'_{p,\omega}(\Phi_n)\Phi_n^- \end{aligned} \tag{3.10}$$

Since

$$\pi'_{p,\omega}(\Phi)\psi = 2\sum_k e_p(\sigma_k) Re(\Phi_k, \psi_k) , \tag{3.11}$$

the last term is nonnegative and we get, with $c_1 = \left(1 - \frac{(\frac{\pi}{2}+\frac{2}{\pi})\alpha \max(Z,N)}{2}\right)$,

$$\left[\sum_k ||\varphi_{k,n}||^2_{E_\omega}\right]^{\frac{1}{2}} \leq c_1^{-1} \left(\sum_k e_p(\sigma_{k,n})\sigma_{k,n} + \mathcal{P}'_\omega(\Phi_n).(\Phi_n^+ - \Phi_n^-)\right) , \tag{3.12}$$

Using (3.5), we estimate the last term, and get, for every $\varepsilon_0 < c_1$,

$$\left[\sum_k ||\varphi_{k,n}||^2_{E_\omega}\right]^{\frac{1}{2}} \leq (c_1 - \varepsilon_0)^{-1} \sum_k e_p(\sigma_{k,n})\sigma_{k,n} . \tag{3.13}$$

This and (3.9) imply that $[\sum_k ||\varphi_{k,n}||_{E_\omega}]^{\frac{1}{2}}$ and $\sum_k e_p(\sigma_{k,n})\sigma_{k,n}$ are both bounded. We call the bound $\bar{K}(M, \nu)$. Since $e_p(t) \to +\infty$ as $t \to 1^-$, this implies the estimate

$$\sigma_{N,n} \leq \bar{\sigma}(M, \nu, p) < 1 . \tag{3.14}$$

and the proof of Lemma 2.5 is over.$\diamond$

To prove Lemma 2.6, it is sufficient to apply Lemma 2.5 to a Palais-Smale sequence for $\mathcal{P}_\omega$ in $B_{\delta,\omega}$. Then, using the usual Sobolev inequalities, implying compact embeddings in the periodic case, the precompactness claimed is proved.$\diamond$

3.3 Proof of Lemma 2.8

After extraction of a subsequence, we may impose

$$\varepsilon_{k,n} = e_p(\sigma_{k,n}) \xrightarrow{n\to\infty} \varepsilon_k \leq b_0 \,.$$

Consider a sequence of critical points (Φ_n) satisfying (2.28) and (2.29). Using the Euler-Lagrange equation (2.23), their corresponding critical values are bounded by Nb_0, and Lemma 3.1 gives a bound of the norm of (Φ_n) in $E^N_{\omega_n}$. We may cut these functions and consider them as functions in $H^{\frac{1}{2}}((-\frac{L_n}{2},\frac{L_n}{2})^3,\mathbb{C}^4) \subset L^2(\mathbb{R}^3,\mathbb{C}^4)$, with $L_n = \frac{2\pi}{\omega_n}$. We apply Lemma 3.1 (ii) and obtain that the sequence Φ_n is precompact in $H^{\frac{1}{2}}_{loc}$. Then, using arguments similar to [6, Proof of Lemma 2.1 (b)], we find that the cut functions actually converge in E to critical points for $\mathcal{F}_{\nu,p}$, with the bound b_0 on each energy level ε_k.

3.4 Proof of Lemma 2.9

In order to prove this lemma, we take advantage of the smoothing of the potential $G_{\nu,\omega}$. We will obtain a contraction coefficient depending on ν. Indeed, we may write, calling λ the cut-off frequency,

$$\begin{aligned}
||\mathcal{I}(\Xi_1)-\mathcal{I}(\Xi_2)||_{L^2_{per}} \quad &\leq \quad H_0^{-1}\Lambda_U\,\big[\big(M_{\rho(\bar\Phi+\Xi_1)}\xi_{1,k} - M_{\rho(\bar\Phi+\Xi_2)}\xi_{2,k}\big) \\
&\qquad + \big(N_{R(\bar\Phi+\Xi_1)}\xi_{1,k} - N_{R(\bar\Phi+\Xi_2)}\xi_{2,k}\big) \\
&\qquad + \left(\frac{\partial\pi_{p,\omega}}{\partial\varphi_k}(\bar\Phi+\Xi_1) - \frac{\partial\pi_{p,\omega}}{\partial\varphi_k}(\bar\Phi+\Xi_2)\right)\big] \\
&\leq \quad \frac{1}{\tilde\lambda}\mathcal{K}_3(\nu,p,\omega,\mu)||\Xi_1-\Xi_2||_{L^2_{per}}\,,
\end{aligned}$$

where $\mathcal{K}_3$ is obtained with the use of Lemma 2.4 (the tedious but straightforward details of this computation are left to the reader). Then, defining $\tilde\lambda = (\mathcal{K}_3+1)^{-1}$, we obtain the desired contraction property.

The proof of the stability property is based on the same kind of estimate: for $\tilde\lambda$ large enough, we have for example $\mathcal{I}_{\bar\Phi}(0) \in B_{L^2_{per}}(0,\frac{\mu}{10})$.$\diamond$

4 The linking construction

This section is devoted to the proof of Lemma 2.11. Recall that we now consider a functional $\mathcal{Q}_\omega$ defined on a subset of a finite dimensional space $(\Lambda_D E_\omega)^N$, and ν, p, ω, $\tilde\lambda$ are fixed. Let $2m(\omega,\tilde\lambda)$ be the real dimension of $\Lambda_D E_\omega$. We recall that, due to the Lyapunov-Schmidt reduction, $\mathcal{Q}_\omega$ is defined on $\mathcal{A}_\mu$, where $\mathcal{A}_\mu$ denotes

(4.1) $$\mathcal{A}_\mu = \left\{\Phi \in (\Lambda_D E_\omega)^N \,|\, \mathrm{Gram}_{L^2_{per}}\Phi < (1-\mu)\mathbb{1}\right\}\,.$$

In this definition, μ is very small and will be chosen later. Note that $\mathrm{Gram}_{L^2_{per}} \Phi$ may be degenerate, if $\Phi \in \mathcal{A}_\mu$. According to Lemma 2.5, the limitation $\mathrm{Gram}_{L^2_{per}} \Phi < (1-\mu)\mathbb{1}$ is not restrictive, since we know that there is no critical point outside $\mathcal{A}_\mu$, for μ sufficiently small. On the contrary, this limitation parametrized with μ is a protection against a diverging $\pi_{p,\omega}$-term or a diverging $||\Phi||_{E^N_\omega}$. We define the degenerate set $\mathcal{D}$ in $\mathcal{A}_\mu$,

$$\mathcal{D} = \left\{ \Phi \in \mathcal{A}_\mu \mid \det \mathrm{Gram}_{L^2_{per}} \Phi = 0 \right\} . \tag{4.2}$$

We will define pairs of submanifolds $(\mathcal{V}_j, \Sigma_j^+)_{1 \le j \le J(\omega)}$ which link together, following [6], but we first explain the idea of our linking procedure with the pair corresponding to $j = 0$. At the end of this section, we will check that the pairs defined for the other linkings satisfy the same properties. Define, for $\delta \in (0,1)$ such that $\delta > \mu$, the following $\mathcal{U}(N)$-invariant manifold without boundary

$$\Sigma_\delta^+ = \left\{ \Phi \in \Lambda^+ \mathcal{A}_\mu \,|\, \mathrm{Gram}_{L^2_{per}} \Phi = (1-\delta)\mathbb{1} \right\} , \tag{4.3}$$

and, if V denotes a linear subspace of $\Lambda^+ E_\omega$, with (complex) dimension N,

$$\mathcal{V} = \mathcal{A}_\mu \cap (\Lambda^- E_\omega \oplus V)^N . \tag{4.4}$$

Under these conditions, the submanifolds Σ_δ^+ and $\partial \mathcal{V}$ link, i.e. $\Sigma_\delta^+ \cap \partial\mathcal{V} = \emptyset$ and

$$\# \left\{ \left(\Sigma_\delta^+ \cap \mathcal{V} \right) / \mathcal{U}(N) \right\} = 1 . \tag{4.5}$$

Indeed $\Lambda^- E_\omega \oplus V$ and $\Lambda^+ E_\omega$ intersect transversally (as linear subspaces of E_ω). Their intersection is a complex subspace of dimension N (namely V), and the intersection above is exactly one orbit by the $\mathcal{U}(N)$ action.

