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Solutions of the Dirac–Fock Equations for Atoms and Molecules

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Abstract: The Dirac–Fock equations are the relativistic analogue of the well-known Hartree–Fock equations. They are used in computational chemistry, and yield results on the inner-shell electrons of heavy atoms that are in very good agreement with experimental data. By a variational method, we prove the existence of infinitely many solutions of the Dirac–Fock equations "without projector", for Coulomb systems of electrons in atoms, ions or molecules, with $Z \le 124$, $N \le 41$, $N \le Z$. Here, Z is the sum of the nuclear charges in the molecule, N is the number of electrons.

1. Introduction

In relativistic quantum mechanics [5], 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. This wave satisfies the free Dirac equation:

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

Here, we have chosen a system of units such that $\hbar = c = 1$, the mass m_e of the electron has also been normalized to 1.

Before going further, let us fix some notations. In the whole paper, the conjugate of $z \in \mathbb{C}$ will be denoted by z^*. For $X = \begin{pmatrix} z_1 \\ \vdots \\ z_4 \end{pmatrix}$ a column vector in $\mathbb{C}^4$, we denote by X^* the row covector $(z_1^*, \dots, z_4^*)$. Similarly, if $A = (a_{ij})$ is a 4×4 complex matrix, we denote by A^* its adjoint, $(A^*)_{ij} = a_{ji}^*$.

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We denote by (X, X') the Hermitian product of two vectors X, X' in $\mathbb{C}^4$, and by $|X|$, the norm of X in $\mathbb{C}^4$, i. e. $|X|^2 = \sum_{i=1}^{4} X_i X_i^*$. The usual Hermitian product in $L^2(\mathbb{R}^3, \mathbb{C}^4)$ is denoted

$$(\varphi, \psi)_{L^2} = \int_{\mathbb{R}^3} \Big(\varphi(x), \psi(x)\Big) d^3x. \qquad (1.2)$$

In the Dirac equation, $\alpha_1, \alpha_2, \alpha_3$ and β are 4×4 complex matrices, whose standard form (in 2×2 blocks) is

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} , \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \qquad (k = 1, 2, 3),$$

with

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

One can easily check the following relations:

$$\begin{cases} \alpha_k = \alpha_k^*, \quad \beta = \beta^*, \\ \alpha_k \alpha_\ell + \alpha_\ell \alpha_k = 2\delta_{k\ell}, \quad \alpha_k \beta + \beta \alpha_k = 0. \end{cases} \qquad (1.3)$$

These algebraic conditions are here to ensure that H_0 is a symmetric operator, such that

$$H_0^2 = -\Delta + 1. \qquad (1.4)$$

Let us now consider an electron near a nucleus of atomic number Z. We assume that the nucleus is point-like and is situated at the origin of coordinates, and we take the system of units of Eq. (1.1). The Hamiltonian of the electron, in the coulombic field created by the nucleus, is then

$$H_Z = H_0 - \alpha Z V(x), \quad \text{with} \quad V(x) = \frac{1}{|x|}. \qquad (1.5)$$

Here, α is a positive dimensionless constant. Its physical value is $\alpha \approx \frac{1}{137}$.

Lemma 1.1 lists some properties of H_0 and $V(x)$, that will be useful in this paper.

Lemma 1.1. **(P1)** *H_0 is a self-adjoint operator on $L^2(\mathbb{R}^3, \mathbb{C}^4)$, with domain $\mathcal{D}(H_0) = H^1(\mathbb{R}^3, \mathbb{C}^4)$. 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*

$$\begin{cases} H_0 \Lambda^+ = \Lambda^+ H_0 = \sqrt{1-\Delta}\,\Lambda^+ = \Lambda^+ \sqrt{1-\Delta} \\ H_0 \Lambda^- = \Lambda^- H_0 = -\sqrt{1-\Delta}\,\Lambda^- = -\Lambda^- \sqrt{1-\Delta}. \end{cases} \qquad (1.6)$$

(P2) *The coulombic potential $V(x) = \frac{1}{|x|}$ satisfies the following Hardy-type inequalities:*

$$\Big(\varphi, (\mu * V)\,\varphi\Big)_{L^2} \leq \frac{1}{2}\Big(\frac{\pi}{2} + \frac{2}{\pi}\Big)\Big(\varphi, |H_0| \varphi\Big)_{L^2}, \qquad (1.7)$$

for all $\varphi \in \Lambda^+(H^{1/2}) \cup \Lambda^-(H^{1/2})$ and for all probability measures μ on $\mathbb{R}^3$. Moreover,

$$\Big(\varphi, (\mu * V)\,\varphi\Big)_{L^2} \leq \frac{\pi}{2}\Big(\varphi, |H_0| \varphi\Big)_{L^2}, \forall \varphi \in H^{1/2}, \qquad (1.8)$$

$$\| (\mu * V)\,\varphi \|_{L^2} \leq 2 \|\nabla \varphi\|_{L^2}, \quad \forall \varphi \in H^1. \qquad (1.9)$$

In the particular case where μ is equal to the Dirac mass at the origin δ_0, an inequality more precise than (1.7) was proved in [8, 47, 48]. This inequality reads as follows:

$$\left(\left(H_0 - \frac{\alpha Z}{|x|}\right)\varphi, \varphi\right) \geq ((1-\alpha Z)\varphi, \varphi) \ ,$$

for all $Z \leq Z_c := \frac{2}{(\frac{\pi}{2}+\frac{2}{\pi})\alpha}$, for all $\varphi \in \Lambda^+(H^{1/2}(\mathbb{R}^3, \mathbb{C}^4))$. The technique used in [8, 47, 48] is based on ideas introduced by Evans-Perry and Siedentop in [18]. We refer to [27, 30] for inequality (1.8) in the case $\mu = \delta_0$. Thaller's book [46] gathers many results on the Dirac operator, including (P1) and the standard Hardy inequality (1.9) for $\mu = \delta_0$, with references. The extension of (1.7), (1.8) and (1.9) from $\mu = \delta_0$ to a general probability measure μ is immediate, since the projectors $\Lambda^{\pm}$, the gradient ∇ and the free Dirac operator H_0 commute with translations. For completeness, we shall give the explicit form of the projectors Λ^+, Λ^- in Sect. 3.

For $\varphi \in L^2(\mathbb{R}^3, \mathbb{C}^4)$, let us denote $\varphi^+ = \Lambda^+\varphi, \quad \varphi^- = \Lambda^-\varphi$. Let

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

E is a Hilbert space with Hermitian product

$$\left(\varphi, \psi\right)_E = \left(\varphi, \sqrt{1-\Delta}\psi\right)_{L^2} = \left(\varphi^+, \psi^+\right)_E + \left(\varphi^-, \psi^-\right)_E. \tag{1.10}$$

Since H_0 is unbounded from below, it is difficult to define a ground state for relativistic atoms and molecules. In order to study the stability of relativistic molecules from a mathematical viewpoint, various simplified models have been introduced. In the simplest one, H_0 is replaced by the positive definite Hamiltonian $\sqrt{1-\Delta}$. See for instance [27, 14, 37, 34], and the Selecta of E.H. Lieb [33] for a more detailed list of references on this topic.

A more realistic model due to Brown and Ravenhall [6] uses projection operators: $\Lambda^+(H_0 + V)\Lambda^+$ replaces $H_0 + V$, i. e., the one-particle Hilbert space is $\Lambda^+ L^2$ instead of L^2. The above projected operator and its multi-particle counterpart was widely discussed by J. Sucher in [43, 44]. In [26], Hardekopf and Sucher investigated numerically the operator $B := \Lambda^+(H_0 - \alpha Z|x|^{-1})\Lambda^+$, and they claimed that its ground state energy vanishes when $Z = Z_c := \frac{2}{(\frac{\pi}{2}+\frac{2}{\pi})\alpha}$. The first mathematical study on the semiboundedness of B appeared in [18]. In [18], Evans, Perry and Siedentop proved that on the space of rapidly decaying smooth spinors, B is bounded from below by $\alpha Z(1/\pi - \pi/4)$ if the charge Z does not exceed Z_c and unbounded from below if Z is larger than Z_c. As already mentioned, several authors [8, 47, 48] improved this result later by showing that B is positive and bounded from below by $(1-\alpha Z)$ whenever $Z \leq Z_c$. For results concerning multi-particle versions of B, see for instance [35].

The Dirac–Fock (DF) functional was first introduced by Swirles [45] as an approximation for the energy of a system of N electrons in an atom of large nuclear charge Z. In such atoms, the inner-shell electrons have relativistic energies, and the standard Hartree–Fock (HF) approximation, based on the nonrelativistic Schrödinger equation, is no longer valid. The Euler–Lagrange equations of the DF energy functional can be solved numerically. The solutions represent stationary states of the electrons in the atom. The numerical results are in very good agreement with experimental data (see e.g. [32, 23, 15, 38, 31, 22]). In [43, 44, 41, 24, 10], the relationship between Dirac–Fock and quantum electrodynamics is studied.

In the Dirac–Fock model, the N electrons are represented by a Slater determinant of N functions $\varphi_k \in E$, subjected to the normalization constraints

$$\Big(\varphi_\ell, \varphi_k\Big)_{L^2} = \delta_{k\ell}. \tag{1.11}$$

We shall denote $\Phi = (\varphi_1, \cdots, \varphi_N)$, and the constraints above will be written in the shorter form $\mathrm{Gram}\,\Phi = 1\!\!1$, with

$$\Big[\mathrm{Gram}\,\Phi\Big]_{k\ell} := \Big(\varphi_\ell, \varphi_k\Big)_{L^2}. \tag{1.12}$$

We consider a molecule, with:

- 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 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 $Z = \sum_{i=1}^m Z_i$.
- N relativistic electrons.

We assume that the interaction between these particles is purely electrostatic. The DF energy of the N electrons in the molecule, is

$$\begin{aligned} \mathcal{E}(\Phi) = &\sum_{\ell=1}^N \Big(\varphi_\ell, H_0\varphi_\ell\Big)_{L^2} - \alpha Z \sum_{\ell=1}^N \Big(\varphi_\ell, (\mu * V)\,\varphi_\ell\Big)_{L^2} \\ &+ \frac{\alpha}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} V(x-y)\Big[\rho(x)\rho(y) - \mathrm{tr}\Big(R(x,y)R(y,x)\Big)\Big]\,d^3x\,d^3y. \end{aligned} \tag{1.13}$$

Here, ρ is a scalar and R is a 4×4 complex matrix, given by

$$\rho(x) = \sum_{\ell=1}^N \Big(\varphi_\ell(x), \varphi_\ell(x)\Big)\ , \quad R(x,y) = \sum_{\ell=1}^N \varphi_\ell(x) \otimes \varphi_\ell^*(y), \tag{1.14}$$

ρ is the electronic density, R is the exchange matrix which comes from the antisymmetry of the Slater determinant. Note that $R(y,x) = R(x,y)^*$, so that $\mathrm{tr}\Big(R(x,y)R(y,x)\Big) = \sum_{i,j} |R(x,y)_{ij}|^2$.

The main difference with the more standard HF functional, is that the kinetic energy term $(\varphi_k, -\Delta\varphi_k)_{L^2}$ in HF is replaced by $(\varphi_k, H_0\varphi_k)_{L^2}$ in DF. This changes completely the nature of the functional, which becomes strongly indefinite: it is not bounded below, and any of its critical points has an infinite Morse index.

The DF functional is invariant under the action of the group $\mathcal{U}(N)$:

$$u \cdot \Phi = \Big(\sum_\ell u_{1\ell}\varphi_\ell, \ldots, \sum_\ell u_{N\ell}\varphi_\ell\Big), u \in \mathcal{U}(N), \Phi \in E^N. \tag{1.15}$$

We denote

$$\Sigma = \Big\{\Phi \in E^N \,/\, \mathrm{Gram}\,\Phi = 1\!\!1\Big\}. \tag{1.16}$$

Using inequality (1.8), one can easily prove that the DF functional $\mathcal{E}$ is smooth on E^N. A critical point of $\mathcal{E}|_\Sigma$ is a weak solution of the following Euler–Lagrange equations:

$$\overline{H}_\Phi \varphi_k = \sum_{\ell=1}^{N} \lambda_{k\ell}\varphi_\ell, k = 1, \ldots, N. \tag{1.17}$$

Here,

$$\begin{aligned} \overline{H}_\Phi \psi = H_0\psi\ &-\alpha Z\,(\mu * V)\,\psi \\ &+\alpha(\rho * V)\psi - \alpha \int_{\mathbb{R}^3} R(x,y)\psi(y)V(x-y)\,dy. \end{aligned} \tag{1.18}$$

Since $\overline{H}_\Phi$ is self-adjoint from $H^{1/2}$ to its dual $H^{-1/2}$, $\Lambda = (\lambda_{k\ell})$ is a self-adjoint $(N \times N)$ complex matrix. It is the matrix of Lagrange multipliers associated to the constraints $(\varphi_\ell, \varphi_k)_{L^2} = \delta_{k\ell}$.

For $\Phi \in \Sigma$ a critical point whose matrix of multipliers is Λ, and $u \in \mathcal{U}(N)$, the matrix of multipliers of the critical point $\tilde{\Phi} = u \cdot \Phi$ is $\tilde{\Lambda} = u\Lambda u^*$. So any $U(N)$-orbit of critical points of $\mathcal{E}|_\Sigma$ contains a weak solution of the following system of nonlinear eigenvalue problems, called the Dirac–Fock equations:

$$\overline{H}_\Phi \varphi_k = \epsilon_k \varphi_k, \quad k = 1, \ldots, N. \tag{1.19}$$

Physically, $\overline{H}_\Phi$ represents the Hamiltonian of an electron in the mean field due to the nuclei and the electrons. The eigenvalues $\epsilon_1, \ldots, \epsilon_N$ are the energies of each electron in this mean field.

