A mean-field model in Quantum Electrodynamics*

Julien Sabin

January 8, 2010

*M2 Internship spent under the direction of Mathieu Lewin (Cergy/CNRS) at the University Paris-Dauphine, from May 2009 to–

Contents

1 Introduction

Quantum Electrodynamics (or QED) is a branch of Quantum Field Theory which modelizes more particularly the interactions between matter and light. It has been mainly developed by Dyson, Feynman, Schwinger, and Tomonaga. These last three's contribution has even been awarded by a Nobel prize in 1965. It is a theory with an unknown number of particles which has a remarkable ability of numerical prediction, even if its mathematical background is yet to be found. A perturbative approach leads to very accurate results but there is still no satisfying variational formulation of QED. Therefore, we will introduce in this paper a mean-field approximation of QED which is fully non-perturbative. It has been developed by Hainzl, Lewin, Séré and Solovej [HLS05b, HLS07, HLS09, HLS05a] after the influence of Chaix, Iracane, and Lions [CI89, CIL89] and the previous works of Bach, Barbaroux, Helffer and Siedentop [BBHS99]. A review of these results can be found in [Lew09].

The model we are going to describe is an approximation of the full QED, where we will neglect photons and where there is no magnetic field. As a consequence, we cannot expect any quantitative resut from this approach since most of the physical effects are due to the presence of photons. However, many qualitative aspects of Quantum Field Theory are present in this theory, such as renormalization. It is therefore of interest to study such a model. Finally, a variational formulation may be interesting algorithm-wise, since we minimize a functional.

1.1 The inner difficulties of relativistic models

There exists several ways to establish a N-body relativistic quantum model. First of all, it seems quite natural to try to adapt the non-relativistic theory to the relativistic case. The energy operator (or *Hamiltonian*) of N non-relativistic quantum particles moving in $\mathbb{R}^3$ acts on $L^2(\mathbb{R}^3;\mathbb{C})^{\otimes N}$. It can be written

$$H_N = \sum_{i=1}^{N}(E_i^k + V_i) + \sum_{i\neq j}\Omega_{ij},$$

where E_i^k represents the kinetic energy of the i-th particle, V_i its potential energy, and Ω_{ij} the interaction between the particles i and j (Coulombian for instance). The state of a N-body quantum system is represented in a general manner by a function $\psi \in L^2(\mathbb{R}^3;\mathbb{C})^{\otimes N}$ of norm 1, called the *wave function* of this quantum system. As it is, it does not represent anything physically but contains all the information of the considered quantum system. Indeed, the quantity $|\psi(x_1,\dots,x_N)|^2\mathrm{d}x_1\dots\mathrm{d}x_N$ represents the probability to find the first particle in position $x_1 \in \mathbb{R}^3$ with $\mathrm{d}x_1$ for error, the second in x_2 with $\mathrm{d}x_2$ for error, and so on. More precisely, $|\psi|^2$ represent the presence probability density of the particle. Conversely, the square norm of the Fourier transform $|\widehat{\psi}(p)|^2$ is the probability density of momentum p for the particle. The non-relativistic kinetic energy operator of the particle i is then

$$E_i^k : \psi \mapsto -\frac{1}{2m_i}\Delta_{x_i}\psi,$$

where m_i is the mass of the i-th particle, and Δ_{x_i} is the Laplacian with respect to the variable $x_i \in \mathbb{R}^3$. In the relativistic case, the one-particle energy operator does not act on $L^2(\mathbb{R}^3;\mathbb{C})$ anymore, but on $L^2(\mathbb{R}^3;\mathbb{C}^4)$, and is written

$$D_c := -ic\boldsymbol{\alpha}\cdot\nabla + mc^2\beta = -ic\sum_{k=1}^{3}\alpha_k\partial_k + mc^2\beta.$$

The α_k and the β are 4×4 self-adjoint matrices, c is the speed of light, m is the mass of the considered particle, i is the complex number, and ∇ the gradient operator. More precisely,

$$\beta = \begin{bmatrix} I_2 & 0 \\ 0 & -I_2 \end{bmatrix}, \quad \alpha_k = \begin{bmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{bmatrix},$$

where the $(\sigma_k)_{k=1,2,3}$ are the Pauli matrices defined by

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

This operator has been introduced by Dirac, and his particularity lies in its spectrum which is nothing but

$$\sigma(D_c) = (-\infty; -mc^2] \cup [mc^2; +\infty),$$

where the non-relativistic spectrum is

$$\sigma(-\Delta) = [0; +\infty).$$

This difference is fundamental. Indeed, according to a quantum mechanics postulate, the energy of a quantum system can only be an element of the Hamiltonian's spectrum. Furthermore, the study of the state of lowest energy the system can reach (or *ground state*) is of the greatest importance for the understanding of the stability of matter. In the non-relativistic case, the kinetic energy operator is bounded from below, and so is the total Hamiltonian under some conditions. We are therefore capable of proving the stability of a non-relativisitic molecule. However, the relativistic kinetic energy is not bounded from below, even for one body. Also, there is no state of lowest energy and one has to adapt the model.

Remark 1.1. *Dirac chose this operator for several reasons. He wanted first an operator which verifies*

$$(D_c)^2 = -c^2\Delta + m^2c^4,$$

in order to adapt the classical relativistic formula $E^2 = c^2p^2 + m^2c^4$ with the quantum correspondance $p \leftrightarrow -i\nabla$. This relation explains the form of the spectrum of D_c. Moreover Dirac was looking for a local operator, that is a polynomial in the spatial derivatives. Since $(D_c)^2$ is of order two, Dirac looked for an operator of order one. However, the lowest dimension where these equations have a solution is 4. That's why the (α_k) and β are 4×4 matrices. The fact that wave functions must then have 4 components is relevant physically: it may be interpreted as the spin (up or down) distinction and the matter/antimatter (electron/positron) distinction. One may be careful with the notion of positron which is not really clear though, but this distinction remains of first importance.

Remark 1.2. *If one ignores the negative part of the Dirac operator's spectrum, one can see that it corresponds to a well-known relativistic result: an electron cannot have a kinetic energy lower than mc^2, which is its mass energy.*

Dirac's idea was to interpret the form of his spectrum in the following way. Even if negative kinetic energy elecrons are not observable, Dirac conjectured the existence of "virtual" electrons which occupy the negative kinetic energy states of his operator. Moreover, the Pauli principle forbids two different electrons to occupy the same energy state. Therefore, a "real" electron could not have a negative kinetic energy since all these states should be already occupied by "virtual" electrons. This interpretation gives a chance to develop a relativistic theory relevant

from a variational point of view, that is where the ground state actually minimizes the energy of the system.

These negative kinetic energy electrons are usually refered to as the *Dirac sea*. One may infer that if we give to one of these electrons an energy greater than $2mc^2$, it may have a positive energy and change side of the spectrum. A hole would then be created in the negative spectrum, and such a hole would have a positive energy with respect to the Dirac sea. This positive energy pair of a "virtual" particle which becomes an electron by switching to the positive side of the spectrum and the hole thus created is called an *electron/positron* pair. Dirac actually predicted their existence:

> Admettons que dans l'Univers tel que nous le connaissons, les états d'energie négative soient presque tous occupés par des électrons, et que la distribution ainsi obtenue ne soit pas accessible à notre observation à cause de son uniformité dans toute l'étendue de l'espace. Dans ces conditions, tout état d'energie négative non occupé représentant une rupture de cette uniformité, doit se révéler à l'observation comme une sorte de lacune. Il est possible d'admettre que ces lacunes constituent les positrons.
>
> Dirac, P.A.M.: Théorie du Positron, *Solvay Report XXV*, pp. 203-212, 1934.

Remark 1.3. *Notice the importance given by Dirac to the* uniform *aspect of the Dirac sea, which makes it not observable. Later on, we will characterize this property by the term* translation invariant*, and notice that the vacuum we will build satisfies this property which is physically relevant.*

This idea allows a better understanding of the one-particle Dirac operator. However, we cannot adapt this interpretation when we deal with several bodies. For instance, let us consider a two-body system, without external potential and where interactions are neglected. The Hamiltonian of this sytem described by a wave function in $L^2(\mathbb{R}^3;\mathbb{C}^4)\otimes L^2(\mathbb{R}^3;\mathbb{C}^4)$ is

$$H_2 = D_c \otimes \mathrm{Id} + \mathrm{Id} \otimes D_c,$$

where Id is the identity operator of $L^2(\mathbb{R}^3;\mathbb{C}^4)$. We can deduce the spectrum of H_2 with respect to the one of D_c. Indeed, one can easily see that for operators A, B,

$$\sigma(\mathrm{Id} \otimes A + B \otimes \mathrm{Id}) = \sigma(A) + \sigma(B).$$

So that $\sigma(H_2) = \sigma(D_c) + \sigma(D_c) = \mathbb{R}$. The two-body energy operator spectrum allows any energy level, and Dirac's interpretation is not clear anymore: shall we again fill all the negative energy states, in which case the energy of a molecule would be always positive and thus there would be no bound state for electrons attracted by a nucleus? Shall we then fill only some of the negative energy states? If we do, which ones? One may realize the issues involved by such choices, both mathematically and physically speaking. We thus have to choose another model.