The key point of the proof of Lemma 2.11 is the construction of a pseudo-gradient vector field $\mathcal{X}$ in $\mathcal{A}_\mu = \left\{ \Phi \in (\Lambda_D E_\omega)^N \,|\, 0 \le \mathrm{Gram}_{L^2_{per}} \Phi < (1-\mu)\mathbb{1} \right\}$ having good properties with respect to the degenerate set $\mathcal{D}$. Following a linking idea, the image of $\mathcal{V}$ by the flow of this pseudogradient will always intersect Σ_δ^+. Let us define the vector field $\mathcal{X}$. Let $\theta_\varepsilon : \mathbb{R} \to [0,1]$ be a smooth real function satisfying

$$\begin{cases} \theta_\varepsilon(s) = 0 \text{ for } s \le \frac{\varepsilon}{2} , \\ \theta_\varepsilon(s) = 1 \text{ for } s \ge \varepsilon , \\ \theta_\varepsilon'(s) > 0 \text{ for } s \in (\frac{\varepsilon}{2}, \varepsilon) . \end{cases} \tag{4.6}$$

Let $\Phi \in \mathcal{A}_\mu$. We consider $\Phi^+ = \Lambda^+ \Phi = (\varphi_1^+, ..., \varphi_N^+)$, and

$$\mathcal{O}^+ = \left\{ \Phi \in \mathcal{A}_\mu \,|\, \mathrm{Gram}_{L^2_{per}} \Phi^+ = \mathrm{Diag}(\sigma_1^+, ..., \sigma_N^+) \right\} . \tag{4.7}$$

Let $\Phi \in \mathcal{O}^+$, with $\mathrm{Gram}_{L^2_{per}} \Phi^+ = \mathrm{Diag}(\sigma_1^+, ..., \sigma_N^+)$. With $\Psi = (\psi_k)_{1 \le k \le N} = \Phi + h_{\bar\lambda}(\Phi)$, we define the function

$$\tau(\Phi) = \theta_1 \left(\left(\sum_k ||\psi_k||^2_{E_\omega} \right)^{\frac{1}{2}} - K_b(V) \right) ,$$

where $K_b(V) \ge \bar K(N, \nu)$ will be defined more precisely later, and $\bar K$ is defined in (2.25). The vector field $\mathcal{X}$ is given by

$$\begin{aligned} \mathcal{X}_k(\Phi) \quad := \quad & \theta_1(\mathcal{Q}_\omega(\Phi) + 2) \Big((\theta_\varepsilon(\sigma_k^+) + \tau(\Phi)) \left[-\frac{\partial \mathcal{Q}_\omega}{\partial \varphi_k}(\Phi) \right] + \\ & (1 - \tau(\Phi))(1 - \theta_\varepsilon(\sigma_k^+)) \left[\Lambda^- \varphi_k - \Lambda^+ \varphi_k \right] \Big) \ . \end{aligned} \tag{4.8}$$

Remark that we are only interested in positive levels for $\mathcal{Q}_\omega$, so we define a nonzero $\mathcal{X}$ at points Φ where $\mathcal{Q}_\omega > -2$. The function τ gives the following indication: $\tau(\Phi) > 0$ and $\mathcal{Q}_\omega(\Phi) \le N$ implies that $||\mathcal{Q}'_\omega(\Phi)||_{(E^N_\omega)^*} \ge \varepsilon_0$, according to Lemma 2.5. The main feature of this vector field is that it is a positive linear combination of the gradient $-\frac{\partial \mathcal{Q}_\omega}{\partial \varphi_k}$ of $\mathcal{Q}_\omega$ and the gradient $\Lambda^- \varphi_k - \Lambda^+ \varphi_k$ of the periodic free Hamiltonian.

As every $\Phi \in \mathcal{A}_\mu$ is obtained by the action of $\mathcal{U}(N)$ on $\mathcal{O}^+$, we may then extend $\mathcal{X}$ to an equivariant vector field, for $u \in \mathcal{U}(N)$,

$$\mathcal{X}(u.\Phi) := u(\mathcal{X}(\Phi)) \,. \tag{4.9}$$

By construction, this vector field is locally Lipschitz.

Lemma 4.1. *The vector field $-\mathcal{X}$ is a pseudogradient for $\mathcal{Q}_\omega$, i.e. it is locally Lipschitz and there exists $\kappa > 0$ such that for every $\Phi \in \mathcal{A}_\mu$,*

$$\frac{\partial \mathcal{Q}_\omega}{\partial \varphi_k}(\Phi).\mathcal{X}_k \le -\kappa || \frac{\partial \mathcal{Q}_\omega}{\partial \varphi_k}(\Phi) ||_{E^*_\omega} ||\mathcal{X}_k||_{E_\omega} \,. \tag{4.10}$$

Moreover, there exists θ_1, $\theta_2 > 0$ such that, for $\mathcal{Q}_\omega(\Phi) \ge -1$,

$$\theta_1 || \frac{\partial \mathcal{Q}_\omega}{\partial \varphi_k} ||_{E^*_\omega} \le ||\mathcal{X}_k||_{E_\omega} \le \theta_2 || \frac{\partial \mathcal{Q}_\omega}{\partial \varphi_k} ||_{E^*_\omega} \,. \tag{4.11}$$

Proof. We just have to prove (4.10) for $\Phi \in \mathcal{O}^+$ since $\mathcal{Q}_\omega$ is invariant by the $\mathcal{U}(N)$ action. Let $\Phi \in \mathcal{O}^+$ satisfy $\mathrm{Gram}_{L^2} \Phi^+ = \mathrm{Diag}(\sigma_1^+, ..., \sigma_N^+)$. there is nothing to prove if every σ_k^+ is greater than ε: in this case, $\mathcal{X}$ is the gradient of $\mathcal{Q}_\omega$. Suppose now that $0 \le \sigma_k^+ \le \varepsilon$. Using the chain rule, we get

$$\begin{aligned} \frac{\partial \mathcal{Q}_\omega}{\partial \varphi_k}(\Phi).\xi_k \quad &= \quad \frac{\partial \mathcal{P}_\omega}{\partial \varphi_k}(\Phi + h_{\bar\lambda}(\Phi)).(\xi_k + Dh_{\bar\lambda}(\xi_k)) \,, \\ &= \quad \frac{\partial \mathcal{P}_\omega}{\partial \varphi_k}(\Phi + h_{\bar\lambda}(\Phi)).\xi_k \,, \end{aligned} \tag{4.12}$$

by construction of the Lyapunov-Schmidt reduction. Recall that $h_{\tilde{\lambda}}$ has been defined after Lemma 2.9 and is bounded, by construction

$$||h_{\tilde{\lambda}}(\Phi)||_{E^N_\omega} \leq \frac{C_3}{\tilde{\lambda}}||\Phi||_{E^N_\omega}\,. \tag{4.13}$$

Using this inequality and Lemma 3.1, one finds

$$\frac{\partial\mathcal{E}_{\nu,\omega}}{\partial\varphi_k}(\Phi + h_{\tilde{\lambda}}(\Phi)).\left(\Lambda^+\varphi_k - \Lambda^-\varphi_k\right) \geq$$
$$(1-\frac{C_5}{\tilde{\lambda}})\left[1-\frac{(\frac{\pi}{2}+\frac{2}{\pi})\alpha\max(N,Z)}{2} - \omega\max(NC_1, ZC_2)\right]||\varphi_k||^2_{E_\omega}\,. \tag{4.14}$$

There remains to compute the terms involving $\pi_{p,\omega}$. To do this, we need to extend some definitions. We define, for Q a $N\times N$ hermitian matrix such that $0 \leq Q < \mathbb{1}$:

$$S_p(Q) = \mathrm{tr}\left[Q^p(\mathbb{1}-Q)^{-1}\right] = \sum_{n\geq p}\mathrm{tr}(Q^n)\,, \tag{4.15}$$

$$e_p(Q) = \left[pQ^{p-1} - (p-1)Q^p\right]\left[\mathbb{1}-Q\right]^{-2} = \sum_{n\geq p} nQ^{n-1}\,. \tag{4.16}$$