In the HF model, the Euler–Lagrange equations have a form similar to (1.19), with $-\Delta$ instead of H_0 in the expression of $\overline{H}_\Phi$. The physically interesting states correspond to $\epsilon_1 \le \cdots \le \epsilon_N < 0$, and the ground state minimizes $\mathcal{E}_{HF}$ on Σ, which implies that $\epsilon_1, \ldots, \epsilon_N$ are the N first eigenvalues of $\overline{H}_\Phi$ (see [36]). In the DF model, the physically interesting states correspond to $0 < \epsilon_k < 1$: a positive energy inferior to the rest mass of the electron. The definition of a ground state is less clear: the DF functional has no minimum on Σ. This fact is at the origin of serious difficulties in the numerical implementation, as well as the interpretation, of the DF equations (see [10] and references therein). One way to deal with this problem, is to restrict the energy functional to the space $(\Lambda^+ E)^N$, Λ^+ being, as defined above, the projector on the space of positive states of the free Dirac operator [43, 44]: this corresponds to a Hartree–Fock reduction of the already mentioned Brown-Ravenhall model. The associated Euler–Lagrange equations are the "projected" Dirac–Fock equations

$$\Lambda^+ \, \overline{H}_\Phi \, \Lambda^+ \varphi_k = \epsilon_k \varphi_k. \tag{1.20}$$

Note that, in the case $\epsilon_k > 0$, (1.19) can be written formally as

$$\Lambda^+_\Phi \, \overline{H}_\Phi \, \Lambda^+_\Phi \, \varphi_k = \epsilon_k \varphi_k. \tag{1.21}$$

Here, Λ^+_Φ is the projector on the positive space associated to $\overline{H}_\Phi$. Numerical computations using (1.19) rather than (1.20), give results that are in very good agreement with experimental data (see e.g. [23, 38]). This is not very surprising: in the presence of strong electric fields, the projector Λ^+_Φ seems physically more adequate than the free-energy projector Λ^+ (see [28]). In [41] Mittleman derived the DF equations with "self-consistent projector" (1.21), from a variational procedure applied to a QED Hamiltonian in Fock space, followed by the standard Hartree–Fock approximation.

Important existence results are known on the HF equations. Lieb and Simon [36] proved the existence of a ground state of $\mathcal{E}_{HF}$ on Σ, provided $N < Z + 1$, where Z is the total nuclear charge, P.-L. Lions [39] proved the existence of infinitely many excited states if $N \leq Z$. Using inequality (1.7), one can easily extend the results of [36, 39] to the projected equations (1.20), assuming that

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

The only difference is that $\frac{1}{|x|}$ is not a compact perturbation of H_0, but this does not create any important difficulty.

In the present paper, we give the first existence result for solutions of the DF equations "without projector" (1.19). Our assumptions are

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

Since we find positive eigenvalues ϵ_k, the equations we solve are formally equivalent to the DF equations with "self-consistent projector" (1.21).

The condition $\alpha(3N - 1) < \frac{2}{\pi/2+2/\pi}$ is rather restrictive, and we do not have a clear definition of the "ground state". But we hope that this first study will stimulate further mathematical research on Dirac–Fock. Our main theorem is the following:

Theorem 1.2. *Assume that* $\alpha \max(Z, 3N - 1) < \frac{2}{\pi/2+2/\pi}, N < Z + 1$, *with* $Z > 0$ *the total nuclear charge. The nuclear charge density is* $Z\mu$, *where* μ *is a fixed probability measure on* $\mathbb{R}^3$. *Then, there is an infinite sequence* $(\Phi^j)_{j\geq 0}$ *of critical points of the DF functional* $\mathcal{E}$ *on*

$$\Sigma = \left\{ \Phi \in E^N \,/\, \mathrm{Gram}\,\Phi = \mathbb{1} \right\}.$$

The functions $\varphi_1^j, \cdots, \varphi_N^j$ *satisfy the normalization constraints (1.11) and they are strong solutions, in* $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \cap \bigcap_{1\leq q<3/2} W^{1,q}(\mathbb{R}^3, \mathbb{C}^4)$, *of the Dirac–Fock equations*

$$\overline{H}_{\Phi^j} \varphi_k^j = \epsilon_k^j \varphi_k^j, \quad 1 \leq k \leq N, \tag{1.22}$$

$$0 < \epsilon_1^j \leq \cdots \leq \epsilon_N^j < 1. \tag{1.23}$$

Moreover,

$$0 < \mathcal{E}(\Phi^j) < N, \tag{1.24}$$

$$\lim_{j\to\infty} \mathcal{E}(\Phi^j) = N. \tag{1.25}$$

Remark 1. With the physical value $\alpha \approx \frac{1}{137}$ and Z an integer, our conditions become

$$Z \leq 124, \quad N \leq 41, \quad N \leq Z.$$

Remark 2. Since μ is arbitrary, our assumptions contain the case of point-like nuclei as well as more realistic nuclear potentials, of the form $-\alpha \sum_i \rho_i(x) * \dfrac{1}{|x|}$, where $\rho_i \in L^\infty \cap L^1,\ \rho_i \geq 0,\ \sum_i \int_{\mathbb{R}^3} \rho_i = Z$.

Remark 3. The first solution Φ^0 is a good candidate for a ground state. Indeed, in the nonrelativistic limit ($\alpha \to 0$), it converges, after rescaling, to a ground state of Hartree–Fock. This will be proved in a forthcoming paper.

Remark 4. In the case $N = 1$, the Dirac–Fock equations are linear and correspond to an eigenvalue problem for Dirac operators with scalar potentials. For variational results in this case, see [17, 25, 16].

Remark 5. The functions $\varphi_1^j, \cdots, \varphi_N^j$ of Theorem 1.2 are smooth outside $\operatorname{supp} \mu$. Moreover, if $\operatorname{supp} \mu$ is compact, they decay exponentially fast, as well as their derivatives, when $|x|$ goes to infinity.

Our main theorem is the analogue, for the DF model, of P.-L. Lions' result for HF [39]. In order to control the Lagrange multipliers ϵ_k (they should be negative in his case), Lions uses an estimate on the Morse index of the critical points. Such an estimate can be obtained for a critical point associated to a "finite-dimensional" min-max, if the functional satisfies the Palais–Smale compactness condition (see e.g. [2, 3, 4, 11, 49]). However, the HF functional does not satisfy the Palais–Smale compactness condition: since the essential spectrum of $-\Delta$ is $[0, \infty)$, only Palais–Smale sequences with negative Lagrange multipliers ϵ_k are precompact. Lions works on approximate functionals that satisfy Palais–Smale, finds critical points of these functionals with Morse index estimates, and passes to the limit. In [19, 21], Fang and Ghoussoub give general existence results on Palais–Smale sequences with Morse-type information, for functionals that do not satisfy Palais–Smale. As an application, they rewrite Lions' proof, working directly with the HF functional.

For DF, we also need a control on $\epsilon_k : 0 < \epsilon_k < 1$. Moreover, the essential spectrum of H_0 is $\mathbb{R} \setminus (-1, 1)$, so that the only precompact Palais–Smale sequences for DF, are such that $|\epsilon_k| < 1$. So a natural approach is to adapt the above ideas to DF. To realize this program, we faced several difficulties.

The first (and smallest) difficulty is that $\mu * \frac{1}{|x|}$ is not a compact perturbation of H_0. This creates some technical problems. They are easily solved, replacing $V = \frac{1}{|x|}$ by a regularized potential V_ν. At the end of the proof, we can pass to the limit $\nu \to 0$, thanks to inequality (1.7).

The second difficulty is that the Morse index estimates can only give upper bounds on the multipliers in [39]. But in the DF case, we want to ensure that $\epsilon_k > 0$. To overcome this problem, we replace the constraint Gram $(\Phi) = \mathbb{1}$ by a penalization term $\pi_p(\Phi)$, subtracted from the energy functional. The new Euler equations are $\overline{H}_\Phi \varphi_k = \partial_{\varphi_k} \pi_p$ (no more Lagrange multipliers). The eigenvalue ϵ_k is now an explicit function of φ_k, which appears in the expression of the derivative $\partial_{\varphi_k} \pi_p$. This function has only positive values, so we automatically get $\epsilon_k > 0$.

The third difficulty with DF, is that all critical points have an infinite Morse index. This kind of problem is often encountered in the theory of Hamiltonian systems and in certain elliptic PDEs. One way of dealing with it is to use a concavity property of the functional to get rid of the "negative directions": see e.g. [1, 7, 9]. We shall use this method. We get a reduced functional $I_{\nu,p}$. A min-max argument gives us Palais–Smale sequences $\Phi_{n,\nu,p}$ for $I_{\nu,p}$ with finite "Morse index", thanks to [19]. Adapting the arguments of [39], we prove that the ϵ_k's of such sequences are smaller than 1. Then we pass to the limit $(\nu, n, p) \to (0, \infty, \infty)$, and get the desired solutions of DF, with $0 < \epsilon_k < 1$.

Our concavity argument works only if $\alpha(3N-1) < \frac{2}{\pi/2+2/\pi}$. In the last 20 years, very powerful methods have been developed to deal with strongly indefinite functionals, that do not present any concavity property [42, 13, 20, 29]. This suggests that it might be possible to weaken the assumptions on N in Theorem 1.2.

2. Sketch of the Proof of Theorem 1.2

As announced in the Introduction, we replace $V(x) = \frac{1}{|x|}$, in the expression of $\mathcal{E}$ (1.13), by the regularized potential

$$V_\nu(x) = \frac{1}{(2\pi\nu)^{3/2}} e^{-|x|^2/2\nu} * V(x), \quad \nu > 0. \tag{2.1}$$

This replacement is made for the attractive potential of the nucleus, as well as for the electronic repulsion and exchange terms. The regularized DF functional is denoted $\mathcal{E}_\nu$, and the associated one-particle Hamiltonian (1.18) is denoted $\overline{H}^\nu_\Phi$.

The Gaussian $\frac{1}{(2\pi\nu)^{3/2}} e^{-|x|^2/2\nu}$ is normalized in L^1, so that V_ν satisfies the same inequalities (1.7–8–9) as V.

We also replace the constraint "$\Phi \in \Sigma$" by a penalization term π_p. The penalization parameter p is a positive integer. The penalized functional

$$\mathcal{F}_{\nu,p} = \mathcal{E}_\nu - \pi_p \tag{2.2}$$

is defined in the domain

$$A = \Big\{\Phi \in E^N \,/\, 0 < \mathrm{Gram}\,\Phi < 1\!\!1\Big\}, \tag{2.3}$$

where $\mathrm{Gram}\,\Phi$ is the $N \times N$ matrix $\big((\varphi_i, \varphi_j)_{L^2}\big)_{1\le i,j\le N}$. The penalization term has the form

$$\pi_p(\Phi) = \mathrm{tr}\Big[\Big(\mathrm{Gram}\,\Phi\Big)^p \Big(1\!\!1 - \mathrm{Gram}\,\Phi\Big)^{-1}\Big]. \tag{2.4}$$

Note that $\mathcal{F}_{\nu,p}$ is invariant under the $\mathcal{U}(N)$ action (1.15). It is easy to see that $\mathcal{F}_{\nu,p}$ is well-defined and smooth on A. We are going to construct approximate critical points of $\mathcal{F}_{\nu,p}$. As $\nu \to 0$ and $p \to \infty$, these points will converge to critical points of $\mathcal{E}|_\Sigma$.

Any $\mathcal{U}(N)$ orbit in A contains a point Φ such that Gram Φ is diagonal, with eigenvalues in nondecreasing order:

$$\mathrm{Gram}\,\Phi = \mathrm{Diag}(\sigma_1, \ldots, \sigma_N), 0 < \sigma_1 \le \cdots \le \sigma_N < 1. \tag{2.5}$$

We call $\mathcal{O}$ the set of points $\Phi \in A$, satisfying (2.5). If $\Phi \in \mathcal{O}$, then

$$\frac{\partial \mathcal{F}_{\nu,p}}{\partial \varphi_k}(\Phi) = \overline{H}^\nu_\Phi \varphi_k - \epsilon_k \varphi_k, \tag{2.6}$$

with

$$\epsilon_k = e_p(\sigma_k), \quad e_p(x) = \frac{d}{dx}\Big(\frac{x^p}{1-x}\Big) = \frac{px^{p-1} - (p-1)x^p}{(1-x)^2}. \tag{2.7}$$

The function e_p is positive and increasing on $(0, 1)$, so that $0 < \epsilon_1 \leq \cdots \leq \epsilon_N$. This is one of the advantages of the penalized functional $\mathcal{F}_{\nu,p}$: its critical points in $\mathcal{O}$ are solutions of a nonlinear eigenvalue problem, with positive eigenvalues.

In the proof of Theorem 1.2, we need to control not only the critical points of $\mathcal{F}_{\nu,p}$, but also its Palais–Smale sequences. Of course, we just need to study Palais–Smale sequences in $\mathcal{O}$, thanks to the $\mathcal{U}(N)$ invariance. Unfortunately, the Palais–Smale condition does not hold for $\mathcal{F}_{\nu,p}$, exactly as in the case of the HF functional. But it can be replaced by the following lemma, which is related to the spectral properties of the Dirac operator with a potential. Its proof is based on inequality (1.7).

Lemma 2.1 (Convergence of approximate solutions). *Assume that* $\alpha \max(Z, N) < \frac{2}{\pi/2+2/\pi}$.

(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*

$$\mathrm{Gram}\,\Phi_n = \mathrm{Diag}(\sigma_{1,n}, \ldots, \sigma_{N,n}), 0 < \sigma_{1,n} \leq \cdots \leq \sigma_{N,n} < 1.$$

We denote $\epsilon_{k,n} = e_{p_n}(\sigma_{k,n})$, *with* $e_{p_n}(x) = \frac{d}{dx}\left(\frac{x^{p_n}}{1-x}\right)$. *We assume that*

$$\mathcal{F}'_{\nu_n,p_n}(\Phi_n) \underset{n\to\infty}{\longrightarrow} 0 \tag{2.8}$$

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*

$$\liminf_{n\to\infty} \sigma_{1,n} > 0. \tag{2.9}$$

Then,

$$\liminf_{n\to\infty} \epsilon_{1,N} \geq h_0, \tag{2.10}$$

where $h_0 \in (0, 1)$ *is a constant which depends only on* $\alpha Z, \alpha N$.