There are many consequences of Dirac's interpretation. First of all, the fact that the Dirac sea is by default filled by infinitely many particles, though virtual, implies that this sea has infinite charge and energy. We may overcome this difficulty by redefining the energy, the charge, or any other physical quantity by its value with respect to the Dirac sea. From a physical point of view, it is not shocking since this sea is not obsvervable and thus all the measures are done with respect to a state of reference, the one of the vacuum present by default. Furthermore, we may notice that virtual particles must interact with the real ones. Also, the study of a quantum system in the vacuum should always take into account infinetely many particles. The functional work space should thus be modified. Finally, these vacuum particles should also feel the influence of an electromagnetic external field as any charged particle. We call this phenomenon the *vacuum polarization*, which has already been observed experimentally.

1.2 Infinitely many-body models

As we have seen, QED must deal with infinitely many particles. Speaking differently, a state of the system can have an infinite number of particle. We thus have to define a functional space which allows states with an infinite number of particles. If $\mathfrak{h}$ denotes the Hilbert space describing the one-particle states, then the N-body fermionic Hilbert space is

$$\mathfrak{h}_N := \bigwedge_{i=1}^{N} \mathfrak{h},$$

which is the $\mathbb{C}$-vector space spanned by the Slater determinants of the form $\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_N}$, where the (φ_i) are a Hilbertian basis of $\mathfrak{h}$. Physically, it means that the first particle is in the state φ_{i_1}, the second in the state φ_{i_2} and so on. We call it "fermionic" because fermions are particles which satisfy the Pauli principle, ie two different fermions cannot be in the same state. Indeed, if two fermions are both in the state φ, we can see that the Slater determinant $\cdots \wedge \varphi \wedge \cdots \wedge \varphi \wedge \cdots = 0$. Therefore the Pauli principle is kind of implemented in the building of the N-body space.

Example 1.1. *If $\mathfrak{h} = L^2(\mathbb{R}^3; \mathbb{C})$, then $\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_N}(x_1, \ldots, x_N) = \det(\varphi_{i_k}(x_l))_{1 \leqslant k,l \leqslant N}$, hence the name Slater determinant.*

We then define the Fock space $\mathcal{F}$, which contains all the N-particles spaces,

$$\mathcal{F} := \bigoplus_{N=0}^{\infty} \mathfrak{h}_N.$$

Here we have taken the definition $\mathfrak{h}_0 := \mathbb{C}$.

Usually, the state of a system in quantum mechanics is a normalized vector of the underlying Hilbert space, here $\varphi \in \mathcal{F}, \|\varphi\|_{\mathcal{F}} = 1$. In the following, we will use the usual "bra-ket" notation, where $|\varphi\rangle$ denotes the vector φ and $\langle\varphi|$ denotes the linear form $|\psi\rangle \mapsto \langle\varphi|\psi\rangle_{\mathcal{F}}$, where $\langle\cdot|\cdot\rangle_{\mathcal{F}}$ is the scalar product in the Fock space. For instance, the notation $|\varphi\rangle\langle\varphi|$ denotes the orthogonal projector on $\mathrm{span}(\varphi)$, that is the map $|\psi\rangle \mapsto \langle\varphi|\psi\rangle_{\mathcal{F}}|\varphi\rangle$. In this study we will use a larger class of states, defined for instance in [BLS94].

Definition 1.1. *Let $\mathcal{B}(\mathcal{F})$ denote the set of all bounded operators on $\mathcal{F}$. Then a* **state** *Ω is a linear form on $\mathcal{B}(\mathcal{F})$ satisfying $\Omega(Id) = 1$ and $\Omega(A^*A) \geqslant 0$ for all $A \in \mathcal{B}(\mathcal{F})$.*

Example 1.2. *Any $\varphi \in \mathcal{F}$ normalized can be seen as such a state by the map $A \mapsto \langle\varphi|A\varphi\rangle_{\mathcal{F}}$. Such states are called* pure states. *That is why this definition is a generalization of the usual concept of state.*

We also recall the following quantum mechanics postulate. For any physical quantity a (position, momentum, energy,...) corresponds a selfadjoint operator A on the underlying Hilbert space. For instance, we saw that the corresponding operator for the energy is the Hamiltonian operator. If the state of the system is a vector φ of the Hilbert space, then the average value (or *expectation value*) of a for the system is $\langle\varphi|A\varphi\rangle$. If Ω is a state as defined earlier, then the expectation value of a is $\Omega(A)$.

1.3 Mean-field (Hartree-Fock) approximation

In this study, we will focus on the problem of finding the fundamental state of a given Hamiltonian. However, this goal is quite difficult to attain even in an N-body non-relativistic theory.

Numerical issues have led to consider a simpler problem where we minimize the energy over a smaller set.

More precisely, let us take the example of a N electrons system. The Pauli principle imposes the wave function describing the system to be antisymmetric, so that the work space is not $L^2(\mathbb{R}^3;\mathbb{C})^{\otimes N}$ but $L^2(\mathbb{R}^3;\mathbb{C})^{\wedge N}$. The average energy of a N-body quantum system in the state ψ is given by

$$E^N(\psi) = \langle H_N\psi, \psi\rangle,$$

where we recall that H_N denotes the N-body Hamiltonian. The search for a ground state consists in solving the following minimization problem

$$E_0^N := \inf_{\substack{\psi\in L^2(\mathbb{R}^3;\mathbb{C})^{\wedge N}\\ \|\psi\|=1}} E^N(\psi).$$

A minimizer for this problem is called a *ground state*. The mean-field approximation called *Hartree-Fock* chooses to pose this problem on a subset of $L^2(\mathbb{R}^3;\mathbb{C})^{\wedge N}$. Indeed, we only consider functions given by a single Slater determinant, that is functions of the form $\psi_1\wedge\cdots\wedge\psi_N$ where $\psi_i \in L^2(\mathbb{R}^3;\mathbb{C})$, $\|\psi\| = 1$. Such states are called *Hartree-Fock* states. This approximation seems simpler since we drastically limit the test functions, but one has to notice that the set of minimization is *not* linear, so that the model becomes non-linear.

One can show that for such states, the energy only depends on the orthogonal projector on $\mathrm{span}(\psi_i)$

$$P = \sum_i |\psi_i\rangle\langle\psi_i|.$$

Hartree-Fock theories have been widely studied in other contexts, see [LS77, BLS94].

In the case of QED, we work in a space with an infinite number of particles. We may also define Hartree-Fock states in this space. The key property of such states is that the energy will also only depend of the orthogonal projector on $\mathrm{span}(\psi_i)$. This property is very useful since this projector P acts on the one-body space which is much simpler than the huge Fock space containing all the N-body spaces.

A more precise description of Hartree-Fock states can be found in the appendix.

1.4 The Hainzl, Lewin, Séré and Solovej approach

The model we are going to introduce has been inspired by an article of Chaix and Iracane [CI89]. According to them, the unboundedness from below of the Dirac makes the Dirac interpretation mandatory. The issue is to find the right way to implement this interpretation in the formulation of QED, the aim being to obtain an energy functional which is bounded from below. Hainzl, Lewin, Séré and Solovej propose the following method, which generalizes in a way the work of Chaix and Iracane. The first step is to define what is the vacuum, which will be a fixed reference state for all the measures of physical quantities. According to Dirac, it is made of virtual particles which are not observable. Hainzl, Lewin, Séré and Solovej propose to define the energy in the following way. If $\mathbb{H}^{\mathrm{QED}}$ is the QED Hamiltonian and if $|0\rangle$ is the vacuum, the effective Hamiltonian $\widetilde{\mathbb{H}}^{\mathrm{QED}}$ is defined as

$$\widetilde{\mathbb{H}}^{\mathrm{QED}} := \mathbb{H}^{\mathrm{QED}} - \langle 0|\mathbb{H}^{\mathrm{QED}}|0\rangle.$$

There is several issues with this method. First, one has to choose a right reference for the vacuum. The choice of Chaix and Iracane is the spectral projector of the Dirac operator $P^0 := \chi_{(-\infty;0]}(D)$, which corresponds to the choice of Dirac. In this study, we will motivate the

choice of this vacuum as the minimizer of a certain energy, such that the Dirac interpretation is not an input but a consequence of the theory. Note that in the work of Hainzl, Lewin, Séré and Solovej, the energy they define is different from the one we will choose in this study, so that P^0 is not their choice for a reference state. Secondly, we have to give a sense to the expression $\langle 0|\mathbb{H}^{\mathrm{QED}}|0\rangle$, because we saw that the vacuum had an infinite energy. We will tackle this issue by defining our energy in a box and by obtaining results in the whole space with a method called a *thermodynamic limit*, which consists in studying the limit of the energy and its minimizers as the size of the box grows.

This method has been used by Hainzl, Lewin, Séré and Solovej to develop a variational approach to QED. In this study, we will present this method.