Then we may write $S'_p(Q).h = \mathrm{tr}(e_p(Q).h)$ and $\pi_{p,\omega} = S_p \circ \mathrm{Gram}_{L^2_{per}}$. This allows to write the remaining terms like

$$\frac{\partial\pi_{p,\omega}}{\partial\varphi_k}(\Phi + h_{\tilde{\lambda}}(\Phi)).\xi_k = \mathrm{tr}\left(e_p\left(\mathrm{Gram}_{L^2_{per}}(\Phi + h_{\tilde{\lambda}}(\Phi))\right)\mathcal{M}_k(\Phi + h_{\tilde{\lambda}}(\Phi), \xi_k)\right) + O(\frac{|\xi_k|}{\tilde{\lambda}})\,, \tag{4.17}$$

where the last term comes from the Lyapunov Schmidt reduction, and does not change the result, if $\tilde{\lambda}$ is large enough. Moreover $\mathcal{M}_k(\zeta,\xi_k)$ is the following $N\times N$ complex matrix, with $\alpha_j = (\zeta_j, \xi_k)$, :

$$\mathcal{M}_k(\xi,\zeta) = \begin{pmatrix} O & \alpha_1 & O \\ & \vdots & \\ \alpha_1^*\ldots & 2Re(\alpha_k) & \ldots\alpha_N^* \\ & \vdots & \\ O & \alpha_N & O \end{pmatrix}.$$

For the sake of simplicity, we put $\Psi = \Phi + h_{\tilde{\lambda}}(\Phi)$, and explain the computations in the case $k=1$, the other values of k implying the same calculations. With the notation $e_{ij} = (e_p(\mathrm{Gram}_{L^2_{per}}\Psi))_{ij}$, the coefficients of the matrix, we have

$$\begin{aligned} \frac{\partial\pi_{p,\omega}}{\partial\varphi_1}(\Psi).\xi_1 &= \sum_j e_{j1}(\xi_1,\psi_j) + \sum_j e_{1j}(\psi_j,\xi_1) \\ &= 2Re\left(\sum_j e_{1j}(\psi_j, \Lambda^+\varphi_1 - \Lambda^-\varphi_1)\right)\,, \end{aligned} \tag{4.18}$$

replacing $\xi_1 = \Lambda^+\varphi_1 - \Lambda^-\varphi_1$. We may write

$$\begin{aligned}
\frac{\partial \pi_{p,\omega}}{\partial \varphi_1}(\Psi).(\Lambda^+\varphi_1 - \Lambda^-\varphi_1) &= 2Re(e_{11}\sigma_1^+) - 2Re\left(\sum_{i=1}^N e_{1i}(\Lambda^-\varphi_i, \Lambda^-\varphi_1)\right) \\
&= 4Re(e_{11}\sigma_1^+) - 2Re\left(\sum_{i=1}^N e_{1i}(\varphi_i, \varphi_1)\right), \qquad (4.19)
\end{aligned}$$

because $(\varphi_i, \varphi_1) = (\Lambda^+\varphi_i, \Lambda^+\varphi_1) + (\Lambda^-\varphi_i, \Lambda^-\varphi_1) = \delta_{i1}\sigma_1^+ + (\Lambda^-\varphi_i, \Lambda^-\varphi_1)$, and this is due to the diagonalization of the Λ^+-terms. But

$$(4.20) \qquad \sum_{i=1}^N e_{1i}(\varphi_i, \varphi_1) = \left[e_p(\mathrm{Gram}_{L^2_{per}}\Psi)\mathrm{Gram}_{L^2_{per}}\Phi\right]_{11} \geq 0\,,$$

and the sum is nonnegative because it is a diagonal term of a positive hermitian matrix. Hence,

$$(4.21) \qquad \frac{\partial \pi_{p,\omega}}{\partial \varphi_1}(\Psi).(\Lambda^+\varphi_1 - \Lambda^-\varphi_1) \leq 4Re(e_{11}\sigma_1^+)\,,$$

Now, we claim that e_{11} (and, for $k \neq 1$, e_{kk}) is bounded above with a constant depending only on μ, on the set where $\mathcal{X} \neq 0$ and $\theta_\varepsilon(\sigma_1^+) \geq 0$ (resp. $\theta_\varepsilon(\sigma_k^+) \geq 0$). Indeed, for μ close enough to 1, for any Ψ such that $\mathrm{Gram}_{L^2_{per}}\Psi \geq (1-\mu)\mathbb{1}\}$, we get either $\mathcal{P}_\omega(\Psi) < -2$ or $(\sum_k ||\psi_k||^2_{E_\omega})^{\frac{1}{2}} > \bar{K}(N,\nu)$. The last alternative is given by a simple comparison between the $\mathcal{E}_{\nu,\omega}$-term and the $\pi_{p,\omega}$-term in the functional.

In both cases, the coefficient of $\Lambda^+\varphi_k - \Lambda^-\varphi_k$ in the vector field $\mathcal{X}$ is zero, hence the only set where $\Lambda^+\varphi_k - \Lambda^-\varphi_k$ occurs in $\mathcal{X}$ is $\Psi \in \{\Phi \in \mathcal{A}_\mu \,|\, \mathrm{Gram}_{L^2_{per}}\Phi \leq (1-\mu)\mathbb{1}\}$, where we get an uniform estimate for e_{11}: if $\mathrm{Gram}_{L^2_{per}}\Phi \leq (1-\mu)\mathbb{1}$, then

$$(4.22) \qquad e_{11} \leq C''(\mu)\,.$$

Then we prove, using this result, that $Re(e_{11}\sigma_1^+)$ is bounded above with a function of ε going to 0 as ε goes to 0. Indeed, either $||\varphi_1||^2_{L^2_{per}} \geq \sqrt{\varepsilon}$, and we get the estimate

$$\begin{aligned}
Re(e_{11}\sigma_1^+) &\leq |e_{11}|||\varphi_1^+||^2_{L^2_{per}} \\
&\leq \sqrt{\varepsilon}C''(\mu)||\varphi_1||^2_{L^2_{per}}\,,
\end{aligned}$$

or $||\varphi_1||^2_{L^2_{per}} \leq \sqrt{\varepsilon}$. In this case, we may use a property of the function e_p, given in the following proposition, whose proof is left to the reader:

Proposition 4.2. *Let $\mu \in (0,1)$. There exists a nondecreasing continuous function $\bar{\chi}_\mu : \mathbb{R}^+ \to \mathbb{R}^+$, such that $\lim_{s\to 0}\bar{\chi}_\mu(s) = 0$ and, given any self-adjoint $N \times N$ matrix $A = (a_{ij})$ satisfying $0 \leq A \leq (1-\mu)\mathbb{1}$, we get*

$$(4.23) \qquad [e_p(A)]_{11} \leq \bar{\chi}_\mu(a_{11})\,.$$

Then we may write

$$e_{11} \leq \bar{\chi}_\mu(\frac{C_3}{\tilde{\lambda}}\sqrt{\varepsilon}) \,,$$

and

$$Re(e_{11}\sigma_1^+) \leq \bar{\chi}_\mu(\frac{C_3}{\tilde{\lambda}}\sqrt{\varepsilon})||\varphi_1||^2_{L^2_{per}} \,. \tag{4.24}$$

In any case, we get the following bound

$$\frac{\partial \pi_{p,\omega}}{\partial \varphi_1}(\Psi).(\Lambda^+\varphi_1 - \Lambda^-\varphi_1) \leq \chi_\mu(\varepsilon)||\varphi_1||^2_{L^2_{per}} \,, \tag{4.25}$$

with $\chi_\mu(\varepsilon) = \max(\sqrt{\varepsilon}C''(\mu), \bar{\chi}_\mu(\frac{C_3}{\tilde{\lambda}}\sqrt{\varepsilon}))$, and $\lim_{\varepsilon\to 0}\chi_\mu(\varepsilon) = 0$.