(b) If, moreover,

$$\limsup_{n\to\infty} \epsilon_{N,n} < 1, \tag{2.11}$$

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

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

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

$$\overline{H}_\Phi \varphi_k = \epsilon_k \varphi_k, \quad \epsilon_k = \lim_{n\to\infty} \epsilon_{k,n} \in [h_0, 1), \tag{2.12}$$

and the DF energy of Φ *is*

$$\mathcal{E}(\Phi) = \lim_{n\to\infty} \mathcal{F}_{\nu_n,p_n}(\Phi_n). \tag{2.13}$$

Lemma 2.1 will be proved in Sect. 3. Our problem now is to find sequences Φ_n satisfying the assumptions of this lemma. Assumption (2.11) is the most difficult to check.

In the HF case, a similar question was solved by P.-L.Lions [39]: if Φ^* is a critical point of $\mathcal{E}_{HF}$ on Σ, the associated multipliers $\epsilon_1 \leq \cdots \leq \epsilon_N$ are eigenvalues of $\overline{H}^{HF}_{\Phi^*}$. Let us denote $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \leq \cdots < 0$ the sequence of negative eigenvalues of $\overline{H}^{HF}_{\Phi^*} = -\Delta - \frac{Z}{|x|} + \ldots$ (assuming $N < Z$). If $\epsilon_k < 0$, there is an integer $n(k)$ such that $\epsilon_k = \lambda_{n(k)}$. Moreover, we may impose $n(k+1) > n(k)$. If $\epsilon_k \geq 0$, we take $n(k) = +\infty$. Lions proved the following inequality:

$$m(\Phi^*) \geq \max_{1 \leq k \leq N} \Big[n(k) - k \Big], \tag{2.14}$$

where $m(\Phi^*)$ is the Morse index of Φ^*.

As a consequence, if Φ^* is a minimizer of $\mathcal{E}_{HF}$ on Σ, then $n(k) = k$ $(\forall k)$. This particular case of (2.14) was proved earlier by Lieb and Simon [36].

In the DF case, we would also like to control the ϵ_k's, using the Morse index for $\mathcal{F}_{\nu,p}$. Unfortunately, the functional $\mathcal{F}_{\nu,p}$ is strongly indefinite, as mentioned in the introduction. We overcome this difficulty thanks to a concavity argument, as in [1, 7, 9].

Lemma 2.2 (Concavity in the E^- directions). *Assume that $\alpha(3N-1) < \frac{2}{\pi/2+2/\pi}$. Then there is a constant $s > 0$, independent of ν, p, such that, for any $\Phi \in A$ and $\Psi^- \in (E^-)^N$,*

$$\mathcal{F}''_{\nu,p}(\Phi) \cdot \left[\Psi^-, \Psi^-\right] \leq -s \sum_{k=1}^{N} ||\psi_k^-||^2_E. \tag{2.15}$$

Lemma 2.2 will be proved in Sect. 4, where an explicit formula for $\mathcal{F}''_{\nu,p}$ will be given. Now, let

$$A^+ = A \cap (E^+)^N = \Big\{ \Phi^+ \in (E^+)^N \,/\, 0 < \mathrm{Gram}(\Phi^+) < \mathbb{1} \Big\}. \tag{2.16}$$

For $\Phi^+ \in A^+$, let

$$\Gamma(\Phi^+) = \Big\{ \chi^- \in (E^-)^N \,/\, \mathrm{Gram}(\Phi^+) + \mathrm{Gram}(\chi^-) < \mathbb{1} \Big\}$$
$$= \Big\{ \chi^- \in (E^-)^N \,/\, \Phi^+ + \chi^- \in A \Big\}. \tag{2.17}$$

One can easily see that $\Gamma(\Phi^+)$ is an open convex subset of $(E^-)^N$, and that $\mathcal{F}_{\nu,p}(\Phi^+ + \chi^-)$ converges to $-\infty$ as χ^- approaches the boundary of $\Gamma(\Phi^+)$, for Φ^+ fixed.

So, Lemma 2.2 has the following consequence:

Corollary 2.3. *Assume that $\alpha(3N-1) < \frac{2}{\pi/2+2/\pi}$. Then, for any $\Phi^+ \in A^+$, the functional*

$$\chi^- \in \Gamma(\Phi^+) \mapsto \mathcal{F}_{\nu,p}(\Phi^+ + \chi^-)$$

has a unique maximizer $h_{\nu,p}(\Phi^+) \in \Gamma(\Phi^+)$. The mapping $h_{\nu,p} : A^+ \to (E^-)^N$ is smooth for the $(H^{1/2})^N$ norm, and equivariant under the $\mathcal{U}(N)$ action (1.15).

We denote

$$I_{\nu,p}(\Phi^+) = \mathcal{F}_{\nu,p}\Big(\Phi^+ + h_{\nu,p}(\Phi^+)\Big), \quad \Phi^+ \in A^+. \tag{2.18}$$

$I_{\nu,p}$ is well-defined and smooth on A^+. Since $h_{\nu,p}$ is $\mathcal{U}(N)$ equivariant, $I_{\nu,p}$ is invariant, and any $\mathcal{U}(N)$ orbit in A^+ contains a point Φ^+ such that $\Phi = \Phi^+ + h_{\nu,p}(\Phi^+)$ satisfies (2.5). By definition of $h_{\nu,p}$, for all $\Psi^- \in (E^-)^N$, $\mathcal{F}'_{\nu,p}(\Phi^+ + h_{\nu,p}(\Phi^+)) \cdot \Psi^- = 0$. As a consequence, if Φ^+ is a critical point of $I_{\nu,p}$, then, $\Phi = \Phi^+ + h_{\nu,p}(\Phi^+)$ is a critical point of $\mathcal{F}_{\nu,p}$. So we just have to look for critical points of $I_{\nu,p}$. This is much more comfortable, because this reduced functional is not strongly indefinite. We now give a relationship between Morse-type information on a Palais–Smale sequence Φ_n^+ for $I_{\nu,p}$, and the estimate (2.11) on the ϵ_k's. Unfortunately, we do not have a precise inequality like (2.14).

Lemma 2.4 (The Morse index controls the ϵ_k's). *Assume that* $\alpha(3N-1) < \frac{2}{\pi/2+2/\pi}$, $N < Z+1$. *Let* $\nu \in (0,1)$, $p \geq 2$, $M > 0$, *and* (Φ_n^+) *a sequence in* A^+. *Denoting*

$$\Phi_n = \Phi_n^+ + h_{\nu,p}(\Phi_n^+),$$

we assume that $\Phi_n \in \mathcal{O}$, *i.e.*

$$\mathrm{Gram}\,\Phi_n = \mathrm{Diag}(\sigma_{1,n},\dots,\sigma_{N,n}), \quad \textit{with} \quad 0 < \sigma_{1,n} \leq \cdots \leq \sigma_{N,n} < 1.$$

Suppose that

$$I_{\nu,p}(\Phi_n^+) \leq M, \quad I'_{\nu,p}(\Phi_n^+) \to 0, \quad \liminf \sigma_{1,n} > 0, \tag{2.19}$$

and that the quadratic form on $(E^+)^N$:

$$Q_n(\Psi^+) = I''_{\nu,p}(\Phi_n^+)\Big[\Psi^+,\Psi^+\Big] + \delta_n \sum_{k=1}^{n} ||\psi_k^+||_E^2 \tag{2.20}$$

has a negative space of dimension at most m, *for a sequence* $\delta_n \to 0$. *Then, there is a constant* $b_m \in (0,1)$, *independent of* $\nu, p, M, \Phi_n^+, \delta_n$, *such that*

$$\limsup_{n\to\infty} \epsilon_{N,n} \leq b_m, \quad with \quad \epsilon_{N,n} = e_p(\sigma_{N,n}). \tag{2.21}$$

The last step in the proof of Theorem 1.2 is to find Palais–Smale sequences for $I_{\nu,p}$, with Morse-type information. For this purpose, we look for positive min-max levels of $I_{\nu,p}$ in A^+. Note that A^+ is an open subset of E^N, whose boundary is $\partial A^+ = G^1 \cup G^2$, with

$$\begin{cases} G^1 = \Big\{\Phi^+ \in (E^+)^N \,/\, \mathrm{Gram}\,\Phi^+ \leq \mathbb{1}, \det \mathrm{Gram}\,\Phi^+ = 0\Big\} \\ G^2 = \Big\{\Phi^+ \in (E^+)^N \,/\, \mathrm{Gram}\,\Phi^+ \leq \mathbb{1}, \det(\mathbb{1} - \mathrm{Gram}\,\Phi^+) = 0\Big\} \end{cases}.$$

If $I_{\nu,p}$ were negative for Φ^+ close to ∂A^+, the existence of positive min-max levels for $I_{\nu,p}$ would be a direct consequence of the topology of $(A^+, \partial A^+)$. We have

$$I_{\nu,p}(\Phi^+) \longrightarrow -\infty \quad \text{as} \quad \mathrm{dist}_{L^2}(\Phi^+, G^2) \longrightarrow 0,$$

with $||\Phi^+||_{E^N}$ bounded. But $I_{\nu,p}(\Phi^+)$ may remain positive when Φ^+ is close to G^1. Following [12, 13, 40], we solve this difficulty by studying the gradient vector field of $I_{\nu,p}$ near G^1. We prove that this field "points inward", in the following sense:

Lemma 2.5 (A pseudo-gradient pointing inward near G^1). *Assume that*

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

Take $\nu > 0$. *Then there are* $d(\nu), e(\nu) > 0$ *such that,*

$$\text{if}\, \Phi^+ \in A^+ \quad \text{satisfies} \quad \det\,(\mathrm{Gram}\,\Phi^+) \in [d(\nu), 2d(\nu)]$$

then one can find a vector $X \in (E^+)^N$, *with*

$$\begin{cases} I'_{\nu,p}(\Phi^+)\cdot X \geq e(\nu)\|X\|_{(E)^N} \quad (\forall p \geq 2), \\ \Delta'(\Phi^+)\cdot X \quad > 0, \quad \textit{where} \quad \Delta(\Phi^+) = \det(\mathrm{Gram}\,\Phi^+). \end{cases} \tag{2.22}$$

Note that in Lemma 2.5 there is a constant, $d(\nu)$, which depends on ν. We have been unable to make d independent of ν.

Now, let $\alpha_\nu \in C^\infty\Big((d(\nu),1),\mathbb{R}\Big)$ be such that

$$\begin{cases} \alpha_\nu(x) = 0, & \forall x \geq 2d(\nu) \\ \alpha'_\nu(x) > 0, & \forall x < 2d(\nu) \\ \alpha_\nu(x) \to -\infty & \text{as } x \to d(\nu). \end{cases} \tag{2.23}$$

Let $\beta \in C^\infty(\mathbb{R},\mathbb{R})$ be such that

$$\begin{cases} \beta \equiv -1 & \text{on } (-\infty,-1) \\ \beta(t) = t, & \forall t \geq 0 \\ \beta(t) \leq 0, & \forall t \leq 0. \end{cases} \tag{2.24}$$

We define a new functional $J_{\nu,p}$, by

$$\begin{cases} J_{\nu,p}(\Phi^+) = \beta\Big(I_{\nu,p}(\Phi^+) + \alpha_\nu \circ \Delta(\Phi^+)\Big) & \text{if } \Phi^+ \in A^+ \text{ and } \Delta(\Phi^+) > d(\nu), \\ J_{\nu,p}(\Phi^+) = -1 & \text{otherwise} \end{cases} \tag{2.25}$$

It is easy to see that $J_{\nu,p}$ is smooth on $(E^+)^N$. If Φ^+ is a critical point of $J_{\nu,p}$ with $J_{\nu,p}(\Phi^+) \geq 0$, then Φ^+ is also a critical point of $I_{\nu,p} + \alpha_\nu \circ \Delta$, at the same level. From (2.22)–(2.23), this is only possible if $\Delta(\Phi^+) > 2d(\nu)$, hence Φ^+ is a critical point of $I_{\nu,p}$ and $I_{\nu,p}$ coincides with $J_{\nu,p}$ in a neighborhood of Φ^+. The same holds for Palais–Smale sequences.

So we can look for positive min-max levels of $J_{\nu,p}$ instead of $I_{\nu,p}$. This is much more convenient, because $J_{\nu,p}$ is defined on $(E^+)^N$, with $J_{\nu,p} = -1$ on ∂A^+. $J_{\nu,p}$ is invariant under the $\mathcal{U}(N)$ action (1.15).