1.5 Presentation of the study

We will proceed as follows:

- In the whole study, a cutoff Λ is fixed in the Fourier domain. This condition is linked to the renormalization of the physical quantities in QED.
- We start by defining the Hamiltonian of QED in a box $C_L := [-L/2; L/2)^3$ from the formal QED Hamiltonian given by Physics. In this context, it is perfectly well defined.
- We then minimize the energy in a box coming from this Hamiltonian to find the *free vacuum* in a box.
- We define an energy per unit volume in the whole space as the limit of the energy in a box for a certain class of states. This energy is minimized and we prove that its minimizer, the *free vacuum* is the limit as $L \to \infty$ of the minimizer in a box. This is the thermodynamic limit. That is how we justify the choice of P^0 as the free vacuum as the limit of the minimizers in a box and as the minimizer of the energy per unit volume in the whole space.
- We now define the energy of any state by measuring it relatively to the energy of the free vacuum. We do it formally, and it can again be justified by a thermodynamic limit. This energy is called the Bogoliubov-Dirac-Fock (BDF) energy.
- We define the right functional setting where we study the BDF energy. Then, we prove that it is bounded from below on this setting.
- We finally study the existence of atoms and molecules in this model, that is minimizing the BDF energy over a set of states with a fixed charge.

2 Derivation of the reduced model

2.1 Formal derivation of the QED energy

From the formal expression of the QED Hamiltonian given by Physics, we will write the formula for the QED energy in the HF approximation. To give a mathematical meaning to this formula, we will see the usefulness of working in a box with a Fourier cutoff. In this case, the derivation can be done in a rigorous manner.

2.1.1 QED Hamiltonian

In Physics, the QED Hamiltonian without photons in Coulomb gauge and in an external electrostatic field φ is formally written as [Sch48]

$$\mathbb{H}^{\varphi} := \int \psi(x)^* D^0 \psi(x)\,\mathrm{d}x + \int \varphi(x)\rho(x)\,\mathrm{d}x + \frac{\alpha}{2}\iint \frac{\rho(x)\rho(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y, \tag{2.1}$$

where $\psi(x)^*$ is the second-quantized field operator and $\psi(x)$ is its adjoint. More precisely, they are four components vectors with operator entries. For each $\sigma \in \{1,\dots,4\}$, $\psi(x)_\sigma$ acts on the Fock space $\mathcal{F}$ by annihilating a particle in position $x \in \mathbb{R}^3$ with spin[1] σ. Conversely, $\psi(x)^*_\sigma$ creates a particle in position x with spin σ. They satisfy the classical anticommutation relations (CAR)

$$\{\psi(x)^*_\sigma \psi(y)_{\sigma'}\} = \delta_{\sigma,\sigma'}\delta_{x,y},$$

where $\{A,B\} = AB + BA$. In (2.1), D^0 is the one-particle Dirac operator which we have introduced before, and $\rho(x)$ is the density operator defined by

$$\rho(x) = \frac{1}{2}\sum_{\sigma=1}^{4} \psi(x)^*_\sigma \psi(x)_\sigma - \psi(x)_\sigma \psi(x)^*_\sigma. \tag{2.2}$$

Finally, α is the (bare) fine structure constant. Notice that in full QED, one must consider photons and possibly an external magnetic field.

Our main goal will be the search for the ground state of this Hamiltonian under some constraints. Here, the ground state is the state of lowest energy. For instance, the ground state with $\varphi = 0$ is called the *free vacuum*, whereas the ground state with $\varphi \neq 0$ is the *polarized vacuum*. If one wants to study atoms and molecules, the ground state must be studied under charge constraints rather than with a fixed number of particles[2].

However, we will not minimize the energy over the whole Fock space in this work since we will study it in the HF approximation.

2.1.2 Hartree-Fock (mean-field) approximation

We will study the QED Hamiltonian (2.1) over a subset of the Fock space which is formed by Hartree-Fock states. These states have the particularity of being fully described by their one-body density matrix $P(x,y)$ defined for any state Ω by

$$P(x,y)_{\sigma,\sigma'} = \Omega\left(\psi(x)^*_\sigma \psi(y)_{\sigma'}\right).$$

For instance, if $\Omega = \varphi_1 \wedge \cdots \wedge \varphi_N$ is a N-particle Slater determinant, $P(x,y) = \sum_i \varphi_i(x)\overline{\varphi_i(y)}^T$. The one-body density matrix defines an operator P on the one-particle space with kernel $P(x,y)$. This operator satisfies $0 \leqslant P \leqslant I$, where I is the identity operator. In the case of a Slater determinant, P is nothing but the orthogonal projector on the subspace spanned by the (φ_i). Notice that the operator P is defined for *any* state and not only Hartree-Fock states.

[1] The term "spin" is used there in a general meaning, as an inner degree of freedom.

[2] Indeed, it is a well-know fact that the QED Hamiltonian does not conserve the number of particles: electron-positron pair creation may occur. That is why an electron is for instance defined as the ground state of this Hamiltonian with the constraint that the system must have a charge $-e$. Moreover, the actual number of particle of a ground state will be infinite whereas the charge is measured relatively to the vacuum so that it will be finite.

For normalization reasons, the main variable of the energy we will consider is not P but $\gamma := P - I/2$, which we call the *renormalized density matrix*. Via the CAR, one may notice that it is equivalent to define γ by

$$\gamma(x,y)_{\sigma,\sigma'} = \frac{1}{2}\Omega\left([\psi(x)^*_\sigma, \psi(y)_{\sigma'}]\right), \tag{2.3}$$

where $[A,B] = AB - BA$. We will precise this choice later.

2.1.3 Hartree-Fock energy

The Hartree-Fock energy for a Hartree-Fock state with (renormalized) density matrix γ can be formally computed as

$$\mathcal{E}^{\varphi}_{\mathrm{HF}}(\gamma) := \mathrm{tr}(D^0\gamma) + \alpha\int \rho_\gamma(x)\varphi(x)\,\mathrm{d}x + \frac{\alpha}{2}\iint \frac{\rho_\gamma(x)\rho_\gamma(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y - \frac{\alpha}{2}\iint \frac{\|\gamma(x,y)\|^2}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y, \tag{2.4}$$

where $\rho_\gamma(x) = \Omega(\rho(x))$ is the density of charge of γ and $\|A\|^2 = \mathrm{Tr}_{\mathbb{C}^4}(A^*A)$ is the Hilbert-Schmidt norm of A. This energy has the following physical interpretation: the term with D^0 measures the kinetic energy of the system, while the term with φ measures its potential energy. The last two terms measure the *self-energy* of the system, that is the interaction energy between the electrons. In the third term (or direct term), the density of charge ρ_γ interacts with itself through a Coulomb potential. The last term (or exchange term) is a compensation term taking into account the fact that a particle cannot interact with itself.

For the sake of simplicity, we will consider in this study the HF energy when we drop the exchange term. We will however shortly explain how to deal with the complete model (see remark 3.1).

Our first goal will consist in giving a precise mathematical meaning to this energy. As it is written in (2.4), it is not properly defined. Indeed, if P is an orthogonal projector on an infinite dimensional subspace, $\gamma = P - I/2$ is never compact and therefore D^0P is not trace-class. The approach proposed in this study, following [HLS07], is to give a rigourous mathematical meaning to this energy by confining the system in a box $C_L := [-L/2; L/2)^3$ with a cutoff Λ in the Fourier domain. Afterwards, the energy for a system in the whole space will be obtained as a *thermodynamic limit* of the energy in a box when $L \to \infty$. During the thermodynamic limit, we will keep the cutoff Λ, which is actually necessary for a variational formulation of QED [HLS05b, Theorem 2]. Actually, it has been predicted by Landau *et al* that the limit $\Lambda \to \infty$ does not, as such, make sense from a physical point of view. It has also been argued by Dirac in [Dir34] that QED could only be valid up to a certain level of energy, so that the introduction of such a cutoff is justified.

2.2 Rigourous derivation of the QED energy in a box

2.2.1 Notations

We will use the same notations as in [HLS07]. In order to confine the system in the box $C_L := [-L/2; L/2)^3$, we first have to restrain the one-body space from $L^2(\mathbb{R}^3;\mathbb{C}^4)$ to $L^2(C_L;\mathbb{C}^4)$. Furthermore, we choose to add periodic boundary conditions so that the one-body space is in fact $L^2(\mathbb{T}_L;\mathbb{C}^4)$ where $\mathbb{T}_L$ is the torus $\mathbb{R}^3/(L\mathbb{Z}^3)$. Then, any function $\varphi \in L^2(\mathbb{T}_L;\mathbb{C}^4)$ can be written by Fourier transform

$$\varphi(x) = \left(\frac{2\pi}{L}\right)^{3/2} \sum_{k\in(2\pi/L)\mathbb{Z}^3} \widehat{\varphi}(k) e_k(x),$$

where $e_k(x) := e^{ik\cdot x}/L^{3/2}$. The Fourier cutoff Λ is implemented by replacing $L^2(\mathbb{T}_L;\mathbb{C}^4)$ to its following finite-dimensional subspace

$$\mathfrak{H}_\Lambda^L := \mathrm{span}\left\{\varepsilon_\sigma e_k\,;\, k\in\Gamma_\Lambda^L, \sigma\in\{1,\dots,4\}\right\},$$

where

$$\Gamma_\Lambda^L := (2\pi/L)\mathbb{Z}^3\cap B(0,\Lambda),$$

and $(\varepsilon_\sigma)_{\sigma=1,\dots,4}$ is the canonical basis of $\mathbb{C}^4$.