Now, combining (4.14) and (4.25), we get

$$\begin{aligned} &\frac{\partial \mathcal{Q}_\omega}{\partial \varphi_1}(\Psi).(\Lambda^+\varphi_1 - \Lambda^-\varphi_1) \geq \\ &\qquad \Bigg(\frac{C_5}{\tilde{\lambda}}) \left(1 - \frac{(\frac{\pi}{2}+\frac{2}{\pi})\alpha\max(N,Z)}{2} - \omega\max(NC_1, ZC_2)\right) - \chi_\mu(\varepsilon)\Bigg) ||\varphi_1||^2_{E_\omega} \,. \end{aligned} \tag{4.26}$$

The same computation gives the same result for $k \neq 1$.

Taking ε small enough, we obtain a positive lower bound, and (4.10) comes from the estimates

$$||\frac{\partial \mathcal{E}_{\nu,\omega}}{\partial \varphi_i}||_{(E^*_\omega)^N} \leq C_{10}||\varphi_i||_{E_\omega} \,, \tag{4.27}$$

and

$$||\frac{\partial \pi_{p,\omega}}{\partial \varphi_i}||_{E^*_\omega} \leq C_{11}(\mu)||\varphi_i||_{E_\omega} \,. \tag{4.28}$$

Now we prove (4.11). The first inequality comes directly from (4.26). It is sufficient to check the second property with the free Hamiltonian gradient, and

$$\begin{aligned} ||\Lambda^+\varphi_k - \Lambda^-\varphi_k||^2_{E_\omega} &\leq ||\Lambda^+\varphi_k|||^2_{E_\omega} + ||\Lambda^-\varphi_k|||^2_{E_\omega} \\ &\leq ||\varphi_k|||^2_{E_\omega} \\ &\leq C_{12}\frac{\partial \mathcal{Q}_\omega}{\partial \varphi_k}.(\Lambda^+\varphi_k - \Lambda^-\varphi_k) \\ &\leq C_{12}||\frac{\partial \mathcal{Q}_\omega}{\partial \varphi_k}||_{E^*_\omega}||\Lambda^+\varphi_k - \Lambda^-\varphi_k||_{E_\omega} \,, \end{aligned}$$

and the proof is over. $\diamond$

We call η^s the flow of the pseudogradient $\mathcal{X}$. From now on, "flow lines" are meant to be the flow lines of the pseudogradient $-\mathcal{X}$. We define now the constant $K_b(V)$.

Lemma 4.3. *Given the linear subspace V, there exists $K_b(V) \geq \bar{K}(\max_{\mathcal{V}} \mathcal{Q}_\omega, \nu)$ and $\mu \in (0,1)$ such that the flow η^s of the pseudogradient $\mathcal{X}$ (defined with this $K_b(V)$) has the following property:*

> *For any $\Phi \in \mathcal{V}$ such that $\mathcal{Q}_\omega(\Phi) \leq M$, for any $s \geq 0$ such that $\mathcal{Q}_\omega(\eta^s(\Phi)) \geq 0$, we get*
>
> $$0 \leq \mathrm{Gram}_{L^2_{per}}(\eta^s(\Phi)) \leq (1-\mu)\mathbb{1}\,. \tag{4.29}$$

Proof. Let $K' > \bar{K}(\max_{\mathcal{V}} \mathcal{Q}_\omega, \nu)$. Suppose that there exists $0 \leq s_1 \leq s_2$ such that

$$\begin{aligned} \left(\sum_{k=1}^{N} ||(\eta^{s_1}(\Phi))_k||^2_{E_\omega}\right)^{\frac{1}{2}} &= \bar{K}(\max_{\mathcal{V}} \mathcal{Q}_\omega, \nu) \\ \left(\sum_{k=1}^{N} ||(\eta^{s_2}(\Phi))_k||^2_{E_\omega}\right)^{\frac{1}{2}} &= K' \end{aligned}$$

and, for any $s \in [s_1, s_2]$,

$$\left(\sum_{k=1}^{N} ||(\eta^{s_2}(\Phi))_k||^2_{E_\omega}\right)^{\frac{1}{2}} \in [\bar{K}(\max_{\mathcal{V}} \mathcal{Q}_\omega, \nu), K']\,.$$

Since $-\mathcal{X}$ is a pseudogradient for $\mathcal{Q}_\omega$, we know that

$$\mathcal{Q}_\omega(\eta^s(\Phi)) \leq \mathcal{Q}_\omega(\Phi) \leq \max_{\mathcal{V}} \mathcal{Q}_\omega\,.$$

This implies, following Lemma 2.5, that for any $s \geq 0$ such that

$$\left(\sum_{k=1}^{N} ||(\eta^{s}(\Phi))_k||^2_{E_\omega}\right)^{\frac{1}{2}} > \bar{K}(\max_{\mathcal{V}} \mathcal{Q}_\omega, \nu)\,,$$

we have

$$||\frac{\partial \mathcal{Q}_\omega}{\partial \Phi}(\eta^s(\Phi))||_{(E^N_\omega)^*} \geq \varepsilon_0\,.$$

Then,

$$\begin{aligned} \mathcal{Q}_\omega(\eta^{s_2}(\Phi)) - \mathcal{Q}_\omega(\eta^{s_1}(\Phi)) &= \int_{s_1}^{s_2} \frac{\partial \mathcal{Q}_\omega}{\partial \Phi}(\eta^s(\Phi)).\mathcal{X}(\eta^s(\Phi))ds \\ &\leq -\kappa\varepsilon_0 \int_{s_1}^{s_2} ||\mathcal{X}(\eta^s(\Phi))||ds \\ &\leq -\kappa\varepsilon_0(K' + \bar{K}(\max_{\mathcal{V}} \mathcal{Q}_\omega, \nu))\,. \end{aligned}$$

Defining

$$K_b(V) = \bar{K}(\max_{\mathcal{V}} \mathcal{Q}_\omega, \nu) + \frac{2 + \max_{\mathcal{V}} \mathcal{Q}_\omega}{\kappa\varepsilon_0}\,, \tag{4.30}$$

we get that any flow line joining a point of E_ω^N-norm $\bar{K}(\max_{\mathcal{V}} \mathcal{Q}_\omega, \nu)$ to a point of E_ω^N-norm $K_b(V)$ attains this point with

$$\mathcal{Q}_\omega(\eta^{s_2}(\Phi)) \leq -2\,.$$

Hence there exists a $K'' \in [\bar{K}(\max_{\mathcal{V}} \mathcal{Q}_\omega, \nu), K_b(V)]$ such that for every $\Phi \in \mathcal{V}$ and for every $s \geq 0$ verifying $\mathcal{Q}_\omega(\eta^s(\Phi)) \geq 0$, we get

$$\left(\sum_{k=1}^N ||(\eta^s(\Phi))_k||^2_{E_\omega}\right)^{\frac{1}{2}} \leq K''\,,$$

which implies, as in Lemma 2.5, a bound $\bar{\sigma}$ (uniform in s and Φ) depending on $\max_{\mathcal{V}} \mathcal{Q}_\omega$, ν and p, for the eigenvalues of $\mathrm{Gram}_{L^2_{per}}(\eta^s(\Phi))$. Denoting $1-\mu$ this bound, (4.29) is proved.$\diamond$

The pseudogradient $\mathcal{X}$ has the following interesting properties:

Lemma 4.4. *If $\Phi \in \mathcal{O}^+$ satisfies $\sigma_1^+ < \frac{\varepsilon}{2}$, then for any $s \geq 0$, the matrix $\mathrm{Gram}_{L^2_{per}}([\eta^s(\Phi)]^+)$ has an eigenvalue lower than $e^{-s}\sigma_1^+$.*

As a consequence, if $\eta^s(\Phi)$ tends to a critical point Φ_c for $\mathcal{Q}_\omega$ as s goes to $-\infty$, if moreover 0 is an eigenvalue of $\mathrm{Gram}_{L^2_{per}}\Phi_c$, then, for any $s \in \mathbb{R}$, 0 is an eigenvalue of $\mathrm{Gram}_{L^2_{per}}([\eta^s(\Phi)]^+)$.