For F a finite dimensional complex subspace of E^+, let

$$D(F) = \Big\{\Phi^+ \in F^N \,/\, \mathrm{Gram}\,\Phi^+ \leq 1\!\!1\Big\}. \tag{2.26}$$

We say that a homotopy $h \in C\Big([0,1]\times(E^+)^N, (E^+)^N\Big)$ is "admissible " if

$$\begin{cases} h(\lambda, u\cdot\Phi^+) = u\cdot h(\lambda,\Phi^+), & \begin{cases} \forall u \in \mathcal{U}(N) \\ \forall(\lambda,\Phi^+) \in [0,1]\times(E^+)^N \end{cases} \\ h(\lambda,\Phi^+) = \Phi^+, \forall\lambda \in [0,1], & \forall \Phi^+ \in \partial A^+. \end{cases} \tag{2.27}$$

We define the class of sets

$$\mathcal{Q}(F) = \Big\{ Q \subset (E^+)^N \,/\, \text{there is } h, \text{ admissible, such that} \quad h(0,\cdot) = \mathrm{Id}_{(E^+)^N},\, h(1, D(F)) = Q \Big\}. \tag{2.28}$$

Finally, let

$$c_{\nu,p}(F) = \inf_{Q\in\mathcal{Q}(F)} \max_{\Phi^+\in Q} J_{\nu,p}(\Phi^+). \tag{2.29}$$

We have

Lemma 2.6 (The min–max levels). *Assume that*

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

For any integer $j \geq 0$, there is a complex vector space $F_j \subset E^+$ with $\dim_{\mathbb{C}} F_j = N + j$, and three constants

$$\begin{aligned} 0 < \underline{a}(j) < \overline{a}(j) < N, \quad p(j) \geq 1, \quad \textit{such that} \\ \underline{a}(j) \to N \quad \textit{as } j \to \infty, \quad \textit{and} \\ \underline{a}(j) \leq c_{\nu,p}(F_j) \leq \overline{a}(j), \quad (\forall \nu \in (0,1)) \quad (\forall p \geq p(j)). \end{aligned} \tag{2.30}$$

Note that the action of $\mathcal{U}(N)$ is free on the set $\Big\{\Phi^+ \in (E^+)^N \,/\, J_{\nu,p}(\Phi^+) > 0\Big\}$. Moreover, $D(F_j)\,/\,\mathcal{U}(N)$ has dimension $m_j = 2Nj + N^2$. It then follows from arguments by Fang and Ghoussoub [19, 21], that there is a Palais–Smale sequence at the level $c_{\nu,p}(F_j)$, with Morse-type information:

Lemma 2.7 (Palais–Smale sequences with bounded Morse index). *Assume that*

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

Take F_j as in Lemma 2.6, and $\nu \in (0,1), p \geq p(j)$. Then there is a sequence $\Phi_n^+ \in A^+$, with

$$I'_{\nu,p}(\Phi_n^+) \to 0,\, I_{\nu,p}(\Phi_n^+) \to c_{\nu,p}(F_j),\, \Delta(\Phi_n^+) > d(\nu), \tag{2.31}$$

and a sequence $\delta_n > 0, \delta_n \to 0$, such that the quadratic form

$$Q_n(\Psi^+) = I''_{\nu,p}(\Phi_n^+)\Big[\Psi^+, \Psi^+\Big] + \delta_n \sum_{k=1}^N ||\psi_k^+||_E^2, \Big(\Psi^+ \in (E^+)^N\Big) \tag{2.32}$$

has a negative space of dimension at most $m_j = 2Nj + N^2$.

Proof of Theorem 1.2. We now prove Theorem 1.2 as a direct consequence of Lemmas 2.1, 2.4, 2.6 and 2.7. Let $j \geq 0$, $p \geq \max(3, p(j))$ be two integers. Take $\nu = \frac{1}{p} \in (0,1)$. There is a sequence Φ_n^+ satisfying (2.31–32) of Lemma 2.7 and such that $\Phi_n = \Phi_n^+ + h_{1/p,p}(\Phi_n^+)$ satisfies (2.5). Then (2.21) of Lemma 2.4 holds, with $m = m_j$. So, from (b.1) of Lemma 2.1, Φ_n converges, after extraction of a subsequence, to a critical point $\Phi^{j,p}$ of $\mathcal{F}_{1/p,p}$, with

$$\mathcal{F}_{1/p,p}(\Phi^{j,p}) = c_{1/p,p}(F_j)\ , \quad \mathrm{Gram}\,\Phi^{j,p} = \mathrm{Diag}(\sigma_1^p, \cdots, \sigma_N^p),$$
$$0 < \sigma_1^p \leq \cdots \leq \sigma_N^p < 1, \quad h_0 \leq e_p(\sigma_k^p) \leq b_{m_j} < 1.$$

Since e_p converges uniformly to 0 on any interval $[0,s]$, $s < 1$, we have $\lim_{p\to\infty} \sigma_1^p = 1$. Applying (b.2) of Lemma 2.1 to the sequence $\Phi^{j,p}$, for j fixed, we find, after extraction of a subsequence, a limit Φ^j which satisfies the requirements (1.22–25) of Theorem 1.2. $\square$

In Sect. 3, we study the properties of the first derivative of $\mathcal{F}_{\nu,p}$, and we prove Lemma 2.1.

In Sect. 4, we compute the Hessian of $\mathcal{F}_{\nu,p}$, and we prove Lemmas 2.2 and 2.4.

In Sect. 5, we study the min-max argument, and prove Lemmas 2.5 and 2.6.

3. The First Derivative of $\mathcal{F}_{\nu,p}$

Our first task is to prove property (P1) of Lemma 1.1. For this purpose, we write H_0 in Fourier space:

$$\widehat{H_0\psi}(\xi) = \Big(\sum_{k=1}^{3}\alpha_k\xi_k + \beta\Big)\widehat{\psi}(\xi) = \begin{pmatrix} 1 & \xi\cdot\sigma \\ \xi\cdot\sigma & -1 \end{pmatrix}\widehat{\psi}(\xi) \tag{3.1}$$

We denote by $\widehat{H}_0(\xi)$ the matrix $\begin{pmatrix} 1 & \xi.\sigma \\ \xi.\sigma & -1 \end{pmatrix}$, with the standard notation $\xi\cdot\sigma = \sum_{k=1}^{3}\xi_k\sigma_k$. $\widehat{H}_0(\xi)$ is a self-adjoint 4×4 matrix, and we have: $\widehat{H}_0(\xi)^2 = (1+|\xi|^2)\mathbb{1}_{\mathbb{C}^4}$. Taking

$$\begin{cases} \widehat{\Lambda^+}(\xi) = \dfrac{\widehat{H}_0(\xi) + \sqrt{1+|\xi|^2}\,\mathbb{1}}{2\sqrt{1+|\xi|^2}} = \\[2ex] \quad = \dfrac{1}{2}\left(\begin{array}{c|c} \frac{1}{\sqrt{1+|\xi|^2}} + 1 & \frac{\xi.\sigma}{\sqrt{1+|\xi|^2}} \\ \hline \frac{\xi.\sigma}{\sqrt{1+|\xi|^2}} & -\frac{1}{\sqrt{1+|\xi|^2}} + 1 \end{array}\right) \end{cases} \tag{3.2}$$

and

$$\begin{cases} \widehat{\Lambda^-}(\xi) = \dfrac{-\widehat{H}_0(\xi) + \sqrt{1+|\xi|^2}\,\mathbb{1}}{2\sqrt{1+|\xi|^2}} = \\[2ex] \quad = \dfrac{1}{2}\left(\begin{array}{c|c} -\frac{1}{\sqrt{1+|\xi|^2}} + 1 & -\frac{\xi.\sigma}{\sqrt{1+|\xi|^2}} \\ \hline -\frac{\xi.\sigma}{\sqrt{1+|\xi|^2}} & \frac{1}{\sqrt{1+|\xi|^2}} + 1 \end{array}\right), \end{cases} \tag{3.3}$$

we find that $\widehat{\Lambda^+}(\xi), \widehat{\Lambda^-}(\xi)$ are two orthogonal projectors of rank 2, with

$$\begin{cases} \widehat{\Lambda^+}\widehat{H_0}(\xi) & = \widehat{H_0}\widehat{\Lambda^+}(\xi) = \sqrt{1+|\xi|^2}\,\widehat{\Lambda^+}(\xi) \\ \widehat{\Lambda^-}\widehat{H_0}(\xi) & = \widehat{H_0}\widehat{\Lambda^-}(\xi) = -\sqrt{1+|\xi|^2}\,\widehat{\Lambda^-}(\xi) \\ \widehat{\Lambda^+}\widehat{\Lambda^-}(\xi) & = \widehat{\Lambda^-}\widehat{\Lambda^+}(\xi) = 0 \\ \widehat{\Lambda^+}(\xi) + \widehat{\Lambda^-}(\xi) = \mathbb{1}_{\mathbb{C}^4} \end{cases} . \tag{3.4}$$

Finally, if we define Λ^+, Λ^- on $L^2(\mathbb{R}^3, \mathbb{C}^4)$ by

$$\begin{cases} \widehat{\Lambda^+\psi}(\xi) = \widehat{\Lambda^+}(\xi)\widehat{\psi}(\xi) \\ \widehat{\Lambda^-\psi}(\xi) = \widehat{\Lambda^-}(\xi)\widehat{\psi}(\xi) \end{cases} \tag{3.5}$$

we easily obtain (P1) of Lemma 1.1, as a consequence of (3.4). □

We now give a first consequence of inequality (1.7).

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

(i) *There is a constant* $h_0 > 0$*, such that for any* $\nu \in [0,1]$*,* $\Phi \in E^N$ *such that* $\mathrm{Gram}(\Phi) \leq \mathbb{1}$*, and* $\psi \in E$*,*

$$h_0||\psi||_{H^{1/2}} \leq ||\overline{H}^{\nu}_{\Phi}\psi||_{H^{-1/2}}. \tag{3.6}$$

In other words, $\overline{H}^{\nu}_{\Phi}$ *is a self-adjoint isomorphism between* $H^{1/2}$ *and its dual* $H^{-1/2}$*, whose inverse is bounded independently of* Φ, ν*.*

(ii) *Take* $\nu \in [0,1]$*,* $\Phi \in E^N$ *with* $\mathrm{Gram}(\Phi) \leq \mathbb{1}$*, and* $\psi \in E$*, such that* $\overline{H}^{\nu}_{\Phi}\psi \in L^2(\mathbb{R}^3, \mathbb{C}^4)$*. Then* $\psi \in \bigcap_{1 \leq q < 3/2} W^{1,q}_{loc}(\mathbb{R}^3, \mathbb{C}^4)$*.*

(iii) *Let* $\nu_n \in [0,1]$*, and* $\Phi_n \in E^N$ *with* $\mathrm{Gram}(\Phi_n) \leq \mathbb{1}$*. We assume that* $\|\varphi_{k,n}\|_E$ *is a bounded sequence, for* $k = 1, \cdots, N$*. Let* $\psi_n \in E$ *be such that the sequence* $\|\overline{H}^{\nu_n}_{\Phi_n}\psi_n\|_{L^2}$ *is bounded. Then* ψ_n *is precompact in* $H^{1/2}_{\mathrm{loc}}(\mathbb{R}^3, \mathbb{C}^4)$*.*

Proof. (i) Let $\psi^+ = \Lambda^+\psi$, $\psi^- = \Lambda^-\psi$. From inequality (1.7), we have

$$\begin{cases} (\psi^+, \overline{H}^{\nu}_{\Phi}\psi^+)_{E\times E^*} \geq (1 - \dfrac{(\pi/2 + 2/\pi)\alpha Z}{2})||\psi^+||^2_E, \\ -(\psi^-, \overline{H}^{\nu}_{\Phi}\psi^-)_{E\times E^*} \geq (1 - \dfrac{(\pi/2 + 2/\pi)\alpha N}{2})||\psi^-||^2_E \end{cases} \tag{3.7}$$

Let us choose $h_0 = 1 - \frac{(\pi/2+2/\pi)\alpha \max(Z,N)}{2}$. We get

$$\begin{aligned} \|\psi\|_E\|\overline{H}^{\nu}_{\Phi}\psi\|_{H^{-1/2}} &\geq Re(\psi^+ - \psi^-, \overline{H}^{\nu}_{\Phi}\psi)_{E\times E^*} \\ &= (\psi^+, \overline{H}^{\nu}_{\Phi}\psi^+)_{E\times E^*} - (\psi^-, \overline{H}^{\nu}_{\Phi}\psi^-)_{E\times E^*} \\ &\geq h_0\|\psi\|^2_E, \end{aligned} \tag{3.8}$$

hence (3.6). Now, $\overline{H}^{\nu}_{\Phi}$ is obviously self-adjoint from $H^{1/2}$ to its dual $H^{-1/2}$, so it is Fredholm of index 0. Equation (3.6) tells us that $\overline{H}^{\nu}_{\Phi}$ is injective, so it is an isomorphism, and the norm of its inverse is less than or equal to $1/h_0$.

(ii) ψ and $\varphi_1, \cdots, \varphi_N$ are in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, so they are in $L^r(\mathbb{R}^3, \mathbb{C}^4)$, for any $2 \leq r < 3$. V_ν is in the Marcinkiewicz space $\mathcal{M}^3$, so $(\mu * V_\nu)\psi$ is in any

$L^q_{loc}(\mathbb{R}^3,\mathbb{C}^4)$, $1 \le q < 3/2$, and $(\rho_\Phi * V_\nu)\psi - \int R_\Phi(x,y)\psi(y)dy$ is in any $L^{q'}_{loc}(\mathbb{R}^3,\mathbb{C}^4)$, $1 \le q' < 3$. As a consequence,

$$\psi = H_0^{-1}\left(\alpha Z(\mu * V_\nu)\psi - \alpha(\rho_\Phi * V_\nu)\psi + \alpha\int R_\Phi(x,y)\psi(y)dy + \overline{H}^\nu_\Phi\psi\right)$$

is in $\bigcap_{1\le q<3/2} W^{1,q}_{loc}(\mathbb{R}^3,\mathbb{C}^4)$.

(iii) From (i), $\|\psi_n\|_E$ is a bounded sequence. $\|\varphi_{k,n}\|_E$ is also bounded. ψ_n and $\varphi_{k,n}$ are thus precompact in any $L^r_{loc}(\mathbb{R}^3,\mathbb{C}^4)$, $2 \le r < 3$. So, refining the arguments in the proof of (ii), we see that ψ_n is precompact in $H^{1/2}_{\rm loc}(\mathbb{R}^3,\mathbb{C}^4)$. $\square$

We are now going to prove Lemma 2.1.