Remark 2.1. *This a key fact for the definition of the model that $\mathfrak{H}_\Lambda^L$ is finite-dimensional.*

With this definition of the coefficients $\widehat{\varphi}(k)$ we have the following Parseval equality

$$\langle\varphi,\psi\rangle_{L^2(\mathbb{T}_L;\mathbb{C})} = \left(\frac{2\pi}{L}\right)^3 \sum_{k\in\Gamma_\Lambda^L} \widehat{\varphi}(k)\overline{\widehat{\psi}(k)}, \tag{2.5}$$

and the following convolution equality

$$\widehat{\varphi\star\psi}(k) = (2\pi)^{3/2}\widehat{\varphi}(k)\widehat{\psi}(k). \tag{2.6}$$

Definition 2.1 (Kernel operators)**.** *Let (X,μ) be a measured space. An operator Q on $L^2(X,\mu)$ is a **kernel operator** if there exists $q\in L^2(X\times X)$ so that for every $f\in L^2(X,\mu)$ we have*

$$Qf(x) = \int_X q(x,y)f(y)\,d\mu(y).$$

*The function q is called the **kernel** of the operator Q.*

Remark 2.2. *For the sake of simplicity, we will often denote the operator and its kernel by the same letter, but we have to keep in mind that they are not the same mathematical objects.*

Any operator Q on $\mathfrak{H}_\Lambda^L$ has a matrix kernel of the form

$$Q(x,y) = \sum_{k,\ell\in\Gamma_\Lambda^L} \widehat{Q}(k,\ell)e_k(x)\overline{e_\ell(y)},$$

where $\widehat{Q}(k,\ell)$ is a 4×4 matrix defined by the following decomposition on the Fourier basis

$$Q(\varepsilon_\sigma e_k) = \sum_{\sigma'=1}^4 \sum_{\ell\in\Gamma_\Lambda^L} \widehat{Q}(k,\ell)_{\sigma'\sigma}\varepsilon_{\sigma'}e_\ell. \tag{2.7}$$

Definition 2.2 (Density of an operator)**.** *Let Q be an operator on $\mathfrak{H}_\Lambda^L$. Its **density** ρ_Q is then defined as*

$$\rho_Q(x) := \mathrm{Tr}_{\mathbb{C}^4}\left(Q(x,x)\right). \tag{2.8}$$

We have the following useful lemma:

Lemma 2.1. *Let Q be any operator on $\mathfrak{H}_\Lambda^L$. Then we have the equality*

$$\int_{\mathbb{T}_L}\rho_Q(x)dx = \mathrm{tr}(Q). \tag{2.9}$$

Proof. Any operator Q on $\mathfrak{H}_\Lambda^L$ has a matrix kernel of the form

$$Q(x,y) = \sum_{k,\ell \in \Gamma_\Lambda^L} \widehat{Q}(k,\ell) e_k(x) \overline{e_\ell(y)}, \tag{2.10}$$

From (2.10) we have on the one hand

$$\begin{aligned} \int_{\mathbb{T}_L} \mathrm{Tr}_{\mathbb{C}^4}\left(Q(x,x)\right) \mathrm{d}x &= \sum_{k,\ell \in \Gamma_\Lambda^L} \mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{Q}(k,\ell)\right) \langle e_k, e_\ell \rangle_{L^2(\mathbb{T}_L;\mathbb{C})} \\ &= \sum_{k \in \Gamma_\Lambda^L} \mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{Q}(k,k)\right). \end{aligned}$$

On the other hand, from (2.7), we have

$$\mathrm{tr}(Q) := \sum_{\sigma=1}^{4} \sum_{k \in \Gamma_\Lambda^L} \langle Q(e_k \varepsilon_\sigma), e_k \varepsilon_\sigma \rangle = \sum_{\sigma=1}^{4} \sum_{k \in \Gamma_\Lambda^L} \widehat{Q}(k,k)_{\sigma\sigma} = \sum_{k \in \Gamma_\Lambda^L} \mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{Q}(k,k)\right).$$

□

Remark 2.3. *Note that the equality (2.9) is non-trivial in the whole space (because then we are not in a finite dimensional setting), and it will have its importance later. Note that this lemma holds in the case of trace-class operators.*

Definition 2.3 (Translation-invariant operators)**.** *An operator T on $\mathfrak{H}_\Lambda^L$ is said to be* ***translation-invariant*** *if it is a multiplication operator in Fourier space. More precisely, there exists a family $(g(k))_{k \in \Gamma_\Lambda^L}$ of 4×4-matrices such that for any $\varphi \in \mathfrak{H}_\Lambda^L$,*

$$\widehat{T\varphi}(k) = g(k) \widehat{\varphi}(k).$$

If then one denotes

$$\check{g}(x) := \left(\frac{2\pi}{L}\right)^{3/2} \sum_{k \in \Gamma_\Lambda^L} g(k) e_k(x),$$

one can easily check that

$$T(x,y) = (2\pi)^{-3/2} \check{g}(x-y), \tag{2.11}$$

so that translation-invariant operators are those which act by convolution on $\mathfrak{H}_\Lambda^L$.

Corollary 2.1. *Any translation-invariant operator has a constant density.*

Proof. Let T be a translation-invariant operator. Then by (2.8) and (2.11) we have

$$\rho_T(x) = \mathrm{Tr}_{\mathbb{C}^4}\left(T(x,x)\right) = (2\pi)^{-3/2} \mathrm{Tr}_{\mathbb{C}^4}\left(\check{g}(0)\right) = L^{-3} \sum_{k \in \Gamma_\Lambda^L} \mathrm{Tr}_{\mathbb{C}^4}\left(g(k)\right). \tag{2.12}$$

□

Remark 2.4. *The last corollary justifies the use of the term* translation-invariant *for such operators since their density is uniform. It can also be justified by the fact that such operators commute with translations.*

Example 2.1. *The identity operator I_Λ^L on $\mathfrak{H}_\Lambda^L$ is a translation-invariant operator, whose kernel is*

$$I_\Lambda^L(x,y) = L^{-3} \sum_{k \in \Gamma_\Lambda^L} I_4 e^{ik\cdot(x-y)},$$

where I_4 is the identity 4×4 matrix since

$$\int_{\mathbb{T}_L} I_\Lambda^L(x,y)\varphi(y)\,dy = \frac{(2\pi)^{3/2}}{L^6} \sum_{k,k'\in\Gamma_\Lambda^L} \widehat{\varphi}(k') \int_{\mathbb{T}_L} e^{ik\cdot(x-y)} e^{ik'\cdot y}\,dy = \frac{(2\pi)^{3/2}}{L^3} \sum_{k\in\Gamma_\Lambda^L} \widehat{\varphi}(k) e^{ik\cdot x} = \varphi(x).$$

The density of the identity is thus $\rho_{I_\Lambda^L} = 4|\Gamma_\Lambda^L|/L^3$. We will use the notation

$$\rho_\Lambda^L = \frac{\rho_{I_\Lambda^L}}{2} = \frac{2|\Gamma_\Lambda^L|}{L^3}. \tag{2.13}$$

Definition of operators in the torus. In order to define the restriction of the Hamiltonian (2.1) to the torus, we have to precise the Dirac operator in the box and to periodize the Coulomb potential as well as the external potential φ.

The Dirac operator was previously defined as

$$D^0 = -i\boldsymbol{\alpha}\cdot\nabla + m\beta,$$

where m is the (bare) mass of an electron and $\boldsymbol{\alpha} = (\alpha_1,\alpha_2,\alpha_3), \beta$ are the Dirac matrices. One can see that the Dirac operator is a multiplication operator by $D^0(k) = \boldsymbol{\alpha}\cdot k + m\beta$ in the Fourier domain, so that the Dirac operator on the torus will just be the multiplication operator in the Fourier domain by the matrices $(\boldsymbol{\alpha}\cdot k + m\beta)_{k\in\Gamma_\Lambda^L}$. The Dirac operator on the torus will be denoted as D^L.

The Coulomb potential $|x|^{-1}$ which appears for instance in the last term of (2.1) needs to be periodized. To do so, following [HLS07], we remark that for the usual Fourier transform

$$\widehat{|\cdot|^{-1}}(k) = \frac{4\pi}{|k|^2},$$

so that we define the periodized Coulomb potential W_L by the formula

$$W_L(x) := \frac{1}{L^3}\left(\sum_{\substack{k\in\Gamma_\Lambda^L\\ k\neq 0}} \frac{4\pi}{|k|^2} e^{ik\cdot x} + \mu L^2\right),$$

where $\mu > 0$ is chosen so that $\min_{C_L} W_L = 0$.