This is very important for our linking procedure: according to this lemma, there is no flow line going from a point in a ε-neighborhood of $\mathcal{D}$ to a point in Σ_δ^+. In particular, the flow lines joining $\mathcal{V}$ to Σ_δ^+ stay away from $\mathcal{D}$, at a distance of at least ε.

Proof of Lemma 4.4. It is sufficient to prove that, calling $\sigma^+(s)$ the smallest eigenvalue of $\mathrm{Gram}_{L^2_{per}}([\eta^s(\Phi)]^+)$, we get,

$$\lim \sup_{h>0, h\to 0} \frac{\sigma^+(s+h)-\sigma^+(s)}{h} \leq -\sigma^+(s)\,.$$

We can take $\Phi \in \mathcal{O}^+$ after action of an element in $\mathcal{U}(N)$. We put then

$$\mathrm{Gram}_{L^2_{per}}([\eta^s(\Phi)]^+) = \mathrm{Diag}\left(\sigma^+(s), \sigma_2^+(s), ..., \sigma_N^+(s)\right)\,. \tag{4.31}$$

Then

$$\begin{aligned}
\sigma^+(s+h) &= \inf_{x\in\mathbb{C}^N, ||x||=1} ||\sum_i x_i \Lambda^+\eta^{s+h}(\Phi)_i||^2_{L^2_{per}} \\
&\leq ||\Lambda^+\eta^{s+h}(\Phi)_i||^2_{L^2_{per}} \\
&\leq ||\Lambda^+\eta^s(\Phi)_i||^2_{L^2_{per}} + 2h\left(\Lambda^+\eta^s(\Phi)_i, -\Lambda^+\eta^s(\Phi)_i\right)_{L^2_{per}} + o(h)\,,
\end{aligned}$$

and we conclude

$$\lim \sup_{h>0, h\to 0} \frac{\sigma^+(s+h)-\sigma^+(s)}{h} \leq -\sigma^+(s) < 0\,, \tag{4.32}$$

which implies the lemma. $\diamond$

For the linking procedure, we follow now ideas inspired by [15]. We will suppose that $\mathcal{Q}_\omega$ is a Morse function; if it is not true, we will indicate later the means to overcome the problem. It is possible, since we work on a finite dimensional setting, to perturb slightly $\mathcal{V}$ into $\bar{\mathcal{V}}$ such that it is transverse to every stable manifold of any critical point for $\mathcal{Q}_\omega$.

Consider the image $\eta^s(\bar{\mathcal{V}})$ for $s \geq 0$. From the linking property, given any $s \geq 0$, we have

$$\#\left\{\left(\eta^s(\mathcal{V}) \cap \Sigma_\delta^+\right)/\mathcal{U}(N)\right\} = 1.$$

As $\overline{\mathcal{V}}$ is compact, there is a limit point $\bar{\Phi}$ in the sequence

$$\left\{\eta^{-s}\left(\left(\eta^s(\bar{\mathcal{V}}) \cap \Sigma_\delta^+\right)/\mathcal{U}(N)\right)\right\}\,,$$

as s goes to infinity. We now consider the following point:

$$\bar{\Phi}_* = \lim_{s\to+\infty} \eta^s(\bar{\Phi})\,, \tag{4.33}$$

and claim that

Lemma 4.5. *$\bar{\Phi}_*$ is a critical point for $\mathcal{Q}_\omega$, and*

$$\mathcal{Q}_\omega(\bar{\Phi}_*) \geq c = \min_{\Phi\in\Sigma_\delta^+} (\mathcal{Q}_\omega(\Phi)) > 0\,.$$

Moreover, $\bar{\Phi}_* \notin \mathcal{D}$ and its Morse index is bounded above by the real dimension of $\mathcal{V}/\mathcal{U}(N)$, i.e. $Nm(\omega,\tilde{\lambda}) + N^2$.

Proof. The fact that $\bar{\Phi}_*$ is a critical point for $\mathcal{Q}_\omega$ is a consequence of the linking property, and the pseudogradient properties of $\mathcal{X}$. The inequality $\mathcal{Q}_\omega(\bar{\Phi}_*) \geq c > 0$ also follows from this linking property.

We have to prove that $\bar{\Phi}_* \notin \mathcal{D}$: actually, this is due to the construction of $\mathcal{X}$. Looking at the flow lines issued from $\eta^{-s}\left(\left(\eta^s(\mathcal{V}) \cap \Sigma_\delta^+\right)/\mathcal{U}(N)\right)$, they are all connecting a point in $\mathcal{V}/\mathcal{U}(N)$ to a point in $\Sigma_\delta^+/\mathcal{U}(N)$. Since flow lines arriving at $\Sigma_\delta^+/\mathcal{U}(N)$ cannot come close to $\mathcal{D}$, it is impossible for $\bar{\Phi}$ to belong to $\mathcal{D}$.

Finally, $\mathcal{V}/\mathcal{U}(N)$ intersects the stable manifold of the critical point $\bar{\Phi}_*$, and, by assumption, the intersection is transverse, but this is only possible if

$$\mathrm{codim} W^s(\bar{\Phi}_*) \leq \dim\left(\mathcal{V}/\mathcal{U}(N)\right) \tag{4.34}$$

and, since $\mathcal{Q}_\omega$ is a Morse function, the codimension above is exactly the Morse index of $\bar{\Phi}_*$ for this function.$\diamond$

If $\mathcal{Q}_\omega$ is not a Morse function, it is possible , adding a small $\mathcal{U}(N)$-invariant perturbation τ_n acting on $\mathcal{A}_\mu$, to change $\mathcal{Q}_\omega$, when acting on $\mathcal{A}_\mu/\mathcal{U}(N)$, into a Morse function $\mathcal{Q}_\omega+\tau_n$. From the Morse Lemma, we may even impose τ_n to be as small as we want, for example we take

$$\lim_{n\to+\infty}||\tau_n||_{C^1}=0\,.$$

We also replace $\mathcal{X}$ by the vector field $\mathcal{X}_n$ obtained from $\mathcal{Q}_\omega+\tau_n$ with formula (4.8). We obtain a nondegenerate critical point $\bar{\Phi}_n$, exactly as above. There remains then to pass to the limit as n goes to infinity. This is an easy task: since we work in a finite dimensional setting, the bounded sequence $\bar{\Phi}_n$ is precompact, and a subsequence converges, say, to $\bar{\Phi}_*$. Now,

$$\mathcal{Q}'_\omega(\bar{\Phi}_n)=-\tau'_n(\bar{\Phi}_n)\xrightarrow{n\to+\infty}0\,,$$

hence $\bar{\Phi}_*$ is a critical point for $\mathcal{Q}_\omega$. Since the distance between $\mathcal{D}$ and $\bar{\Phi}_n$ is uniformly bounded below, $\bar{\Phi}_*\notin\mathcal{D}$. Finally, since we consider only strict Morse index (i.e. the number of strictly decreasing directions, or negative eigenvalues of the Hessian matrix) of a finite dimensional function, the equation (4.34) still holds true.