(a) First of all, (2.8) gives

$$\overline{H}^{\nu_n}_{\Phi_n}\varphi_{k,n} = \epsilon_{k,n}\varphi_{k,n} + \delta_{k,n}, \tag{3.9}$$

with $\lim_{n\to\infty} ||\delta_{k,n}||_{H^{-1/2}} = 0$. As a consequence,

$$||\overline{H}^{\nu_n}_{\Phi_n}\varphi_{k,n}||_{H^{-1/2}} \le \epsilon_{k,n}||\varphi_{k,n}||_{L^2} + ||\delta_{k,n}||_{H^{-1/2}}. \tag{3.10}$$

Using (3.6) of Lemma 3.1, we get

$$h_0||\varphi_{k,n}||_E \le \epsilon_{k,n}||\varphi_{k,n}||_{L^2} + ||\delta_{k,n}||_{H^{-1/2}}. \tag{3.11}$$

But we assume (2.9), i.e. lim inf $||\varphi_{1,n}||_{L^2} > 0$. So we must have lim inf $\epsilon_{1,n} \ge h_0$, and (2.10) follows from (2.8) (2.9), with the same h_0 as in Lemma 3.1.

(b) Under the additional assumption (2.11), i.e. lim sup $\epsilon_{N,n} < 1$, let us study the convergence of $\varphi_{k,n}$ for the $H^{1/2}$ topology. After extraction of a subsequence, we may impose

$$\epsilon_{k,n} \underset{n\to\infty}{\longrightarrow} \epsilon_k \in [h_0, 1) \quad \text{and} \quad \nu_n \quad \nu \in [0,1].$$

$\|\epsilon_{k,n}\varphi_{k,n}\|_{L^2}$ is a bounded sequence. So (3.11) implies that $\|\varphi_{k,n}\|_E$ is bounded uniformly in n.

Let $\chi_{k,n} \in H^{1/2}$ be defined by $H^{\nu_n}_{\Phi_n}\chi_n = \epsilon_{k,n}\varphi_{k,n}$. By (iii) of Lemma 3.1, we may impose, after extraction of a subsequence, $\chi_{k,n} \underset{n\to\infty}{\longrightarrow} \varphi_k$ in $H^{1/2}_{\rm loc}(\mathbb{R}^3,\mathbb{C}^4)$.

On the other hand, we may write

$$\overline{H}^{\nu_n}_{\Phi_n}(\varphi_{k,n} - \chi_{k,n}) = \delta_{k,n} \underset{n\to\infty}{\longrightarrow} 0 \quad \text{in} \quad H^{-1/2}(\mathbb{R}^3,\mathbb{C}^4).$$

So $\Delta_{k,n} = \varphi_{k,n} - \chi_{k,n} \to 0$ in $H^{1/2}(\mathbb{R}^3,\mathbb{C}^4)$, and $\varphi_{k,n} = \chi_{k,n} + \Delta_{k,n} \underset{n\to\infty}{\longrightarrow} \varphi_k$, in $H^{1/2}_{\rm loc}(\mathbb{R}^3,\mathbb{C}^4)$.

Then $\Phi = (\varphi_1,\ldots,\varphi_N)$ is a strong solution, in $\left(E \cap \bigcap_{1\le q<3/2} W^{1,q}_{\rm loc}(\mathbb{R}^3,\mathbb{C}^4)\right)^N$, of

$$\overline{H}^\nu_\Phi\varphi_k = \epsilon_k\varphi_k, (\forall k).$$

Our goal is to prove that $\varphi_{k,n}$ converges to φ_k in $H^{1/2}(\mathbb{R}^3,\mathbb{C}^4)$. Let $\psi_{k,n} = \varphi_{k,n} - \varphi_k$. Let us denote

$$\tilde\rho_n = \sum_k |\psi_{k,n}(x)|^2, \tilde R_n(x,y) = \sum_k \psi_{k,n}(y)^* \otimes \psi_{k,n}(x). \tag{3.12}$$

For $\psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, let

$$L_{k,n}\psi = H_0\psi + \alpha\Big(\tilde{\rho}_n * V_{\nu_n}\Big)\psi - \alpha \int \tilde{R}_n(x,y)\psi(y)V_{\nu_n}(x-y)dy - \epsilon_k\psi. \tag{3.13}$$

We have

$$\lim_{n\to\infty} ||L_{k,n}\psi_{k,n}||_{H^{-1/2}} = 0.$$

Now, from inequality (1.7) and our assumptions, it is easy to see that the map

$$\psi^- \in E^- \mapsto F_{k,n}(\psi^-) = \Big(\psi_{k,n} + \psi^-, L_{k,n}(\psi_{k,n} + \psi^-)\Big)_{L^2}$$

is strictly concave. So, denoting $\psi^{\pm}_{k,n} = \Lambda^{\pm}\psi_{k,n}$,

$$F_{k,n}(-\psi^-_{k,n}) \le F_{k,n}(0) - F'_{k,n}(0).\psi^-_{k,n} \le 3||\psi_{k,n}||_E ||L_{k,n}\psi_{k,n}||_{H^{-1/2}}, \tag{3.14}$$

hence $\limsup_{n\to\infty} F_{k,n}(-\psi^-_{k,n}) \le 0$. But if we define $\delta = 1 - \epsilon_N$, we have

$$F_{k,n}(-\psi^-_{k,n}) = \Big(\psi^+_{k,n}, L_{k,n}\psi^+_{k,n}\Big)_{L^2} \ge \Big(\psi^+_{k,n}, \delta\sqrt{1-\Delta}\,\psi^+_{k,n}\Big)_{L^2}. \tag{3.15}$$

As a consequence, $||\psi^+_{k,n}||_E \to 0$ as $n \to \infty$.

So, $||L_{k,n}\psi^-_{k,n}||_{H^{-1/2}} \underset{n\to\infty}{\longrightarrow} 0$ and $\lim_{n\to\infty}\Big(\psi^-_{k,n}, L_{k,n}\psi^-_{k,n}\Big)_{L^2} = 0$. But from inequality (1.7),

$$\Big(\psi^-_{k,n}, L_{k,n}\psi^-_{k,n}\Big)_{L^2} \le -\Big(1 - \frac{\alpha N(\pi/2 + 2/\pi)}{2}\Big)||\psi^-_{k,n}||^2_E. \tag{3.16}$$

So $||\psi^-_{k,n}||_E$ 0, and $||\psi_{k,n}||_E \longrightarrow 0$ as $n \to \infty$.

We have thus proved that $||\varphi_{k,n} - \varphi_k||_E \longrightarrow 0$ as $n \to \infty$.

(b.1) We now assume that $p_n = p$ for n large. Being a limit of Φ_n in the strong E^N-topology, Φ is obviously a critical point of $\mathcal{F}_{\nu,p}$ in A, and from (2.9), Gram $\Phi > 0$. We also have Gram $\Phi = \text{Diag}(\sigma_1, \ldots, \sigma_N)$, $0 < \sigma_1 \le \ldots. \le \sigma_N < 1$. From (2.10),

$$e_p(\sigma_1) = \frac{p\sigma_1^{p-1} - (p-1)\sigma_1^p}{(1-\sigma_1)^2} \ge h_0.$$

There is a unique number $c_p \in (0,1)$ such that $e_p(c_p) = h_0$, and we have $\lim_{p\to\infty} c_p = 1$. Since e_p is increasing on $(0,1)$, we get

$$c_p \mathbb{1} \le \text{Gram}\,\Phi < \mathbb{1}.$$

(b.2) Finally, let us assume that $\nu_n \to 0$ and $p_n \to \infty$. Then

$$1 > \epsilon_{k,n} \ge c_{p_n} \underset{n\to\infty}{\longrightarrow} 1,$$

so $\Phi \in \Sigma$. Obviously, Φ satisfies (2.12), so it is a critical point of $\mathcal{E}|_\Sigma$. Moreover, $\mathcal{E}(\Phi) = \lim_{n\to\infty} \mathcal{E}(\Phi_n)$.

Now, $\pi_{p_n}(\Phi_n) = \sum_k \theta_{p_n}(\sigma_{k,n})$, with $\theta_p(x) = \frac{x^p}{1-x}$.

We recall that $\theta^{'}_{p_n}(\sigma_{k,n}) = \epsilon_{k,n} < 1$. But $\dfrac{\theta^{'}_p(x)}{\theta_p(x)} = \dfrac{p}{x} + \dfrac{1}{1-x} \geq p, \forall x \in (0,1)$. So, $\theta_{p_n}(\sigma_{k,n}) < \dfrac{1}{p_n} \underset{n\to\infty}{\longrightarrow} 0$. As a consequence, $\pi_{p_n}(\Phi_n) \to 0$ and

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

This ends the proof of Lemma 2.1. □

4. The Hessian of $\mathcal{F}_{\nu,p}$

We shall use the following formula for the second derivative of the DF energy:

$$\frac{1}{2}\,\mathcal{E}_\nu^{''}(\Phi)\Big[\Psi,\Psi\Big] = \sum_\ell \;||\psi_\ell^+||_E^2 - ||\psi_\ell^-||_E^2 - \alpha Z\Big(\psi_\ell, (\mu * V_\nu(x))\,\psi_\ell\Big)_{L^2} \\ + \;\; \mathcal{K}_1 - \mathcal{K}_2 + \mathcal{K}_3 - \mathcal{K}_4 + \mathcal{K}_5, \tag{4.1}$$

where

$$\mathcal{K}_1 = \alpha \iint_{\mathbb{R}^3\times\mathbb{R}^3} V_\nu(x-y)\rho_\Psi(x)\rho_\Phi(y) \tag{4.2}$$
$$\rho_\Psi(x) = \sum_\ell |\psi_\ell(x)|^2, \; \rho_\Phi(y) = \sum_m |\varphi_m(y)|^2,$$

$$\mathcal{K}_2 = \alpha \sum_{\ell\neq m} \iint V_\nu(x-y)\Big(\psi_\ell(y),\varphi_m(y)\Big)\Big(\varphi_m(x),\psi_\ell(x)\Big) \\ + \alpha\sum_\ell \iint V_\nu(x-y)\mathrm{Im}\Big(\varphi_\ell(x),\psi_\ell(x)\Big)\mathrm{Im}\left(\varphi_\ell(y),\psi_\ell(y)\right), \tag{4.3}$$

$$\mathcal{K}_3 = \alpha \iint k(x)k(y)V_\nu(x-y), \quad k(x) = \sum_\ell \mathrm{Re}\Big(\varphi_\ell(x),\psi_\ell(x)\Big), \tag{4.4}$$

$$\mathcal{K}_4 = 2\alpha \iint V_\nu(x-y)tr\Big(K(x,y)K(y,x)\Big), \tag{4.5}$$
$$K(x,y) = \frac{1}{2}\sum_\ell \Big(\varphi_\ell^*(y)\otimes\psi_\ell(x) + \psi_\ell^*(y)\otimes\varphi_\ell(x)\Big),$$

$$\mathcal{K}_5 = \alpha \sum_{\ell\neq m} \iint Re\Big(\varphi_\ell(x),\psi_\ell(x)\Big)Re\Big(\varphi_m(y),\psi_m(y)\Big)V_\nu(x-y). \tag{4.6}$$

$\mathcal{E}_\nu$ has a very useful concavity property:

Lemma 4.1. *If* $(3N-1)\alpha < \frac{2}{\pi/2+2/\pi}$*, then for any* $\Phi \in A$*, and any* $\Psi^- \in (E^-)^N, \nu \in [0,1]$,

$$\mathcal{E}_\nu''(\Phi)\Big[\Psi^-,\Psi^-\Big] \leq -s\sum_{k=1}^N ||\psi_k^-||_E^2, \tag{4.7}$$

where $s > 0$ *is a constant independent of* Φ, Ψ, ν.

Proof of Lemma 4.1. We obviously have $(\psi_\ell, (\mu * V_\nu)\psi_\ell)_{L^2} > 0$. The Fourier transform of V_ν is a positive measure, so

$$\iint V_\nu(x-y)f(x)f(y)^* \geq 0, \quad \forall f \in L^1 \cap L^{3/2}(\mathbb{R}^3,\mathbb{C}). \tag{4.8}$$

As a consequence, $\mathcal{K}_2 \geq 0$.
Now, $K(y,x) = K(x,y)^*$, so that

$$\mathrm{tr}\Big(K(x,y)K(y,x)\Big) \geq 0 \quad \forall x, y,$$

hence $\mathcal{K}_4 \geq 0$. We thus have

$$\frac{1}{2}\mathcal{E}''(\Phi)\Big[\Psi,\Psi\Big] \leq \sum_\ell ||\psi_\ell^+||_E^2 - ||\psi_\ell^-||_E^2 + \mathcal{K}_1 + \mathcal{K}_3 + \mathcal{K}_5. \tag{4.9}$$

Now, take $\Phi \in A$ and $\Psi^- \in (E^-)^N$. For $m = 1,\ldots,N$, we have $||\varphi_m||_{L^2} \leq 1$. So, using inequality (1.7), we easily get

$$\mathcal{K}_1 \leq \frac{(\pi/2+2/\pi)\alpha N}{2}\sum_\ell ||\psi_\ell^-||_E^2, \tag{4.10}$$

and

$$\mathcal{K}_5 \leq \frac{(\pi/2+2/\pi)\alpha(N-1)}{2}\sum_\ell ||\psi_\ell^-||_E^2. \tag{4.11}$$

By the Cauchy–Schwarz inequality,

$$\mathcal{K}_3 \leq \mathcal{K}_1. \tag{4.12}$$

Finally, for any $\Phi \in A$ and $\Psi^- \in \Big(E^-\Big)^N$,

$$\begin{aligned}\frac{1}{2}\mathcal{E}_\nu''(\Phi)\Big[\Psi^-,\Psi^-\Big] &\leq -\sum_\ell ||\psi_\ell^-||_E^2 + \frac{(\pi/2+2/\pi)\alpha}{2}(3N-1)\sum_\ell ||\psi_\ell^-||_E^2 \\ &\leq -s\sum_\ell ||\psi_\ell^-||_E^2,\end{aligned} \tag{4.13}$$

with $s = 1 - \frac{(\pi/2+2/\pi)\alpha}{2}(3N-1)$. Note that $s > 0$ provided

$$\alpha(3N-1) < \frac{2}{\pi/2+2/\pi}. \tag{4.14}$$

This proves Lemma 4.1. □

We now compute the second derivative of the penalization term π_p. We write $\pi_p(\Phi) = S_p \circ \mathrm{Gram}(\Phi)$, with

$$\begin{cases} S_p(Q) = \mathrm{tr}\Big[Q^p(1-Q)^{-1}\Big] = \sum_{n\geq p} T_n(Q), \\ T_n(Q) = \mathrm{tr}(Q^n). \end{cases} \tag{4.15}$$