We will consider an external potential φ created by a distribution of charge ν

$$\varphi = -\alpha\nu \star |\cdot|^{-1}.$$

Typically, the distribution of charge can be created by M protons of charge $+e$ placed in positions $(z_i)_{i=1}^M$ so that we have

$$\nu = \sum_{i=1}^M e\chi(\cdot - z_i),$$

where χ is a positive smooth function with compact support and with $\int \chi = 1$. When protons are ponctual, we can replace χ by a Dirac distribution, but in reality the charge distribution of a proton is smooth.

We will not say much here about the living space of ν. We will choose later $\nu \in \mathcal{C}$, the Coulomb space defined in section 4.2.2.

We define the external potential in a box by the formula

$$\nu_L(x) := \frac{(2\pi)^{3/2}}{L^3} \sum_{k \in \Gamma_\Lambda^L} \widehat{\nu}(k) e^{ik\cdot x},$$

which is exactly saying that the Fourier coefficient in $k \in \Gamma_\Lambda^L$ of $\nu_L \in \mathfrak{H}_\Lambda^L$ is the value in k of the Fourier transform of $\nu \in \mathfrak{H}_\Lambda$. The corresponding potential is

$$\varphi_L(x) := -\alpha \nu_L \star W_L(x) = -\alpha \int_{C_L} \nu_L(y) W_L(x-y)\,\mathrm{d}y.$$

Finally, we denote by $D_L(f,f)$ the periodized Coulomb self-interaction for a charge distribution f, it is defined by

$$D_L(f,f) := \iint_{(\mathbb{T}_L)^2} f(x)f(y)W_L(x-y)\,\mathrm{d}x\mathrm{d}y = \left(\frac{2\pi}{L}\right)^3 (2\pi)^{3/2} \sum_{k \in \Gamma_\Lambda^L} |\widehat{f}(k)|^2 \widehat{W_L}(k) \geqslant 0.$$

In the box we denote the Dirac operator with potential by $D_\varphi^L := D^L + \varphi_L$, acting on $\mathfrak{H}_\Lambda^L$.

Fock space, creation and annihilation operators. As we said earlier, QED is a theory which deals with infinitely many particles. The functional space describing an infinite number of particles is built on the one-body space $\mathfrak{H}_\Lambda^L$ and is called the Fock space $\mathcal{F}_\Lambda^L$, defined as

$$\mathcal{F}_\Lambda^L := \mathbb{C} \oplus \bigoplus_{N \geqslant 1} \underbrace{\bigwedge_{n=1}^{N} \mathfrak{H}_\Lambda^L}_{=:\mathfrak{H}_\Lambda^L(N)},$$

where $\mathbb{C}$ denotes by convention the 0-body space and $\mathfrak{H}_\Lambda^L(N)$ the N-body fermionic space. The space $\mathfrak{H}_\Lambda^L$ being finite-dimensional, so is the space $\mathcal{F}_\Lambda^L$. Indeed, $\mathfrak{H}_\Lambda^L(N) = 0$ for $N > \dim(\mathfrak{H}_\Lambda^L)$.

Definition 2.4. *Let $k \in \Gamma_\Lambda^L$ and $\sigma \in \{1,\dots,4\}$. We define the **creation operator** $\boldsymbol{\psi}_{k,\sigma}^*$ which acts on $\mathcal{F}_\Lambda^L$ by creating a particle in the state $\varepsilon_\sigma e_k$. This operator maps $\mathfrak{H}_\Lambda^L(N)$ to $\mathfrak{H}_\Lambda^L(N+1)$ in the following way*

$$\boldsymbol{\psi}_{k,\sigma}^*(\varphi_1 \wedge \cdots \wedge \varphi_N) = (\varepsilon_\sigma e_k) \wedge \varphi_1 \wedge \cdots \wedge \varphi_N.$$

*The adjoint $\boldsymbol{\psi}_{k,\sigma}$ of this operator is called the **annihilation operator**, it maps $\mathfrak{H}_\Lambda^L(N+1)$ to $\mathfrak{H}_\Lambda^L(N)$ by annihilating a particle in the state $\varepsilon_\sigma e_k$. They satisfy the classical anticommutation relation*

$$\{\boldsymbol{\psi}_{k,\sigma}, \boldsymbol{\psi}_{l,\sigma'}^*\} = \delta_{k,l}\delta_{\sigma,\sigma'}. \tag{2.14}$$

Definition 2.5 (Second-quantized field operator)**.** *Let $x \in \mathbb{R}^3$. We define the **second-quantized field operator** $\boldsymbol{\psi}(x)$, which annihilates a particle* in position x*, as an operator-valued 4-component vector by the formula*

$$\boldsymbol{\psi}(x)_\sigma = \sum_{k \in \Gamma_\Lambda^L} e_k(x) \boldsymbol{\psi}_{k,\sigma}, \quad \sigma = 1,\dots,4.$$

The adjoint $\boldsymbol{\psi}(x)^*$ of this operator creates a particle in position x.

Remark 2.5. *Recall that Γ_Λ^L is finite, hence $\boldsymbol{\psi}(x)$ is perfectly well defined.*

2.2.2 Determination of the QED energy in a box

Formula (2.1) becomes in a box

$$\mathbb{H}_L^\varphi := \int_{\mathbb{T}_L} \boldsymbol{\psi}(x)^* D^L \boldsymbol{\psi}(x)\,\mathrm{d}x + \int_{\mathbb{T}_L} \varphi_L(x)\rho(x)\,\mathrm{d}x + \frac{\alpha}{2}\iint_{(\mathbb{T}_L)^2} \rho(x)\rho(y)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y. \quad (2.15)$$

Remark 2.6. *Note that $D^L\boldsymbol{\psi}$ is defined as the operator acting on the Fock space*

$$D^L\boldsymbol{\psi}(x) := \sum_{k\in\Gamma_\Lambda^L} (D^L e_k)(x)\boldsymbol{\psi}_{k,\sigma} = \sum_{k\in\Gamma_\Lambda^L} (\boldsymbol{\alpha}\cdot k + \beta)e_k(x)\boldsymbol{\psi}_{k,\sigma}.$$

Let us compute the expectation value of this Hamiltonian on a Hartree-Fock state Ω with density matrix P. Let us notice that $\boldsymbol{\psi}(x), \boldsymbol{\psi}(x)^*, \rho(x), W_L(x)$ are all bounded functions of x (for the respective norm of their living space). Hence each term of the Hamiltonian is well defined and all the following computations are meaningful.

Proposition 2.1. *Let Ω be a generalized Hartree-Fock state. Then if $\gamma := P - I_\Lambda^L/2$ we have*

$$\Omega(\mathbb{H}_L^\varphi) = \mathcal{E}_\varphi^L(\gamma) + \frac{\alpha}{8}\iint_{(\mathbb{T}_L)^2} \|I_\Lambda^L(x,y)\|^2 W_L(x-y)\,dx\,dy, \quad (2.16)$$

where

$$\boxed{\mathcal{E}_\varphi^L(\gamma) = \mathrm{tr}(D_\varphi^L\gamma) + \frac{\alpha}{2}D_L(\rho_\gamma,\rho_\gamma) - \frac{\alpha}{2}\iint_{(\mathbb{T}_L)^2} \|\gamma(y,x)\|^2 W_L(x-y)\,dx\,dy.} \quad (2.17)$$

Proof. **Kinetic energy.** We will first prove that

$$\boxed{\Omega\left(\int_{\mathbb{T}_L} \boldsymbol{\psi}(x)^* D^L\boldsymbol{\psi}(x)\,\mathrm{d}x\right) = \mathrm{tr}(D^L P).} \quad (2.18)$$

By definition, the kinetic energy of the state Ω is (think of $\boldsymbol{\psi}^*$ as a line vector, $\boldsymbol{\psi}$ as a column vector, and D^L as a matrix)

$$\Omega\left(\int_{\mathbb{T}_L} \boldsymbol{\psi}(x)^* D^L\boldsymbol{\psi}(x)\,\mathrm{d}x\right) = \sum_{\sigma,\sigma'=1}^4 \int_{\mathbb{T}_L} \Omega\left(\boldsymbol{\psi}(x)^*_\sigma D^L_{\sigma\sigma'}\boldsymbol{\psi}(x)_{\sigma'}\right)\,\mathrm{d}x \quad (2.19)$$

$$= \sum_{\sigma,\sigma'=1}^4 \iint_{(\mathbb{T}_L)^2} \Omega\left(\boldsymbol{\psi}(x)^*_\sigma D^{L,y}_{\sigma\sigma'}\boldsymbol{\psi}(y)_{\sigma'}\right)\delta(y-x)\,\mathrm{d}x\,\mathrm{d}y, \quad (2.20)$$

where the notation $D^{L,y}$ is there to keep in mind that D^L acts on the y variable in this expression. Now let us remark that

$$\Omega\left(\boldsymbol{\psi}(x)^*_\sigma D^{L,y}_{\sigma\sigma'}\boldsymbol{\psi}(y)_{\sigma'}\right) = D^{L,y}_{\sigma\sigma'}\Omega\left(\boldsymbol{\psi}(x)^*_\sigma\boldsymbol{\psi}(y)_{\sigma'}\right) = D^{L,y}_{\sigma\sigma'}P(y,x)_{\sigma'\sigma},$$

since $D^{L,y}$ is a differential operator acting only on the y variable and Ω is linear. Now let us show that

$$\sum_{\sigma'=1}^4 D^{L,y}_{\sigma\sigma'}P(y,x)_{\sigma'\sigma} = (D^L P)(y,x)_{\sigma\sigma}, \quad (2.21)$$

where the last term is the element (σ,σ) of the kernel matrix of the operator $D^L P$. Indeed, by definition of the kernel matrix $P(y,x)$, for any $\varphi \in L^2(\mathbb{T}_L;\mathbb{C}^4)$ we have

$$(P\varphi)(y)_\sigma = \sum_{\sigma'=1}^{4} \int_{\mathbb{T}_L} P(y,x)_{\sigma\sigma'} \varphi(x)_{\sigma'} \,\mathrm{d}x.$$