We may now define precisely the submanifolds $(\mathcal{V}_j,\Sigma_j^+)$, and check that the announced properties are verified. To this aim, we use a periodic version of [6, Lemma 5.2]:

Lemma 4.6. *Assume that* $\alpha Z<\frac{2}{\frac{2}{\pi}+\frac{\pi}{2}}$. *Then there exists a nondecreasing sequence* $\{\lambda_j, j\ge 0\}$ *in* $(0,1)$, *with* $\lim_{j\to+\infty}\lambda_j=1$ *and a sequence* $\{G_{j,\omega}, 0\le j\le J(\omega)\}$ *of complex linear subspaces of* $\Lambda_D E_\omega^+$, *with*

$$\dim_{\mathbb{C}}(\Lambda_D E_\omega^+/G_{j,\omega})=j\,, \tag{4.35}$$

and

$$\left(\varphi^+,H_0-\alpha Z G_{\nu,\omega}\varphi^+\right)_{L^2_{per}}\ge\lambda_j||\varphi^+||_{L^2_{per}}\,,\ \forall\varphi^+\in G_{j,\omega}\,. \tag{4.36}$$

Proof. We refer to [6] or, for a similar but nonperiodic case [17].$\diamond$

We define the following submanifold without boundary

$$\Sigma_j^+=\left\{\Phi^+\in(G_{j,\omega})^N\,|\,\mathrm{Gram}_{L^2_{per}}\Phi^+=\frac{j+1}{j+2}\mathbb{1}\right\}\,. \tag{4.37}$$

Now, if V_j is a linear subspace of Λ^+E_ω, with complex dimension $j+N$, defined as the orthogonal space of $G_{j+N,\omega}$ in $\Lambda_D E_\omega^+$, we may define

$$\mathcal{V}_j=\mathcal{A}_\mu\cap(\Lambda^-E_\omega\oplus V_j)^N\,. \tag{4.38}$$

Now $\mathcal{V}_j$ and Σ_j^+ link and we have the same formula (4.5). The properties of the pseudogradient stay valid, particularly the fact that no flow line can join

$\mathcal{D}$ to Σ_j^+. Given ω and $\tilde{\lambda}$, we may define a $J(\omega) = m(\omega, \tilde{\lambda})$ and a constant K_b uniformly for every linking (i.e. for $1 \leq j \leq J(\omega)$) replacing $K_b(V)$:

$$K_b = \max_{1 \leq j \leq J(\omega)} (K_b(V_j)) .$$

The critical points are obtained exactly in the same way, and the Morse index estimate reads now

$$i_M(\Phi_\omega^j) \leq \dim_{\mathbb{R}} \mathcal{V}_j / \mathcal{U}(N) = Nm(\tilde{\lambda}, \omega) + 2N(N+j) - N^2 , \tag{4.39}$$

and we get (2.34).

Finally, we get (2.32) using Lemma 4.6: we get of course

$$\mathcal{Q}_\omega(\Phi_\omega^j) \geq \min_{\Phi \in \Sigma_j^+} \mathcal{Q}_\omega(\Phi) \tag{4.40}$$

$$\geq N\lambda_j \frac{j+1}{j+2} , \tag{4.41}$$

as soon as the j-th linking is possible. We define $\underline{c}_j = N\lambda_j \frac{j+1}{j+2}$ and this gives (2.32). Now, using μ defined in Lemma 4.3 and $\hat{\lambda}$ large enough, we may define

$$\Psi_\omega^j = \Phi_\omega^j + h_{\hat{\lambda}}(\Phi_\omega^j) , \tag{4.42}$$

which satisfies the conditions of Lemma 2.11.$\diamond$

5 Morse-type estimates

In this section, devoted to the proof of Lemma 2.12, we look at the Morse index of the critical point and min-max sequences developed in the preceding section, in order to get some a priori estimates on the eigenvalues ε_k. Obtaining estimates from Morse-type information is now a usual technique (see [7], or [8] for a complete exposition). Thanks to the $\mathcal{U}(N)$ invariance, we consider Φ_ω^j one of the critical points found in the last section for $\mathcal{Q}_\omega$, such that

$$\mathrm{Gram}_{L^2_{per}} \Phi_\omega^j = \mathrm{Diag}(\sigma_1, ..., \sigma_N) , \text{ with } 0 < \sigma_1 \leq ... \leq \sigma_N < 1 . \tag{5.1}$$

We denote its Morse index by k_0. To get the upper bound for the corresponding eigenvalues ε_k of the infinite dimensional problem, we will use the definition of the Morse index: if V is a linear subspace of $(\Lambda_D E_\omega)^N$ such that $\dim V \geq k_0 + 1$, then $\mathcal{Q}''_\omega(\Phi_\omega^j)$ cannot be negative on the whole space V. Therefore we are going to construct a subspace V of $(\Lambda_D E_\omega)^N$, whose dimension will be greater than $k_0 + 1$ and where we have an estimate like

$$\exists 0 < b(k_0) < 1, \ \forall \Psi \in V, \ \mathcal{Q}''_\omega(\Phi_\omega^j).\Psi^2 < (b(k_0) - \varepsilon_N)||\Psi||^2 . \tag{5.2}$$

As $\mathcal{Q}''_\omega$ cannot be negative on V, there exists a $\Psi \neq 0$ in V such that $\mathcal{Q}''_\omega(\Phi_\omega^j).\Psi^2 \geq 0$ and thus $\varepsilon_N \leq b(k_0) < 1$.

In order to construct such a subspace, we need the following preliminary result:

Proposition 5.1. *Recall that ν and p are fixed. There exists $m(\nu) \in \mathbb{N}$ such that, given any critical point Ψ^j_ω of $\mathcal{P}_\omega$ that we found, there exists a subspace $W_{\Phi^j_\omega}$ of E^N_ω, with dimension m, such that*

$$(E_L^-)^N = W_{\Psi^j_\omega} \overset{\perp}{\oplus} F^-_{\Psi^j_\omega} \,,$$

and

$$\forall \chi \in F^-_{\Psi^j_\omega}\,,\ \mathcal{P}''_\omega(\Psi^j_\omega).\chi^2 \leq -\frac{1}{2}||\chi||^2 \,. \tag{5.3}$$

Proof. Using the Cauchy-Schwarz inequality, one can easily prove the estimate, for any $\chi \in (\Lambda^- E_\omega)^N$,

$$\begin{aligned}
\mathcal{P}''_\omega(\Psi^j_\omega).\chi^2 &\leq -\sum_{k=1}^N (\chi_k, \sqrt{1-\Delta}\chi_k) + 3\iint \rho_{\Psi^j_\omega}(x)\rho_\chi(y)G_{\nu,\omega}(x-y)dxdy \\
&\leq \sum_{k=1}^N \Big(\chi_k, \Big[-\sqrt{1-\Delta} + 3(\rho_{\Psi^j_\omega} * G_{\nu,\omega})\Big]\chi_k\Big) \,. \qquad (5.4)
\end{aligned}$$

Define

$$W_{\Psi^j_\omega} = \sum_{\lambda \leq \frac{1}{2}, \lambda \in \sigma(\sqrt{1-\Delta} - 3(\rho_{\Psi^j_\omega} * G_{\nu,\omega}))} Ker\Big[\sqrt{1-\Delta} - 3(\rho_{\Psi^j_\omega} * G_{\nu,\omega}) - \lambda Id\Big] \,.$$

Since $\nu \in (0,1)$ is fixed, we may see $U^j_{\nu,\omega} = 3(\rho_{\Psi^j_\omega} * G_{\nu,\omega})$ as a compact perturbation of $\sqrt{1-\Delta}$. Hence, by a classical argument of spectral theory, $W_{\Psi^j_\omega}$ is finite dimensional. But we can say more: its dimension may be bounded above with a constant m depending on ν. This comes from the fact that, for each $q \geq 1$, there is a constant $C_{\nu,q}$ such that

$$||(U^j_{\nu,\omega} - \frac{1}{2})_+||_{L^q_{per}} \leq C_{\nu,q} \,, \tag{5.5}$$

where $(U)_+$ denotes the positive part of U. Then, [4, Section 2] gives the estimate (to use this result, it is in fact sufficient to get a L^3 bound). Then, the orthogonal space of $W_{\Psi^j_\omega}$ in $(\Lambda^- E_\omega)^N$ satisfies (5.3).$\diamond$

Note that by construction, the vectors in $W_{\Psi^j_\omega}$ are regular functions: indeed, for ν fixed, one can easily prove, by a bootstrap method, that for each $q \geq 1$, there is a constant $C'_{\nu,q}$ such that, for all $\chi \in W_{\Phi^j_\omega}$,

$$||\chi||_{W^{1,q}_{per}} \leq C'_{\nu,q}||\chi||_{L^2_{per}} \,. \tag{5.6}$$

Thanks to this estimate, we get

$$||\Lambda_U|_{W_{\Psi^j_\omega}}||_{\mathcal{L}(E_\omega, E_\omega)} = O(\frac{1}{\tilde{\lambda}}) \,,$$

so we can replace $W_{\Phi_\omega^j}$ by $\Lambda_D W_{\Phi_\omega^j} = \tilde{W}_{\Phi_\omega^j}$, and consider $F'_{\Phi_\omega^j}$, or simply F' for convenience, the orthogonal space of $\tilde{W}_{\Phi_\omega^j}$ in $\Lambda_D\Lambda^- E_\omega$. Given $\tilde{\lambda}$ great enough, an estimate like (5.3) is conserved:

$$\forall \chi \in F'_{\Phi_\omega^j}\,,\ \mathcal{Q}''_\omega(\Psi_\omega^j).\chi^2 \leq -\frac{1}{4}||\chi||^2\,. \tag{5.7}$$