Since π_p is $\mathcal{U}(N)$ invariant, we just need an expression of $\pi_p^{''}(\Phi)$ when $\Phi \in \mathcal{O}$, i.e.

$$Q = \mathrm{Gram}\,\Phi = \mathrm{Diag}(\sigma_1, \dots, \sigma_N), 0 < \sigma_1 \leq \dots \leq \sigma_N < 1.$$

For any self-adjoint matrix h we have

$$T_n^{'}(Q)\cdot h = \sum_{\alpha+\beta=n-1} \mathrm{tr}(Q^\alpha h Q^\beta) = n\mathrm{tr}(Q^{n-1}h) = n\sum_k \sigma_k^{n-1} h_{kk}, \tag{4.16}$$

and

$$T_n^{''}(Q)\cdot\Big[h,h\Big] = n\sum_{a+b=n-2} \mathrm{tr}(Q^a h Q^b h) = n\sum_{k,\ell}\Big(\sum_{a+b=n-2}\sigma_k^a\sigma_\ell^b\Big)|h_{k\ell}|^2. \tag{4.17}$$

Summing up, we get

$$S_p^{'}(Q)\cdot h = \sum_k e_p(\sigma_k) h_{kk}, \tag{4.18}$$

$$S_p^{''}(Q)\cdot\Big[h,h\Big] = \sum_k e_p^{'}(\sigma_k)|h_{kk}|^2 + \sum_{k\neq\ell}\frac{e_p(\sigma_k)-e_p(\sigma_\ell)}{\sigma_k-\sigma_\ell}|h_{k\ell}|^2, \tag{4.19}$$

with $e_p(t) = \left(\frac{t^p}{1-t}\right)^{'} = \frac{pt^{p-1}-(p-1)t^p}{(1-t)^2}$. Finally we obtain

$$\pi_p^{'}(\Phi)\cdot\psi = 2\sum_k e_p(\sigma_k) Re(\Phi_k,\psi_k), \tag{4.20}$$

$$\begin{aligned}\pi_p^{''}(\Phi).\Big[\Psi,\Psi\Big] &= \sum_k 2e_p(\sigma_k)||\psi_k||_{L^2}^2 + e_p^{'}(\sigma_k)|2Re(\varphi_k,\psi_k)_{L^2}|^2 \\ &\quad + \sum_{k\neq\ell}\frac{e_p(\sigma_k)-e_p(\sigma_\ell)}{\sigma_k-\sigma_\ell}\Big|(\varphi_k,\psi_\ell)_{L^2}+(\psi_k,\varphi_\ell)_{L^2}\Big|^2.\end{aligned} \tag{4.21}$$

The function e_p is positive and strictly increasing on $(0,1)$. As a consequence, we have

Lemma 4.2. *For any $p \geq 1$, the functional π_p is strictly convex on*

$$A = \Big\{\Phi \in E^N \,/\, 0 < \mathrm{Gram}\,\Phi < \mathbb{1}\Big\}.$$

Lemma 2.2 is an immediate consequence of Lemmas 4.1 and 4.2.

Our goal is now to prove Lemma 2.4. We start with an upper bound on the second derivative $I''_{\nu,p}(\Phi^+)\Big[\Psi^+,\Psi^+\Big]$, at a point $\Phi^+ \in A^+$, in a direction $\Psi^+ \in (E^+)^N \cap \Big[H^1(\mathbb{R}^3,\mathbb{C}^4)\Big]^N$, under the orthogonality conditions $(\varphi_k^+,\psi_\ell^+)_{L^2} = 0, \forall k,\ell$.

Lemma 4.3. *Assume that* $\alpha(3N-1) < \frac{2}{\pi/2+2/\pi}$. *Take* $\nu \in (0,1)$ *and* $p \geq 2$. *Consider* $\Phi^+ \in A^+$ *such that*

$$\mathrm{Gram}(\Phi) = \mathrm{Diag}(\sigma_1,\ldots,\sigma_N), 0 < \sigma_1 \leq \cdots \leq \sigma_N < 1, \tag{4.22}$$

where $\Phi = \Phi^+ + h_{\nu,p}(\Phi^+)$. *Let* $\Psi^+ \in \big(E^+ \cap H^1(\mathbb{R}^3,\mathbb{C}^4)\big)^N$ *satisfy*

$$(\varphi_k^+,\psi_\ell^+)_{L^2} = 0, \quad \forall k,\ell. \tag{4.23}$$

Then the following inequality holds:

$$\frac{1}{2}I''_{\nu,p}(\Phi^+)\Big[\Psi^+,\Psi^+\Big] \leq \frac{1}{2}\mathcal{E}''_\nu(\Phi)\Big[\Psi^+,\Psi^+\Big] - \sum_k e_p(\sigma_k)\|\psi_k^+\|^2_{L^2} + \\ + \overline{c}\sum_k \|\nabla\psi_k^+\|^2_{L^2}. \tag{4.24}$$

Here, $\overline{c}$ *depends only on* (Z,N).

Proof. Take $\Phi^+ \in A^+$, $\Psi^+ \in (E^+)^N \cap \Big[H^1(\mathbb{R}^3,\mathbb{C}^4)\Big]^N$, and denote

$$\Phi^- = h_{\nu,p}(\Phi^+), \Psi^- = h'_{\nu,p}(\Phi^+)\Psi^+, \Phi = \Phi^+ + \Phi^-, \Psi = \Psi^+ + \Psi^-. \tag{4.25}$$

We may write

$$\frac{1}{2}I''_{\nu,p}(\Phi^+)\Big[\Psi^+,\Psi^+\Big] = \frac{1}{2}\mathcal{F}''_{\nu,p}(\Phi)\Big[\Psi,\Psi\Big]. \tag{4.26}$$

If we impose the condition (4.23): $\Big(\varphi_k^+,\psi_\ell^+\Big)_{L^2} = 0 \quad \forall k,\ell$, then, from (4.21), we see that, for any $\chi^- \in (E^-)^N$,

$$\pi''_p(\Phi)\Big[\Psi^+ + \chi^-, \Psi^+ + \chi^-\Big] = \sum_k 2e_p(\sigma_k)\|\psi_k^+\|^2_{L^2} + \pi''_p(\Phi)\Big[\chi^-,\chi^-\Big]. \tag{4.27}$$

As a consequence,

$$\frac{1}{2}\mathcal{F}''_{\nu,p}(\Phi)\Big[\Psi,\Psi\Big] = \frac{1}{2}\mathcal{E}''_\nu(\Phi)\Big[\Psi^+,\Psi^+\Big] - \sum_k e_p(\sigma_k)\|\psi_k^+\|^2_{L^2} + \\ + \mathcal{E}''_\nu(\Phi)\Big[\Psi^+,\Psi^-\Big] + \frac{1}{2}\mathcal{F}''_{\nu,p}(\Phi)\Big[\Psi^-,\Psi^-\Big]. \tag{4.28}$$

Now, $\Psi^- = h'_{\nu,p}(\Phi)\Psi^+$ is solution of

$$\mathcal{F}''_{\nu,p}(\Phi)\Big[\Psi^+,\chi^-\Big] + \mathcal{F}''_{\nu,p}(\Phi)\Big[\Psi^-,\chi^-\Big] = 0, \forall\chi^- \in (E^-)^N. \tag{4.29}$$

Note that $\mathcal{F}''_{\nu,p}(\Phi)\Big[\Psi^+,\chi^-\Big] = \mathcal{E}''_\nu\Big[\Psi^+,\chi^-\Big]$, from (4.21) and (4.27). So, applying (4.29) to $\chi^- = \Psi^-$, and using Lemma 2.2, we get

$$s\sum_k \|\psi_k^-\|_E^2 \le \Big|\mathcal{E}''_\nu(\Phi)\Big[\Psi^+,\Psi^-\Big]\Big|. \tag{4.30}$$

From Hardy's inequality (1.9), we have

$$\Big|\mathcal{E}''_\nu(\Phi)\Big[\Psi^+,\Psi^-\Big]\Big| \le C(N,Z)\Big[\sum_k ||\nabla\psi_k^+||_{L^2}^2\Big]^{1/2}\Big[\sum_k ||\psi_k^-||_{L^2}^2\Big]^{1/2}. \tag{4.31}$$

Combining (4.30) (4.31), we get

$$\sum_k \|\psi_k^-\|_E^2 \le C'\sum_k \|\nabla\psi_k^+\|_{L^2}^2, \tag{4.32}$$

and finally

$$\begin{aligned}\frac{1}{2}\mathcal{F}''_{\nu,p}(\Phi)\Big[\Psi,\Psi\Big] \le \frac{1}{2}\mathcal{E}''_\nu(\Phi)\Big[\Psi^+,\Psi^+\Big] - \sum_k e_p(\sigma_k)\|\psi_k^+\|_{L^2}^2 +\\ +\bar{c}\sum_k \|\nabla\psi_k^+\|_{L^2}^2.\end{aligned} \tag{4.33}$$

Now, combining (4.26), (4.33), one easily gets (4.24), and the lemma is proved. □

The next lemma gives an upper estimate on $\mathcal{E}''_\nu(\Phi)\Big[\Psi,\Psi\Big]$ for Ψ of the form $(0,\dots,0,\psi)$, $\psi\in E$, radial. It is inspired by [36, 39].

Lemma 4.4. *For any $\Phi\in A, \nu\in(0,1)$ and $\psi\in E$, of the form $\psi(x) = f(|x|)$, taking $\Psi(x) = (0,\dots,0,\psi(x))$, we have*

$$\begin{aligned}\frac{1}{2}\,\mathcal{E}''_\nu(\Phi)\Big[\Psi,\Psi\Big] \le \Big(\psi,H_0\psi\Big)_{L^2} + \alpha(N-1)\Big(\psi,V_\nu\psi\Big)_{L^2}\\ -\alpha Z\Big(\psi,(\mu*V_\nu)\,\psi\Big)_{L^2}.\end{aligned} \tag{4.34}$$

Proof. We may write

$$\begin{aligned}\mathcal{E}_\nu(\varphi_1\dots\varphi_N) = \mathcal{E}_\nu\Big(\varphi_1\dots\varphi_{N-1}\Big) + \Big(\varphi_N,H_0\varphi_N\Big)_{L^2} - \alpha Z\Big(\varphi_N,(\mu*V_\nu)\,\varphi_N\Big)_{L^2}\\ +\alpha\iint V_\nu(x-y)\sum_{k=1}^{N-1}|\varphi_k(y)|^2|\varphi_N(x)|^2\\ -\alpha\iint V_\nu(x-y)\sum_{k=1}^{N-1}\Big(\varphi_k(y),\varphi_N(y)\Big)\Big(\varphi_N(x),\varphi_k(x)\Big).\end{aligned} \tag{4.35}$$

So $\mathcal{E}_\nu$ is a quadratic form in φ_N, when $\varphi_1,\dots,\varphi_{N-1}$ are fixed. Note that

$$\iint V_\nu(x-y)\Big(\varphi_k(y),\psi(y)\Big)\Big(\psi(x),\varphi_k(x)\Big)$$

is nonnegative, from (4.8). Hence,

$$\frac{1}{2}\mathcal{E}_\nu''(\Phi)\Big[\Psi,\Psi\Big] \le \Big(\psi, H_0\psi\Big)_{L^2} - \alpha Z\Big(\psi, (\mu * V_\nu)\,\psi\Big)_{L^2} + \alpha \iint V_\nu(x-y)\sum_{k=1}^{N-1}|\varphi_k(y)|^2|\psi(x)|^2, \tag{4.36}$$

for any $\Psi = \Big(0,\dots,0,\psi), \psi \in E$.

Now, if $\rho \in L^1(\mathbb{R}^3, \mathbb{R}_+)$ is radial, then an easy computation shows that

$$\int_{\mathbb{R}^3} \rho(x)V_\nu(x-x_0)dx \le \int_{\mathbb{R}^3} \rho(x)V_\nu(x)dx, \quad \forall x_0 \in \mathbb{R}^3. \tag{4.37}$$

As a consequence, if $\psi(x) = f(|x|)$, then

$$\begin{aligned}&\int_{\mathbb{R}^3} dy \sum_{k=1}^{N-1}|\varphi_k(y)|^2 \int_{\mathbb{R}^3} |\psi(x)|^2 V_\nu(x-y)dx \\ &\le \int_{\mathbb{R}^3} dy \sum_{k=1}^{N-1}|\varphi_k(y)|^2 \int_{\mathbb{R}^3} |\psi(x)|^2 V_\nu(x)dx = \\ &= (N-1)\Big(\psi, V_\nu\psi\Big)_{L^2}.\end{aligned} \tag{4.38}$$

Lemma 4.4 follows directly from (4.36) and (4.38). □

We now give an upper bound on $I''_{\nu,p}\cdot(0,\dots,0,\psi^+)^2$ for ψ^+ in a suitably chosen finite dimensional subspace of E^+.

Lemma 4.5. *Assume that* $\alpha(3N-1) < \frac{2}{\pi/2+2/\pi}$, $N < Z+1$. *Then, for any* $m \ge 0$, *there is a real finite dimensional subspace of* E^+ *denoted* X_m, *with* $\dim_{\mathbb{R}} X_m = m+1$ *and a constant* $b_m \in (0,1)$ *such that*

$$\frac{1}{2}I''_{\nu,p}(\Phi^+).\Big(0,\dots,0,\psi^+\Big)^2 \le \Big[b_m - e_p(\sigma_N)\Big]\|\psi^+\|_E^2 \tag{4.39}$$

for any $\nu \in (0,1), p \ge 1$, $\psi^+ \in X_m$, *and any* $\Phi^+ \in A^+$ *such that* Gram Φ = Diag$(\sigma_1,\dots,\sigma_N)$, $0 < \sigma_1 \le \dots \le \sigma_N < 1$, *with the notation* $\Phi = \Phi^+ + h_{\nu,p}(\Phi^+)$.