Applying the matrix D_L to the vector $(P\varphi)(y)$ gives

$$\begin{aligned}
(D^L P\varphi)(y)_\sigma &= \sum_{\sigma''=1}^{4} D^{L,y}_{\sigma\sigma''} (P\varphi)(y)_{\sigma''} \\
&= \sum_{\sigma'',\sigma'=1}^{4} \int_{\mathbb{T}_L} D^{L,y}_{\sigma\sigma''} P(y,x)_{\sigma''\sigma'} \varphi(x)_{\sigma'} \,\mathrm{d}x \\
&= \sum_{\sigma'=1}^{4} \int_{\mathbb{T}_L} \underbrace{\sum_{\sigma''=1}^{4} D^{L,y}_{\sigma\sigma''} P(y,x)_{\sigma''\sigma'}}_{\stackrel{\text{def.}}{=} (D^L P)(y,x)_{\sigma\sigma'}} \varphi(x)_{\sigma'} \,\mathrm{d}x
\end{aligned}$$

Therefore we have shown (2.21). Now let us insert this result in the equality (2.20). We find

$$\begin{aligned}
\Omega\left(\int_{\mathbb{T}_L} \boldsymbol{\psi}(x)^* D^L \boldsymbol{\psi}(x) \,\mathrm{d}x\right) &= \sum_{\sigma=1}^{4} \iint_{(\mathbb{T}_L)^2} (D^L P)(y,x)_{\sigma\sigma} \delta(y-x) \,\mathrm{d}x \,\mathrm{d}y \\
&= \sum_{\sigma=1}^{4} \int_{\mathbb{T}_L} (D^L P)(x,x)_{\sigma\sigma} \,\mathrm{d}x \\
&= \int_{\mathbb{T}_L} \mathrm{Tr}_{\mathbb{C}^4}\left(D^L P(x,x)\right) \mathrm{d}x \\
&\stackrel{\text{def.}}{=} \int_{\mathbb{T}_L} \rho_{D^L P}(x) \,\mathrm{d}x \\
&= \mathrm{tr}(D^L P).
\end{aligned}$$

We thus have proved the equality (2.18).

External field term. We then prove that

$$\boxed{\Omega\left(\int_{\mathbb{T}_L} \varphi_L(x)\rho(x) \,\mathrm{d}x\right) = \int_{\mathbb{T}_L} \varphi_L(x)(\rho_P(x) - \rho^L_\Lambda) \,\mathrm{d}x.} \tag{2.22}$$

The density operator defined in (2.2) can be rewritten thanks to the CAR

$$\rho(x) = \sum_{\sigma=1}^{4} \boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(x)_\sigma - \rho^L_\Lambda.$$

Then the expectation value of the external field term in the QED Hamiltonian applied to the Hartree-Fock state Ω gives

$$\Omega\left(\int_{\mathbb{T}_L} \varphi_L(x)\rho(x) \,\mathrm{d}x\right) = \int_{\mathbb{T}_L} \varphi_L(x)\Omega(\rho(x)) \,\mathrm{d}x.$$

A quick computation leads to

$$\begin{aligned}\Omega(\rho(x)) &= \sum_{\sigma=1}^{4} \underbrace{\Omega(\boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(x)_\sigma)}_{=P(x,x)_{\sigma\sigma}} - \rho_\Lambda^L \underbrace{\Omega(\mathrm{Id})}_{=1} \\ &= \mathrm{Tr}_{\mathbb{C}^4}\left(P(x,x)\right) - \rho_\Lambda^L \\ &= \rho_P(x) - \rho_\Lambda^L.\end{aligned}$$

Finally, we obtain (2.22).

Interaction term. We finally prove that

$$\begin{aligned}\Omega\left(\iint_{(\mathbb{T}_L)^2} \rho(x)\rho(y)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y\right) &= \iint_{(\mathbb{T}_L)^2} \rho_P(x)\rho_P(y)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y \\ &\quad - \iint_{(\mathbb{T}_L)^2} \|P(y,x)\|^2 W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y \\ &\quad + \iint_{(\mathbb{T}_L)^2} \mathrm{Tr}_{\mathbb{C}^4}\left(I_\Lambda^L(x,y)P(y,x)\right)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y \\ &\quad - 2\rho_\Lambda^L \iint_{(\mathbb{T}_L)^2} \rho_P(x)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y + (\rho_\Lambda^L)^2 \iint_{(\mathbb{T}_L)^2} W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y. \quad (2.23)\end{aligned}$$

As for the external field term, all we have to do is compute the expression $\rho(x)\rho(y)$:

$$\rho(x)\rho(y) = \sum_{\sigma,\sigma'=1}^{4} \boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(x)_\sigma \boldsymbol{\psi}(y)^*_{\sigma'} \boldsymbol{\psi}(y)_{\sigma'} - \sum_{\sigma=1}^{4} \rho_\Lambda^L \boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(x)_\sigma - \sum_{\sigma'=1}^{4} \rho_\Lambda^L \boldsymbol{\psi}(y)^*_{\sigma'} \boldsymbol{\psi}(y)_{\sigma'} + (\rho_\Lambda^L)^2. \quad (2.24)$$

Using the CAR we obtain

$$\boldsymbol{\psi}(x)_\sigma \boldsymbol{\psi}(y)^*_{\sigma'} = \delta_{\sigma\sigma'} I_\Lambda^L(x,y)_{\sigma\sigma'} - \boldsymbol{\psi}(y)^*_{\sigma'} \boldsymbol{\psi}(x)_\sigma,$$

thus

$$\sum_{\sigma,\sigma'=1}^{4} \boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(x)_\sigma \boldsymbol{\psi}(y)^*_{\sigma'} \boldsymbol{\psi}(y)_{\sigma'} = \sum_{\sigma=1}^{4} I_\Lambda^L(x,y)_{\sigma\sigma} \boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(y)_\sigma - \sum_{\sigma,\sigma'=1}^{4} \underbrace{\boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(y)^*_{\sigma'} \boldsymbol{\psi}(x)_\sigma \boldsymbol{\psi}(y)_{\sigma'}}_{=:A_{\sigma\sigma'}}.$$

We can easily deduce the expectation value of the first operator for the state Ω by writing

$$\begin{aligned}\Omega\left(\sum_{\sigma=1}^{4} I_\Lambda^L(x,y)_{\sigma\sigma} \boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(y)_\sigma\right) &= \sum_{\sigma=1}^{4} I_\Lambda^L(x,y)_{\sigma\sigma} \Omega\left(\boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(y)_\sigma\right) \\ &= \sum_{\sigma=1}^{4} I_\Lambda^L(x,y)_{\sigma\sigma} P(y,x)_{\sigma,\sigma} \\ &= \mathrm{Tr}_{\mathbb{C}^4}\left(I_\Lambda^L(x,y)P(y,x)\right),\end{aligned}$$

since $I_\Lambda^L(x,y)$ has zero values off the diagonal.

To compute the term $\Omega(A_{\sigma\sigma'})$, we use the relation written in [BLS94, Eq. (2a.12)], following from the definition of a Hartree-Fock state:

$$\Omega(A_{\sigma\sigma'}) = \Omega(\boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(y)^*_{\sigma'})\Omega(\boldsymbol{\psi}(x)_\sigma \boldsymbol{\psi}(y)_{\sigma'}) - \Omega(\boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(x)_\sigma)\Omega(\boldsymbol{\psi}(y)^*_{\sigma'} \boldsymbol{\psi}(y)_{\sigma'}) + \Omega(\boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(y)_{\sigma'})\Omega(\boldsymbol{\psi}(y)^*_{\sigma'} \boldsymbol{\psi}(x)_\sigma). \quad (2.25)$$

Now let us remark that for any Hartree-Fock state Ω,

$$\Omega(\boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(y)^*_{\sigma'}) = \Omega\left(\boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(y)^*_{\sigma'}\right) = 0. \quad (2.26)$$

Indeed, if for instance Ω is a N-body Slater determinant, then $\boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(y)^*_{\sigma'}\Omega$ lives in the $(N+2)$-body space. Hence it is orthogonal to Ω in the Fock space. This result is also true for any Hartree-Fock state that is particle-conserving (i.e. a convex combination of states having a definite number of particles, following [BLS94, p. 12]).