Let U_d be a subspace with dimension d of *radial* smooth functions with exponential decay defined in $\mathbb{R}^3$ and values in $\mathbb{R}$. We may associate, for $u \in \mathbb{N}$, $u > 0$,

$$W_{d,u} = \left\{ \chi = \begin{pmatrix} f(\frac{\cdot}{u}) \\ 0 \\ 0 \\ 0 \end{pmatrix}, f \in U_d \right\}.$$

Since we work in a periodic setting, we have to "periodize" these functions: we consider, for each $\psi \in W_{d,u}$, a corresponding periodic function $\tilde{\psi} \in E_\omega$, such that, for every $x \in (-\frac{\pi}{\omega}, \frac{\pi}{\omega})^3$, we get $\tilde{\psi}(x) = \psi(x)$. We denote $\tilde{W}_{d,u,\omega}$ the vector space spanned by the $\tilde{\psi}$, for $\psi \in W_{d,u}$. We denote W' the image of $\tilde{W}_{d,u,\omega}$ by the projector $\Lambda_D\Lambda^+$.

Define now the following subspace of $(\Lambda_D E_\omega)^N$, for ω small enough

$$V = \{[\{0\} \times ... \times \{0\} \times W'] \oplus F'\} \cap \{\varphi_{1,\omega}^j, ..., \varphi_{N,\omega}^j\}^\perp\,.$$

We have to check that V satisfies the estimate (5.2). The following result will be helpful.

Lemma 5.2. *For any $\Psi \in A_\omega$ and $\varphi \in E_\omega$, of the form $\varphi(x) = f(|x|)$ for every $x \in (-\frac{\pi}{\omega}, \frac{\pi}{\omega})^3$, taking $\Phi(x) = (0, ..., 0, \varphi(x))$, we have*

$$\frac{1}{2}\mathcal{E}''_{\nu,\omega}(\Psi)\,[\Phi,\Phi] \leq (\varphi, H_0\varphi)_{L^2_{per}} + \alpha(1+v(\omega))(N-Z-1)(\varphi, G_{\nu,\omega}\varphi)_{L^2_{per}}\,,$$

with $v(\omega)$ going to 0 as ω goes to 0.

Proof. The proof is the same as in [6, Lemma 4.4], taking into account the fact that we work in a periodic setting. More precisely, we may write

$$\begin{aligned} \mathcal{E}_{\nu,\omega}(\phi_1...\phi_N) &= \mathcal{E}_{\nu,\omega}(\phi_1...\phi_{N-1}) + (\phi_N, H_0\phi_N)_{L^2_{per}} - \alpha Z(\phi_N, G_{\nu,\omega}\phi_N)_{L^2_{per}} \\ &\quad + \alpha \iint G_{\nu,\omega}(x-y) \sum_{k=1}^{N-1} |\phi_k(x)|^2 |\phi_N(x)|^2 \\ &\quad - \alpha \iint G_{\nu,\omega}(x-y) \sum_{k=1}^{N-1} (\phi_k(y), \phi_N(y))\,(\phi_N(x), \phi_k(x))\,. \end{aligned} \tag{5.8}$$

So $\mathcal{E}_{\nu,\omega}$ is a quadratic form in ϕ_N, when $\phi_1, ..., \phi_{N-1}$ are fixed. Note that

$$\iint G_{\nu,\omega}(x-y)\,(\phi_k(y), \psi(y))\,(\psi(x), \phi_k(x))$$

is nonnegative, since the Fourier series associated to $G_{\nu,\omega}$ has only positive coefficients. Hence,

$$\frac{1}{2}\mathcal{E}''_{\nu,\omega}(\Psi)\,[\Phi,\Phi] \leq (\varphi, H_0\varphi)_{L^2_{per}} - \alpha Z(\varphi, G_{\nu,\omega}\varphi)_{L^2_{per}}$$

$$+\alpha \iint_{(-\frac{\pi}{\omega},\frac{\pi}{\omega})^3\times(-\frac{\pi}{\omega},\frac{\pi}{\omega})^3} G_{\nu,\omega}(x-y)\sum_{k=1}^{N-1}|\psi_k(x)|^2|\varphi(x)|^2\,, \tag{5.9}$$

for any $\Phi = (0, ..., 0, \varphi(x))$, with $\varphi \in E_\omega$. Now, if $\rho \in L^1$ is radial and nonnegative, then an easy computation shows that

$$\int_{\mathbb{R}^3} \rho(x)V_\nu(x-x_0)dx \leq \int_{\mathbb{R}^3} \rho(x)V_\nu(x)dx,\ \forall x_0 \in \mathbb{R}^3\,.$$

We deduce the following property for *periodic* functions:

$$\int_{(-\frac{\pi}{\omega},\frac{\pi}{\omega})^3} |\varphi(x)|^2 G_{\nu,\omega}(x-x_0)dx \leq (1+v(\omega))\int_{(-\frac{\pi}{\omega},\frac{\pi}{\omega})^3} |\varphi(x)|^2 G_{\nu,\omega}(x)dx\,, \tag{5.10}$$

with $v(\omega)\geq 0$ going to 0 as ω goes to 0. As a consequence,

$$\begin{aligned}
&\int_{(-\frac{L}{2},\frac{L}{2})^3} dy\sum_{k=1}^{N-1}|\phi_k(y)|^2\int_{(-\frac{L}{2},\frac{L}{2})^3}|\psi(x)|^2G_{\nu,\omega}(x-y)dx \leq\\
&\leq\ (1+v(\omega))\int_{(-\frac{L}{2},\frac{L}{2})^3} dy\sum_{k=1}^{N-1}|\phi_k(y)|^2\int_{(-\frac{L}{2},\frac{L}{2})^3}|\psi(x)|^2G_{\nu,\omega}(x)dx\\
&\leq\ (1+v(\omega))(N-1)(\psi, G_{\nu,\omega}\psi)_{L^2_{per}}\,,
\end{aligned}$$

and the lemma follows.$\diamond$

The space W' is the image of $\tilde{W}_{d,u,\omega}$ by the projector $\Lambda_D\Lambda^+$. For u large enough, $\Lambda_D\Lambda^+|_{\tilde{W}_{d,u,\omega}}$ is close to this identity. Indeed, there exists $c^* > 0$, depending on d, such that, for every $\psi \in \tilde{W}_{d,u,\omega}$,

$$||\Lambda^-\psi||^2_{L^2_{per}} \quad\leq\quad \frac{c^*}{u^2}||\psi||^2_{L^2_{per}}\,. \tag{5.11}$$

Moreover, scaling arguments imply that there exists a constant $0 < c_* < c^*$ depending on d such that, for any $\psi \in W'$ and u large,

$$(H_0\psi,\psi) \quad=\quad ||\psi||^2_{L^2_{per}}\,, \tag{5.12}$$

$$||\nabla\psi||^2_{L^2_{per}} \quad\leq\quad \frac{c^*}{u^2}||\psi||^2_{L^2_{per}}\,, \tag{5.13}$$

$$(\psi, G_{\nu,\omega}\psi) \quad\geq\quad \frac{c_*}{u}||\psi||^2_{L^2_{per}}, -C_0\omega||\psi||^2_{L^2_{per}}\,. \tag{5.14}$$