Proof. Let d be a positive integer. We choose a d-dimensional subspace of

$$H^1\Big(\Big\{[0,\infty), r^2dr\Big\}, \mathbb{R}\Big),$$

denoted V_d. To $f(r) \in V_d$, and $\lambda > 0$, we associate

$$\psi(x) = \begin{pmatrix} f(|x|/\lambda) \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{4.40}$$

Obviously, $\psi \in H^1(\mathbb{R}^3, \mathbb{C}^4)$. We call $W_{d,\lambda}$ the d-dimensional real vector space of functions ψ of the form (4.54), with λ fixed and $f \in V_d$ arbitrary.

It is easy to see that there are two constants $0 < c_*(d) < c^*(d) < \infty$ such that, for any $\psi \in W_{d,\lambda}$ and λ large,

$$(H_0\psi, \psi) = \|\psi\|^2_{L^2}, \tag{4.41}$$

$$\|\nabla\psi\|^2_{L^2} \le \frac{c^*}{\lambda^2}\|\psi\|^2_{L^2}, \tag{4.42}$$

$$\Big(\psi, V_\nu\psi\Big)_{L^2} \ge \frac{c_*}{\lambda}\|\psi\|^2_{L^2}, \forall\nu\in[0,1], \tag{4.43}$$

$$\|\Lambda^-\psi\|^2_{L^2} \le \frac{c^*}{\lambda^2}\|\psi\|^2_{L^2}, \tag{4.44}$$

$$((\mu * V_\nu)\,\psi, \psi)_{L^2} \ge (V_\nu\psi, \psi)_{L^2} - o\left(\frac{1}{\lambda}\right)||\psi||^2_{L^2}, \forall\nu\in[0,1]. \tag{4.45}$$

Inequalities (4.42), (4.43) and (4.45) follow from scaling arguments, and (4.44) is a consequence of formula (3.3).
Now, suppose that $\psi \in W_{d,\lambda}$ satisfies

$$\Big(\varphi_k^+, \psi\Big)_{L^2} = 0, \quad \forall k, \tag{4.46}$$

for some $\Phi^+ = (\varphi_1^+, \dots, \varphi_N^+) \in A^+$, such that Gram $\Phi = (\sigma_1, \dots, \sigma_n)$, $0 < \sigma_1 \le \dots \le \sigma_N < 1$, with $\Phi = \Phi^+ + h_{\nu,p}(\Phi^+)$. Let $\Psi^+ = (0, \dots, \Lambda^+\psi)$. From Lemma 4.3, we have, for any $\nu \in (0,1), p \ge 1$,

$$\begin{aligned}\frac{1}{2}I''_{\nu,p}(\Phi^+)\Big[\Psi^+, \Psi^+\Big] \le \frac{1}{2}\mathcal{E}''_\nu(\Phi)\Big[\Psi^+, \Psi^+\Big] - e_p(\sigma_N)\|\Lambda^+\psi\|^2_{L^2} + \\ + \overline{c}\|\nabla\psi\|^2_{L^2}.\end{aligned} \tag{4.47}$$

From Lemma 2.2,

$$\frac{1}{2}\mathcal{E}''_\nu(\Phi)\Big[\Psi^+, \Psi^+\Big] \le \frac{1}{2}\mathcal{E}''_\nu(\Phi)\Big[\Psi, \Psi\Big] - \mathcal{E}''_\nu(\Phi)\Big[\Psi, \Psi^-\Big], \tag{4.48}$$

where $\Psi = (0, \dots, 0, \psi)$, $\Psi^- = (0, \dots, 0, \Lambda^-\psi)$. But from Hardy's inequality (1.9),

$$\left|\mathcal{E}''_\nu(\Phi)\Big[\Psi, \Psi^-\Big]\right| \le \overline{\overline{c}}\|\nabla\psi\|_{L^2}\|\Lambda^-\psi\|_{L^2}, \tag{4.49}$$

for some $\overline{\overline{c}} > 0$ which depends only on N, Z.
Moreover, using Lemma 4.4, we get

$$\frac{1}{2}\mathcal{E}''_\nu(\Phi)\Big[\Psi, \Psi\Big] \le \Big(\psi, H_0\psi\Big) + \alpha(N-1)(\psi, V_\nu\psi)_{L^2} - \alpha Z\,((\mu * V_\nu)\,\psi, \psi)_{L^2}. \tag{4.50}$$

Finally, combining (4.41, 4.42, ..., 4.50), we get

$$\begin{aligned}\frac{1}{2}I''_{\nu,p}(\Phi)\Big[\Psi^+, \Psi^+\Big] &\le \Big(1 - (Z-N+1)\frac{\alpha c_* + o(1)}{\lambda}\Big)\|\psi\|^2_{L^2} - e_p(\sigma_N)\|\Lambda^+\psi\|^2_{L^2} \\ &\quad + \frac{(\overline{\overline{c}} + \overline{c})c^*}{\lambda^2}\|\psi\|^2_{L^2} \\ &\le \Big(1 - \frac{\alpha c_*(Z-N+1)}{2\lambda} - e_p(\sigma_N)\Big)\|\Lambda^+\psi\|^2_E\end{aligned} \tag{4.51}$$

for $\lambda = \lambda(d)$ large enough.

Now, take $m \geq 0$. Choose X_m as an $(m+1)$-dimensional subspace of $\Lambda^+\Big(W_{d,\lambda(d)} \cap \Big\{\varphi_1^+, \dots, \varphi_N^+\Big\}^\perp\Big)$, where $d = m + 2N + 1$ (such a space always exists). Take $b_m = 1 - \dfrac{\alpha c_*(Z - N + 1)}{2\lambda(d)}$. Then it is easy to check that X_m satisfies (4.39), and Lemma 4.5 is proved. □

Lemma 2.4 is now an immediate consequence of Lemma 4.5.

5. The Min–Max Argument

We start with a proof of Lemma 2.5. We need the following result:

Lemma 5.1. *Assume that* $\alpha(3N - 1) < \frac{2}{\pi/2+2/\pi}$. *Take* $\nu \in (0, 1)$. *There is a constant* $C(\nu) > 0$ *such that, for any* $p \geq 1$ *and* $\Phi^+ \in A^+$,

$$\sigma_1(\Phi^+) \leq C(\nu)\sigma_1^+(\Phi^+). \tag{5.1}$$

Here, $\sigma_1^+(\Phi^+)$ *is the smallest eigenvalue of* Gram Φ^+, *and* $\sigma_1(\Phi^+)$ *is the smallest eigenvalue of* Gram Φ, *where* $\Phi = \Phi^+ + h_{\nu,p}(\Phi^+)$.

Remark. The constant C depends on ν. We have been unable to prove that C remains bounded as ν tends to 0.

Proof of Lemma 5.1. Take $\Phi^+ \in A^+$, i.e. $\Phi^+ \in (E^+)^N$ with $0 < \mathrm{Gram}(\Phi^+) < 1\!\!1$. Using the $\mathcal{U}(N)$ invariance, we just have to prove the lemma when

$$\mathrm{Gram}(\Phi^+) = \mathrm{Diag}(\sigma_1^+, \dots, \sigma_N^+), \quad 0 < \sigma_1^+ \leq \dots \leq \sigma_N^+ < 1. \tag{5.2}$$

We denote

$$h_{\nu,p}(\Phi^+) = \Phi^- = (\varphi_1^-, \dots, \varphi_N^-), \quad \Phi = \Phi^+ + \Phi^- = (\varphi_1, \dots, \varphi_N).$$

We introduce the following functional on E^-:

$$F(\psi^-) = \Big(\varphi_1^+ + \psi^-, H_{\Phi_1}^\nu(\varphi_1^+ + \psi^-)\Big)_{L^2} - \pi_p(\varphi_1^+ + \psi^-, \varphi_2, \dots, \varphi_N). \tag{5.3}$$

Here, $\Phi_1 = (\varphi_2, \dots, \varphi_N) \in E^{N-1}$, and

$$\begin{aligned} H_{\Phi_1}^\nu \psi &= \Big(H_0 - \alpha Z\,(\mu * V_\nu)\Big)\psi \\ &\quad + \alpha \sum_{k=2}^N \iint V_\nu(x-y)\Big(|\varphi_k(y)|^2\psi(x) - (\varphi_k(y), \psi(y))\varphi_k(x)\Big)\,dy. \end{aligned} \tag{5.4}$$

We have extended π_p to E^N, with values in $\overline{\mathbb{R}}$, by defining $\pi_p(\Phi) = +\infty$ when $1\!\!1 - \mathrm{Gram}\,\Phi$ is not positive definite. F is thus well-defined on E^- with values in $\overline{\mathbb{R}}$, and $F''(\psi^-)$ exists when $F(\psi^-) > -\infty$. From Lemma 2.2, F is strictly concave, and

$$F''(\psi^-)\big[\chi^-, \chi^-\big] \leq -s\|\chi^-\|_E^2, \tag{5.5}$$

for any $\chi^- \in E^-$, and $\psi^- \in E^-$ such that $F(\psi^-) > -\infty$. We have

$$\mathcal{F}_{\nu,p}\Big(\varphi_1^+ + \psi^-, \varphi_2, \dots, \varphi_N\Big) = F(\psi^-) + \mathcal{E}_\nu(\Phi_1), \tag{5.6}$$

so φ_1^- is the unique maximizer of F on E^-. From (5.2), $(\varphi_1^+, \varphi_k)_{L^2} = 0$, $\forall k \geq 2$. Therefore, for any $\chi^- \in E^-$,

$$\begin{aligned}
&\pi_p'(\varphi_1^+, \varphi_2, \dots, \varphi_N) \cdot \chi^- = \\
&= \sum_{n\geq p} 2n\mathrm{tr}\left[\begin{pmatrix} (\sigma_1^+)^{n-1} 0 & \dots & 0 \\ 0 & & \\ \vdots & \big(\mathrm{Gram}\ \Phi_1\big)^{n-1} & \\ 0 & & \end{pmatrix}\begin{pmatrix} 0 & Re(\chi^-, \varphi_2^-) \dots Re(\chi^-, \varphi_N^-) \\ Re(\varphi_2^-, \chi^-) & \\ \vdots & 0 \\ Re(\varphi_N^-, \chi^-) & \end{pmatrix}\right] \\
&= 0.
\end{aligned}$$

As a consequence,

$$F'(0)\chi^- = 2Re\Big(\chi^-, H^\nu_{\Phi_1}\varphi_1^+\Big). \tag{5.7}$$

So there is a constant $K_1(\nu) > 0$ such that

$$|F'(0)\chi^-| \leq K_1(\nu)\|\varphi_1^+\|_{L^2}\|\chi^-\|_E, \forall \chi^- \in E^-. \tag{5.8}$$

But (5.5) implies that

$$F(\varphi_1^-) \leq F(0) + F'(0)\varphi_1^- - s\|\varphi_1^-\|_E^2. \tag{5.9}$$

Since $F(\varphi_1^-) \geq F(0)$, (5.8) (5.9) give

$$\|\varphi_1^-\|_E \leq K_2(\nu)\|\varphi_1^+\|_{L^2}. \tag{5.10}$$

Finally, (5.10) gives

$$\sigma_1(\Phi^+) = \inf_{\substack{\xi\in\mathbb{C}^N \\ ||\xi||=1}} \left\|\sum_{k=1}^N \xi_k\varphi_k\right\|_{L^2}^2 \leq \|\varphi_1\|_{L^2}^2 \leq C(\nu)\|\varphi_1^+\|_{L^2}^2 = C(\nu)\sigma_1^+(\Phi^+). \tag{5.11}$$

Lemma 5.1 is proved. □

We are now ready to prove Lemma 2.5.

Using once again the $\mathcal{U}(N)$ invariance, we just have to consider $\Phi^+ \in A^+$ such that, denoting $\Phi = \Phi^+ + \Phi^-$, $\Phi^- = h_{\nu,p}(\Phi^+)$, the following holds:

$$\mathrm{Gram}(\Phi) = \mathrm{Diag}(\sigma_1, \dots, \sigma_N), 0 < \sigma_1 \leq \dots \leq \sigma_N < 1. \tag{5.12}$$

We want to find $X \in (E^+)^N$ satisfying (2.22), assuming that $\Delta(\Phi^+) = \det \mathrm{Gram}\ \Phi^+$ is in $[d(\nu), 2d(\nu)]$. We choose

$$X = (\varphi_1^+, 0, \dots, 0). \tag{5.13}$$

Obviously,

$$\Delta'(\Phi^+) \cdot X = 2\Delta(\Phi^+) > 0. \tag{5.14}$$

Since $\mathcal{F}'_{\nu,p}(\Phi^+)\cdot(\chi^-,0,\dots,0)=0, \forall\chi^-\in E^-$, we may write

$$I'_{\nu,p}(\Phi^+)\cdot X = \mathcal{F}'_{\nu,p}(\Phi)\cdot(\varphi_1^+-\varphi_1^-,0,\dots,0) \tag{5.15}$$
$$= 2\Big(\varphi_1^+, H^\nu_{\Phi_1}\varphi_1^+\Big)_{L^2} - 2\Big(\varphi_1^-, H^\nu_{\Phi_1}\varphi_1^-\Big)_{L^2}$$
$$- 2e_p(\sigma_1)\Big(||\varphi_1^+||^2_{L^2} - ||\varphi_1^-||^2_{L^2}\Big).$$

From inequality (1.7), we have

$$\begin{cases}(\varphi^+, H^\nu_{\Phi_1}\varphi^+)_{L^2} \ge (1-\frac{(\pi/2+2/\pi)\alpha Z}{2})||\varphi^+||^2_E, \forall\varphi^+\in E^+,\\ -(\varphi^-, H^\nu_{\Phi_1}\varphi^-)_{L^2} \ge (1-\frac{(\pi/2+2/\pi)\alpha(N-1)}{2})||\varphi^-||^2_E, \forall\varphi^-\in E^-.\end{cases} \tag{5.16}$$

As a consequence,

$$I'_{\nu,p}(\Phi^+)\cdot X \ge 2\Big[1-\frac{(\pi/2+2/\pi)\,\alpha\,\max(Z,N-1)}{2} - e_p(\sigma_1)\Big]\|\varphi_1^+\|^2_E. \tag{5.17}$$

But $e_p(x)=\dfrac{x^p}{1-x}\le\dfrac{x}{1-x}=e_1(x)$ is small when $x>0$ is small. Moreover, by assumption, $\frac{(\pi/2+2/\pi)\,\alpha\,\max(Z,N-1)}{2}<1$.
From Lemma 5.1,

$$\Delta(\Phi^+)\le\sigma_1(\Phi^+)\le C(\nu)\sigma_1^+(\Phi^+)\le C(\nu)\Big[\Delta(\Phi^+)\Big]^{\frac{1}{N}}. \tag{5.18}$$

Lemma 2.5 is now an immediate consequence of (5.14), (5.17) and (5.18).