Finally we have

$$\Omega(A_{\sigma\sigma'}) = -P(x,x)_{\sigma\sigma}P(y,y)_{\sigma'\sigma'} + P(y,x)_{\sigma'\sigma}P(x,y)_{\sigma\sigma'}.$$

Moreover, as $P^* = P$,

$$P(x,y)_{\sigma\sigma'} = \overline{P(y,x)_{\sigma'\sigma}},$$

hence,

$$\sum_{\sigma,\sigma'=1}^{4} \Omega(A_{\sigma\sigma'}) = -\rho_P(x)\rho_P(y) + \|P(y,x)\|^2.$$

Furthermore, since $W_L(x-y) = W_L(y-x)$ we compute the second and third term of the right-hand side of (2.24) as

$$\Omega\left(\iint_{(\mathbb{T}_L)^2} \left[\sum_{\sigma=1}^{4} \rho^L_\Lambda \boldsymbol{\psi}(x)^*_\sigma \boldsymbol{\psi}(x)_\sigma + \sum_{\sigma'=1}^{4} \rho^L_\Lambda \boldsymbol{\psi}(y)^*_{\sigma'} \boldsymbol{\psi}(y)_{\sigma'}\right] W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y\right) = 2\rho^L_\Lambda \iint_{(\mathbb{T}_L)^2} \rho_P(x) W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y.$$

Regrouping the terms we obtain (2.23).

Remark 2.7. *The relation (2.25) is not written as such in [BLS94]. It is expressed in terms of $\boldsymbol{\psi}(f), \boldsymbol{\psi}(f)^*$ instead of $\boldsymbol{\psi}(x), \boldsymbol{\psi}(x)^*$. The operator $\boldsymbol{\psi}(f)^*$ creates a particle* in the state *f while the operator $\boldsymbol{\psi}(x)^*$ creates a particle* in the position *x (see also [Tha92, Notes of Chap. 10]). The latter is usually used by physicists while mathematicians prefer the former, mainly because the operators $\boldsymbol{\psi}(x), \boldsymbol{\psi}(x)^*$ are often ill-defined. Here, they perfectly make sense since we work in a box with a Fourier cutoff so that the underlying one-body space is finite-dimensional. A proof that (2.25) is equivalent to the relation given in [BLS94] can be found in appendix B.2.*

Remark 2.8. *The relation (2.25) is one of the characteristics of Hartree-Fock states. We have defined the one-body density matrix (which is a 2-point function, acting on the one-body space $\mathfrak{h}$) for Ω, but we could as well define the N-body density matrix ($2N$-point function, acting on the N-body space $\mathfrak{h}^{\wedge N}$). For example, the 2-body density matrix of Ω acting on $\mathfrak{h} \wedge \mathfrak{h}$ is defined as (see [Sol07, sect. 8.1])*

$$\gamma^{(2)}(x,y,z,t)_{\sigma_1\sigma_2\sigma_3\sigma_4} := \Omega\left(\boldsymbol{\psi}(x)^*_{\sigma_1} \boldsymbol{\psi}(z)^*_{\sigma_3} \boldsymbol{\psi}(y)_{\sigma_2} \boldsymbol{\psi}(t)_{\sigma_4}\right).$$

The key property of Hartree-Fock states is that all their N-body density matrices can be expressed in terms of the one-body matrix, the formula being explicit [BLS94, Eq. (2a.11)]. We see that (2.25) uses nothing but the relation which gives the 2-body density matrix in terms of the one-body density matrix of Ω. Roughly speaking, it implies that each term of the Hamiltonian applied to such a state Ω can be written in terms of the one-body density matrix. That is why we talk about mean-field models, the energy only depending on the "density" of the particles and not on their individual behavior.

Remark 2.9. *We may also study a more general class of Hartree-Fock states for which the term in (2.26) is non-zero. It induces a matrix called the pairing matrix. Fortunately, the energy term involving this pairing matrix would be positive in our case, so that the pairing matrix will automatically vanish for a ground state (see [BLS94, Theorem 2.11]). Hence it makes sense to neglect pairing from the beginning.*

Finally, we have the expression of the total energy in a box of a Hartree-Fock state Ω with density matrix P:

$$\mathcal{E}^{\mathrm{QED}}_{L,\varphi}(P) := \Omega\left(\mathbb{H}^{\varphi}_{L}\right) = \mathrm{tr}(D^L P) - \int_{\mathbb{T}_L} \varphi_L(x)(\rho_P(x) - \rho^L_\Lambda)\,\mathrm{d}x + \frac{\alpha}{2}\iint_{(\mathbb{T}_L)^2} \rho_P(x)\rho_P(y)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y$$
$$- \frac{\alpha}{2}\iint_{(\mathbb{T}_L)^2} \|P(y,x)\|^2 W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y + \frac{\alpha}{2}\iint_{(\mathbb{T}_L)^2} \mathrm{Tr}_{\mathbb{C}^4}\left(I^L_\Lambda(x,y)P(y,x)\right)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y$$
$$- \alpha\rho^L_\Lambda \iint_{(\mathbb{T}_L)^2} \rho_P(x)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y + \frac{\alpha}{2}(\rho^L_\Lambda)^2 \iint_{(\mathbb{T}_L)^2} W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y. \quad (2.27)$$

Notice that each term is well-defined since we work in a box with the cutoff Λ.

As mentioned before, our goal is to express this energy with respect to the variable $\gamma := P - I^L_\Lambda/2$. To do so, we have the relations

$$\rho^L_\Lambda = \rho_{I^L_\Lambda/2}, \qquad \mathrm{tr}(D^L I^L_\Lambda) = 0,$$

the last relation holding because the Pauli matrices are traceless. Hence we have

$$\mathrm{tr}(D^L P) - \int_{\mathbb{T}_L} \varphi_L(x)(\rho_P(x) - \rho^L_\Lambda)\,\mathrm{d}x = \mathrm{tr}(D^L\gamma) - \int_{\mathbb{T}_L} \varphi_L(x)\rho_\gamma(x)\,\mathrm{d}x,$$

as well as

$$\iint_{(\mathbb{T}_L)^2} \rho_P(x)\rho_P(y)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y = \iint_{(\mathbb{T}_L)^2} \rho_\gamma(x)\rho_\gamma(y)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y - (\rho^L_\Lambda)^2 \iint_{(\mathbb{T}_L)^2} W_L(x-y)$$
$$+ 2\rho^L_\Lambda \iint_{(\mathbb{T}_L)^2} \rho_P(x)W_L(x-y)\,\mathrm{d}x\,\mathrm{d}y, \quad (2.28)$$

and

$$\|P(y,x)\|^2 = \|\gamma(y,x)\|^2 - \frac{1}{4}\|I^L_\Lambda(x,y)\|^2 + \mathrm{Tr}_{\mathbb{C}^4}\left(I^L_\Lambda(x,y)P(y,x)\right).$$

Fortunately, the expression of the energy is simplified as the appearing terms cancel the existing ones. We thus have proved Proposition 2.1. □

The last term of (2.16) behaves like L^3 when $L \to \infty$ so that we can ignore it for two reasons. First, when L is fixed, the last term in (2.16) is a constant so that the minimizers of $\Omega(\mathbb{H}^{\varphi}_L)$ are the same as those of $\mathcal{E}^L_\varphi(\gamma)$. Secondly, when looking at the thermodynamic limit of the energy per unit volume $\mathcal{E}^L_\varphi(\gamma)/L^3$ the last term of (2.16) behaving like L^3 converges towards a constant. We can discard it because we will then look at differences of energies in the whole space, so that this constant will disappear.

2.3 Main strategy

Since we have computed the energy of a generalized Hartree-Fock state Ω in a box as the expression (2.17) depending only on its renormalized density matrix γ, we are now able to state the minimization problem we will study.

First of all, in [HLS07] Hainzl, Lewin and Solovej minimized the energy $\mathcal{E}^L_\varphi(\gamma)$ while in this study we will neglect the last term of (2.17) that is the exchange term. It will dramatically simplify some of the proofs of the theorems but we will explain quickly how to deal with the full model as remarks. However, many qualitative properties of this so-called *reduced model* (without exchange term) are the same as for the full model. The reference energy we will study is thus

$$\mathsf{E}^L_\varphi(\gamma) := \mathrm{tr}(D^L_\varphi \gamma) + \frac{\alpha}{2} D_L(\rho_\gamma, \rho_\gamma).$$

We will minimize this energy over the space

$$\mathsf{G}^L_\Lambda := \left\{ \gamma \in \mathcal{L}(\mathfrak{H}^L_\Lambda), \quad \gamma^* = \gamma, \quad -\frac{I^L_\Lambda}{2} \leqslant \gamma \leqslant \frac{I^L_\Lambda}{2} \right\},$$

where $\mathcal{L}(\mathfrak{H}^L_\Lambda)$ denotes the set of the linear operators on $\mathfrak{H}^L_\Lambda$. The set G^L_Λ is actually the convex hull of the set $\{P - I^L_\Lambda/2, \quad P \text{ orthogonal projector}\}$ which characterizes usual Hartree-Fock states.