We obtain the estimate (5.2) as follows. In the following, we take the notation $(\chi)_k$ for the k-th coordinate of the vector $\chi \in E_\omega^N$. Note that the decomposition $\chi_u + \chi^-$ follows the splitting in Proposition 5.1. We get:

$$\begin{aligned}
\frac{1}{2}\mathcal{P}''_\omega(\Psi^j_\omega).\chi^2 &= \frac{1}{2}\mathcal{E}''_{\nu,\omega}(\Phi^i)(\chi,\chi) - \frac{1}{2}\pi''_{p,\omega}(\Psi^j_\omega)(\chi,\chi) \\
&= \frac{1}{2}\mathcal{E}''_{\nu,\omega}(\Psi^j_\omega)(\chi_u+\chi^-,\chi_u+\chi^-) - \frac{1}{2}\sum_{k=1}^N 2e_p(\sigma_k)||(\chi)_k||^2_{L^2_{per}},
\end{aligned}$$

this follows form the fact that every $(\Psi)_k$ is orthogonal to every φ^i_k. Now,

$$\begin{aligned}
&\frac{1}{2}\mathcal{P}''_\omega(\Psi^j_\omega).\chi^2 = \\
&= \frac{1}{2}\mathcal{E}''_{\nu,\omega}(\Psi^j_\omega)(\chi_u,\chi_u) + \frac{1}{2}\mathcal{E}''_{\nu,\omega}(\Psi^j_\omega)(\chi^-,\chi^-) + Re\left[\mathcal{E}''_{\nu,\omega}(\Psi^j_\omega)(\chi_u,\chi^-)\right] \\
&\quad -\sum_{k=1}^N e_p(\sigma_k)||(\chi)_k||^2_{L^2_{per}} \\
&\leq (\chi_u, H_0\chi_u) + \alpha(1+v(\omega))(N-Z-1)(\chi_u, G_{\nu,\omega}\chi_u) - \sum_{k=1}^N e_p(\sigma_k)||(\chi)_k||^2_{L^2_{per}} \\
&\quad -\frac{1}{2}||\chi^-||^2_{L^2_{per}} + c_1||\nabla\chi_u||_{L^2_{per}}||\Lambda^-\chi^-||_{L^2_{per}},
\end{aligned}$$

the last inequality is coming from Lemma 5.2, the fact that $\chi^- \in F'$ and Proposition 5.1. The real part term (involving c_1) is obtained with Hardy type inequality. We follow using the estimates (5.12), (5.13), (5.14) and (5.11):

$$\begin{aligned}
&\frac{1}{2}\mathcal{P}''_\omega(\Psi^j_\omega).\chi^2 \leq \\
&\leq ||\chi_u||^2_{L^2_{per}}\left(1 - \frac{\alpha(Z+1-N)}{u}\right) - \frac{1}{2}||\chi^-||^2_{L^2_{per}} + C_0\omega||\chi_u||^2_{L^2_{per}} \\
&\quad +\frac{c^*c_1}{u}||\chi_u||_{L^2_{per}}||\chi^-||_{L^2_{per}} - \sum_{k=1}^N e_p(\sigma_k)||(\chi_u)_k + (\chi^-)_k||^2_{L^2_{per}} \\
&\leq ||\chi_u||^2_{L^2_{per}}\left(1 + C_0\omega - \frac{\alpha(Z+1-N)}{u} - e_p(\sigma_N)\right) - \frac{1}{2}||\chi^-||^2_{L^2_{per}} \\
&\quad +\frac{c^*c_1}{u}||\chi_u||_{L^2_{per}}||\chi^-||_{L^2_{per}} - \sum_{k+1}^N e_p(\sigma_k)||(\chi^-)_k||^2_{L^2_{per}} - 2e_p(\sigma_N)Re(\chi_u,(\chi^-)_N)
\end{aligned}$$

$$
\begin{aligned}
\leq\ & ||\chi_u||^2_{L^2_{per}}\left(1+C_0\omega-\frac{\alpha(Z+1-N)}{u}-e_p(\sigma_N)\right)-\frac{1}{2}||\chi^-||^2_{L^2_{per}}\\
&+\frac{c^*c_1}{u}||\chi_u||_{L^2_{per}}||\chi^-||_{L^2_{per}}+2e_p(\sigma_N)||\Lambda^-\chi_u||_{L^2_{per}}||\chi^-||_{L^2_{per}}\\
\leq\ & ||\chi_u||^2_{L^2_{per}}\left(1+C_0\omega-\frac{\alpha(Z+1-N)}{u}-e_p(\sigma_N)\right)-\frac{1}{2}||\chi^-||^2_{L^2_{per}}+\frac{c'}{u}||\chi_u||_{L^2_{per}}||\chi^-||_{L^2_{per}}\\
\leq\ & ||\chi_u||^2_{L^2_{per}}\left(1+C_0\omega-\frac{\alpha(Z+1-N)}{u}-e_p(\sigma_N)+\frac{(c')^2}{2u^2}\right)\\
\leq\ & ||\chi||^2_{L^2_{per}}\left(1+C_0\omega-\frac{\alpha(Z+1-N)}{u}-e_p(\sigma_N)+\frac{(c')^2}{2u^2}\right).
\end{aligned}
$$

From this computation, we obtain the following estimate on $\mathcal{Q}''_\omega$:

(5.15)
$$
\frac{1}{2}\mathcal{Q}''_\omega(\Phi^j_\omega).\chi^2\leq||\chi||^2_{L^2_{per}}\left(1+C_0\omega-\frac{\alpha(Z+1-N)}{u}-e_p(\sigma_N)+\frac{(c')^2}{2u^2}+O(\frac{1}{\tilde{\lambda}})\right),
$$

where the last term is due to the Lyapunov-Schmidt reduction.

Given $\tilde{\lambda}$ large enough and ω small enough, there exists u such that

$$
C_0\omega-\frac{\alpha(Z+1-N)}{u}-e_p(\sigma_N)+\frac{(c')^2}{2u^2}+O\left(\frac{1}{\tilde{\lambda}}\right)<0\,.
$$

Then we put

$$
b=1+C_0\omega-\frac{\alpha(Z+1-N)}{u}+\frac{(c')^2}{2u^2}+\delta_{\tilde{\lambda}}\in(0,1)\,,
$$

and the estimate follows. Now, for d large enough ($d=m+2N+1$, for example), $\dim V$ is greater than k_0+1. According to our argument, we proved that every ε_k is bounded above by b.

Although the bound b on the eigenvalues ε_k obtained above is not uniform in ν, we still have, for every k, $\varepsilon_k\leq 1$. So, using Lemma 3.1, we find a bound for the E_ω-norm of $(\Psi^j_\omega)_k$ which is independent of ν: $\mathrm{Gram}_{L^2_{per}}\Psi^j_\omega<\mathbb{1}$ implies $||(\Psi^j_\omega)_k||_{L^2_{per}}\leq 1$, then $||\varepsilon_k(\Psi^j_\omega)_k||_{H^{-\frac{1}{2}}}\leq 1$ and this implies, by (3.1),

$$
||(\Psi^j_\omega)_k||_{E_\omega}=||\left(\overline{\Pi}^\omega_{\Psi^j_\omega}\right)^{-1}(\varepsilon_k(\Psi^j_\omega)_k||_{E_\omega}\leq\frac{1}{h_0}\,. \tag{5.16}
$$

This allows to estimate $U^j_{\nu,\omega}=3(\rho_{\Psi^j_\omega}*G_{\nu,\omega})$ in any L^q,for $q\geq 1$, independently of ν. In other terms, the constant $C_{\nu,q}$ in 5.5 may be chosen independent of ν. We get also that $C'_{\nu,q}$ in 5.6 may be chosen independent of ν. This implies that the estimate b is in fact independent of ν. On the other hand, using the equation, we get

$$
\sum_{k=1}^N\varepsilon^j_k\geq\mathcal{P}_\omega(\Psi^j_\omega)\geq\underline{c}_j\,,
$$

the real $\underline{c}_j$ being the constant of Lemma 2.11. So $\varepsilon_k^j \geq \underline{c}_j - N + 1 = a(j)$, with $a(j) \xrightarrow{<} 1$, since $\underline{c}_j \xrightarrow{<} N$, as j goes to infinity, and Lemma 2.12 is proved.

Acknowledgement The author wishes to thank E. Séré for his constant attention and his precious remarks all along this work.

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