Our goal now is to prove Lemma 2.6. We start with a "linear" result that will give us the lower bound $\underline{a}(j)$ in (2.30).

Lemma 5.2. *Assume that $\alpha Z<\frac{2}{\pi/2+2/\pi}$. Then there is a nondecreasing sequence $\{\lambda_j, j\ge 0\}$ in $(0,1)$, with $\lim_{j\to\infty}\lambda_j=1$, and a sequence $\{G_j, j\ge 0\}$ of complex vector subspaces of E^+, with $\dim_{\mathbb{C}}(E^+/G_j)=j$, and*

$$\Big(\varphi^+, (H_0-\alpha Z\,(\mu * V))\,\varphi^+\Big)_{L^2}\ge\lambda_j\|\varphi^+\|^2_{L^2},\quad\forall\varphi^+\in G_j. \tag{5.19}$$

Proof. The arguments below are classical (see [46], 112-117 for a similar situation). The operator $T=\Lambda^+(H_0-\alpha Z\,(\mu*V))\,\Lambda^+$, defined as a Friedrichs extension, is self-adjoint on $\Lambda^+(L^2)$ and has essential spectrum $\sigma_{ess}(T)=[1,+\infty)$. Indeed, the arguments used in [18] to prove the result when μ is a Dirac mass, extend to the more general case. From (1.7), $\sigma(T)\subset(0,\infty)$. As a consequence, $\sigma(T)\cap(-\infty,1)$ consists only of positive eigenvalues with finite multiplicity. One can easily prove, using the Rayleigh quotients, that $\sigma(T)\cap(-\infty,1)=\{\lambda_j, j\ge 0\}$, with $0<\lambda_0\le\cdots\le\lambda_j\le\dots, \lim_{j\to\infty}\lambda_j=1$. Let G_j be the orthogonal space, for the L^2-hermitian product, of

$$K_j=\bigoplus_{k\le j-1}\mathrm{Ker}(T-\lambda_k I_{E^+}). \tag{5.20}$$

Obviously, $E^+/G_j\approx K_j$ has complex dimension j, and (5.19) holds. □

We now construct the space F_j, and we find the upper bound $\overline{a}(j)$.

Lemma 5.3. *Assume that* $\alpha(3N-1) < \frac{2}{\pi/2+2/\pi}, N < 2Z+1$. *There is a sequence* $\{\overline{a}(j), j \geq 0\}$ *in* $(0,N)$ *and a sequence* $\{F_j, j \geq 0\}$ *of complex vector subspaces of* E^+, *with* $\dim_{\mathbb{C}} F_j = j+N$, *and*

$$I_{\nu,p}(\Phi^+) \leq \overline{a}(j), \forall \Phi^+ \in \Big(F_j\Big)^N \cap A^+. \tag{5.21}$$

Proof. Our arguments will be similar to those in the proof of Lemma 2.4, but simpler. We consider the space $W_{d,\lambda}$ of functions ψ of the form (4.40), with λ fixed and $f \in V_d$ arbitrary. We denote $W^+_{d,\lambda} = \Lambda^+(W_{d,\lambda})$. From (4.44), for λ large enough,

$$\dim_{\mathbb{C}} W^+_{d,\lambda} = \dim_{\mathbb{C}} W_{d,\lambda} = d. \tag{5.22}$$

From (4.37), for any $\Phi \in \Big(W_{d,\lambda}\Big)^N$, such that Gram $\Phi \leq 2\Big(\delta_{k\ell}\Big)$,

$$\begin{aligned}\mathcal{E}_\nu(\Phi) = &\sum_k (\varphi_k, H_0\varphi_k) - \alpha Z\,(\varphi_k, (\mu * V_\nu)\,\varphi_k)_{L^2} \\ &+\frac{\alpha}{2}\sum_{k\neq\ell}\iint V_\nu(x-y)\Big\{|\varphi_k(x)|^2|\varphi_\ell(y)|^2 \\ &-\big(\varphi_k(x),\varphi_\ell(x)\big)\big(\varphi_\ell(y),\varphi_k(y)\big)\Big\} \\ \leq &\sum_k\Big(\varphi_k, \Big(H_0 + \frac{\alpha}{2}(N-1)V_\nu\Big)\varphi_k\Big)_{L^2} - \sum_k \alpha Z\,(\varphi_k, (\mu * V_\nu)\,\varphi_k)_{L^2}\,.\end{aligned} \tag{5.23}$$

Moreover, using inequalities (1.7) and (1.9), one can find two constants $a, b > 0$ such that

$$\begin{aligned}|\mathcal{E}'_\nu(\Phi).\Psi^-| \leq\; & a\Big(\sum_k \|\nabla\varphi_k\|^2_{L^2}\Big)^{1/2}\Big(\sum_k \|\psi^-_k\|^2_{L^2}\Big)^{1/2} + \\ &+ b\Big(\sum_k \|\varphi^-_k\|^2_E\Big)^{1/2}\Big(\sum_k \|\psi^-_k\|^2_E\Big)^{1/2},\end{aligned} \tag{5.24}$$

where $\varphi^+_k = \Lambda^+\varphi_k, \varphi^-_k = \Lambda^-\varphi_k$, and $\Psi^- \in (E^-)^N$ is arbitrary. Now, we take $\Phi^+ = (\varphi^+_1, \ldots, \varphi^+_N) \in (W^+_{\lambda,d})^N \cap A^+$.

We recall that $A^+ = \{\Phi^+ \in (E^+)^N \,/\, 0 < \mathrm{Gram}\Phi^+ < \mathbb{1}\}$. From (4.44), for λ large enough, there is $\Phi \in (W_{\lambda,d})^N$, such that $\Lambda^+\varphi_k = \varphi^+_k$ $(\forall k)$ and $\mathrm{Gram}(\Phi) \leq 2(\delta_{k,\ell})$.

Since $\pi_p \geq 0$, we may write

$$I_{\nu,p}(\Phi^+) \leq \mathcal{E}_\nu\Big(\Phi^+ + h_{\nu,p}(\Phi^+)\Big) \leq \sup_{\Psi^- \in (E^-)^N} \mathcal{E}_\nu(\Phi + \Psi^-). \tag{5.25}$$

Combining (5.24), (5.25) and Lemma 4.1, we get, for some $a' > 0$,

$$I_{\nu,p}(\Phi^+) \leq \mathcal{E}_\nu(\Phi) + a'\sum_k \|\nabla\varphi_k\|^2_{L^2} + \|\Lambda^-\varphi_k\|^2_E. \tag{5.26}$$

Finally, combining (5.23), (5.26) and the estimates (4.41), . . . , (4.45), we find,

$$I_{\nu,p}(\Phi^+) \leq N\Big(1 - \alpha(2Z - N + 1)\frac{c_*}{2\lambda} + o\left(\frac{1}{\lambda}\right)\Big). \tag{5.27}$$

We take $\overline{\lambda}(d)$ large enough, and $F_j = W^+_{j+N,\bar{\lambda}(j+N)}$. Then (5.27) gives

$$I_{\nu,p}(\Phi^+) \leq \overline{a}(j) < N, \quad \forall \Phi^+ \in (F_j)^N \cap A^+. \tag{5.28}$$

From (5.22), $\dim_{\mathbb{C}} F_j = j + N$, so Lemma 5.3 is proved. □

We are now ready to prove Lemma 2.6.

We take F_j as in Lemma 5.3. Obviously,

$$\begin{aligned} c_{\nu,p}(F_j) = \inf_{Q\in\mathcal{Q}(F_j)} \max_{\Phi^+\in Q} J_{\nu,p}(\Phi^+) \leq \\ \leq \max_{\Phi^+\in(F_j)^N\cap A^+} J_{\nu,p}(\Phi^+) \leq \overline{a}(j), \end{aligned} \tag{5.29}$$

where for any F, the class of sets $\mathcal{Q}(F)$ is defined in Section 2, formula (2.28). To find a lower estimate on $c_{\nu,p}(F_j)$, we define

$$S_j = \Big\{\Phi^+ \in (G_j)^N \;/\; \mathrm{Gram}\,\Phi^+ = \frac{j+1}{j+2}\mathbb{1}\Big\}. \tag{5.30}$$

Take $\Phi^+ \in S_j$. From Lemma 5.2, we have

$$\mathcal{E}_\nu(\Phi^+) \geq \sum_k \Big(\varphi_k, (H_0 - \alpha Z\,(\mu * V_\nu))\,\varphi_k\Big) \geq N\frac{j+1}{j+2}\lambda_j. \tag{5.31}$$

So there is $p(j)$ such that, if $p \geq p(j)$, then

$$\pi_p\Big(\frac{j+1}{j+2}\mathbb{1}\Big) = N(j+2)\Big(\frac{j+1}{j+2}\Big)^p \leq \frac{1}{j+2}\mathcal{E}_\nu(\Phi^+).$$

Together with (5.31), this gives

$$I_{\nu,p}(\Phi^+) \geq \mathcal{E}_\nu(\Phi^+) - \pi_p(\Phi^+) \geq N\left(\frac{j+1}{j+2}\right)^2 \lambda_j. \tag{5.32}$$

We choose $\underline{a}(j) = N\left(\frac{j+1}{j+2}\right)^2 \lambda_j$. Obviously, $\lim_{j\to\infty} \underline{a}(j) = N$, and Lemma 2.6 is an immediate consequence of the following intersection result:

Lemma 5.4. *For any $Q \in \mathcal{Q}(F_j)$, the intersection $Q \cap S_j$ is non-empty.*

Proof of Lemma 5.4 (hence of Lemma 2.6). The quotient set $S_j/\mathcal{U}(N)$ is a submanifold of the Hilbert manifold $A^+/\mathcal{U}(N)$, and

$$\begin{aligned} \mathrm{codim}_{\mathbb{R}}\Big(S_j/\mathcal{U}(N), A^+/\mathcal{U}(N)\Big) &= \mathrm{codim}_{\mathbb{R}}\Big(S_j, (E^+)^N\Big) = \\ N^2 + \mathrm{codim}_{\mathbb{R}}\Big((G_j)^N, (E^+)^N\Big) &= N\Big(2j + N\Big). \end{aligned} \tag{5.33}$$

Take $\epsilon > 0$ small, and define

$$\mathcal{M}_j(\epsilon) = \Big\{\Phi^+ \in (F_j)^N \cap A^+/\det(\mathrm{Gram}\;\Phi^+)\det(\mathbb{1} - \mathrm{Gram}\;\Phi^+) \geq \epsilon\Big\}. \tag{5.34}$$

$\mathcal{M}_j$ is a manifold with boundary, and

$$\dim_{\mathbb{R}} \mathcal{M}_j = \dim_{\mathbb{R}}(F_j)^N = 2N(j + N).$$

If h is "admissible", then, from (2.27) and by continuity of h, there is $\epsilon_h > 0$ such that

$$h\Big([0,1] \times \partial\mathcal{M}_j(\epsilon_h)\Big) \cap S_j = \emptyset. \tag{5.35}$$

Now, $\mathcal{M}_j/\mathcal{U}(N)$ is a submanifold (with boundary) of $A^+/\mathcal{U}(N)$, and

$$\begin{aligned}\dim_{\mathbb{R}}\mathcal{M}_j/\mathcal{U}(N) &= \dim_{\mathbb{R}}\mathcal{M}_j - \dim_{\mathbb{R}}\mathcal{U}(N)\\ &= N(2j + N) = \operatorname{codim}_{\mathbb{R}}\big(S_j/\mathcal{U}(N), A^+/\mathcal{U}(N)\big).\end{aligned} \tag{5.36}$$

Perturbing slightly F_j if necessary, we may impose that F_j and G_j intersect transversally. Their intersection is then a complex subspace H_j of E^+, of dimension N, and $S_j/\mathcal{U}(N)\cap \mathcal{M}_j/\mathcal{U}(N)$ is a transverse intersection of cardinal 1. Its unique element is the $\mathcal{U}(N)$ class of bases $(\varphi_1^+, \ldots, \varphi_N^+)$ of H_j, such that Gram $(\varphi_1^+, \ldots, \varphi_N^+) = \frac{j+1}{j+2}\mathbb{1}$. So the intersection index of $S_j/\mathcal{U}(N)$ and $\mathcal{M}_j/\mathcal{U}(N)$ (mod 2) is 1. From (5.35), we also have

$$I_{\mathbf{Z_2}}\left(S_j/\mathcal{U}(N), h(1, \mathcal{M}_j)/\mathcal{U}(N)\right) = 1. \tag{5.37}$$

So S_j intersects $Q = h\left(1, D(F_j)\right)$, and Lemma 5.4 (hence Lemma 2.6) is proved. □

This ends the proof of Theorem 1.2.

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