Remark 2.10. *Taking the convex hull of this set is not a simple technical necessity. Indeed, G^L_Λ actually corresponds to the set of the one-body density matrices of quasi-free states which are particle-conserving [BLS94, Theorem 2.3].*

We thus study the following minimzation problem

$$\boxed{E_L(\varphi) = \inf_{\gamma \in \mathsf{G}^L_\Lambda} \mathsf{E}^L_\varphi(\gamma).} \tag{2.29}$$

We study the case with no external field ($\varphi = 0$) and only add an external electric field in the study of atoms and molecules. The study of the case $\varphi = 0$ is crucial since one of the main challenge of QED is to give a sense to the minimisation of the energy of QED in the whole space, which is often unbounded from below. To remove this divergence, we follow the idea of Chaix and Iracane [CI89] who choose to measure the energy of any state relatively to the energy of a reference. Of course, one has to choose a relevant reference state. Following again [HLS07], the reference state we choose is the state of lowest energy without external field, which we call the *free vacuum*.

We first define this free vacuum in a box, as the unique minimizer of $E_L(0)$, which we call γ^0_L. To find the free vacuum in the whole space, we then look for the limit of $\mathsf{E}^L_0(\gamma)/L^3$ for a fixed translation-invariant γ, as the free vacuum is supposed to be. This limit energy is defined as the energy per unit volume in the whole space. The unique minimizer γ^0 of this energy is the free vacuum we are looking for. We will see that $\gamma^0_L \to \gamma^0$ as $L \to \infty$ in a certain sense, so that γ^0 can be seen as the free vacuum in the whole space also as the limit of the free vacuum in a box.

3 Definition of the free vacuum

Recall that the free vacuum is defined as the (unique) minimizer of the reduced Hartree-Fock energy without external field.

3.1 The free vacuum in a box

Theorem 3.1. *Let $L, \Lambda, m > 0$. Then E_0^L has a unique minimizer on G_Λ^L which is $\gamma_0^L := P_0^L - I_\Lambda^L/2$ where $P_0^L = \chi_{(-\infty;0)}(D_L^0)$ is the negative spectral projector of the Dirac operator in a box. The operator γ_0^L is called the* free vacuum *in a box.*

Proof. By lemma A.1, the operator γ_0^L defined in the theorem verifies

$$\operatorname{tr}(D_L^0 \gamma_0^L) = \min_{\gamma \in \mathsf{G}_\Lambda^L} \operatorname{tr}(D_L^0 \gamma), \tag{3.1}$$

We have

$$\gamma_0^L = P_0^L - I_\Lambda^L/2 = \frac{P_0^L - (P_0^L)^\perp}{2}.$$

In the Fourier domain, this is a multiplication operator by

$$\gamma_0^L(k) = -\frac{D_L^0(k)}{2\|D_L^0(k)\|}.$$

In the sense of operators, this implies

$$\gamma_0^L = -\frac{\operatorname{sgn}(D_L^0)}{2}.$$

The Dirac matrices being traceless, we have $\operatorname{Tr}_{\mathbb{C}^4}\left(\gamma_0^L(k)\right) = 0$ and thus $\rho_{\gamma_0^L} = 0$ by the equality (2.12). For any $\gamma \in \mathsf{G}_\Lambda^L$ we have

$$\begin{aligned}
\mathsf{E}_0^L(\gamma) &= \operatorname{tr}(D_L^0\gamma) + \frac{\alpha}{2}\underbrace{D_L(\rho_\gamma, \rho_\gamma)}_{\geqslant 0} && (3.2)\\
&\geqslant \operatorname{tr}(D_L^0\gamma) && (3.3)\\
&\geqslant \operatorname{tr}(D_L^0\gamma_0^L) = \mathsf{E}_0^L(\gamma_0^L) \qquad (\text{because } \rho_{\gamma_0^L} \equiv 0). && (3.4)
\end{aligned}$$

The uniqueness of γ_0^L comes from its uniqueness as minimizer of (3.1). Indeed, for any other minimizer γ of E_0^L, we have $\mathsf{E}_0^L(\gamma) = \mathsf{E}_0^L(\gamma_0^L)$ so that the inequality in (3.4) is in fact an equality. We thus have $\operatorname{tr}(D_L^0\gamma) = \operatorname{tr}(D_L^0\gamma_0^L) = \min_{\Gamma \in \Gamma_\Lambda^L} \operatorname{tr}(D_L^0\Gamma)$. The operator D_L^0 being invertible, the minimizer in (3.1) is unique so that $\gamma = \gamma_0^L$. The free vacuum in a box is thus unique. □

Remark 3.1. *The model including the exchange term is much more complicated because the energy is not convex anymore. The proof actually uses the existence of a minimizer in the whole space. Moreover, the minimizer is not P_0^L anymore and the minimizer satisfies a self-consistent equation. It is also a projector but of a Dirac operator $\mathcal{D}_L^0$ modified by its own presence. Physically, it can be explain by the interaction between these charged virtual particles.*

3.2 The free vacuum in the whole space

To define the free vacuum in the whole space, we first have to find the energy in the whole space. We want to define this energy as the limit of the energy per unit volume in a box as its size grows. We have to choose a test γ defined in the whole space, confine it in a box in a certain sense and determine the limit energy of this restrained operator in terms of γ. First, we have to precise the functional setting in the whole space to then define γ. The one-body space in the whole space is

$$\mathfrak{H}_\Lambda := \left\{\varphi \in L^2(\mathbb{R}^3;\mathbb{C}^4), \quad \operatorname{supp}(\widehat{\varphi}) \subset B(0,\Lambda)\right\}.$$

As we have seen in a box, the free vacuum is translation-invariant. Our test γ will then be chosen as translation-invariant. In the whole space it still means that it is a multiplication operator in the Fourier space. If γ is translation-invariant and self-adjoint, we will denote by $\gamma(p)$ the 4×4 self-adjoint matrix such that for any $\varphi \in \mathfrak{H}_\Lambda$ we have

$$\widehat{\gamma\varphi}(p) = \gamma(p)\widehat{\varphi}(p), \quad p \in B(0;\Lambda).$$

Recall that we have to keep the constraint $-I_\Lambda/2 \leqslant \gamma \leqslant I_\Lambda/2$ as it was the case in a box, where I_Λ denotes the identity operator of $\mathfrak{H}_\Lambda$. The energy in the whole space will then be minimized over the set

$$\mathcal{A}_\Lambda := \{\gamma \,\text{translation-invariant on}\, \mathfrak{H}_\Lambda, \quad \gamma^* = \gamma, \quad -I_\Lambda/2 \leqslant \gamma \leqslant I_\Lambda/2\}\,.$$

For $\gamma \in \mathcal{A}_\Lambda$, the map $\gamma : p \mapsto \gamma(p)$ belongs to the space

$$\text{“}\widehat{\mathcal{A}_\Lambda}\text{”} = \{\gamma \in L^\infty(B(0;\Lambda), \mathcal{S}_4(\mathbb{C})), \quad -I_4/2 \leqslant \gamma \leqslant I_4/2\}\,,$$

where $\mathcal{S}_4(\mathbb{C})$ denotes the set of the 4×4 self-adjoint matrices. For $\gamma \in \mathcal{A}_\Lambda$, its density is still well-defined and constant, passing the formula (2.12) to the limit $L \to \infty$ with a Riemann sum. We have then

$$\rho_\gamma(x) \equiv (2\pi)^{-3} \int_{B(0;\Lambda)} \mathrm{Tr}_{\mathbb{C}^4}\left(\gamma(p)\right) \mathrm{d}p.$$

It is easy to confine a translation-invariant operator in a box since it is a multiplication operator in the Fourier domain. For such a γ, we define the operator $\gamma_L \in \mathsf{G}_\Lambda^L$ by

$$\gamma_L(k) = \gamma(k), \quad k \in \Gamma_\Lambda^L.$$

For our γ test we will moreover assume that $\mathrm{Tr}_{\mathbb{C}^4}(\gamma(p)) = 0$, $\forall p \in B(0;\Lambda)$, as it is the case for the free vacuum in the box and will be the case for the free vacuum in the whole space as we will see. For such a γ we have $\rho_{\gamma_L} \equiv 0$ so that

$$\mathsf{E}_0^L(\gamma_L) = \mathrm{tr}(D_L^0\gamma_L) = \sum_{k\in\Gamma_\Lambda^L} \mathrm{Tr}_{\mathbb{C}^4}\left(D_L^0(k)\gamma_L(k)\right).$$

Hence the limit energy per unit volume is

$$\mathcal{T}(\gamma) := \lim_{L\to\infty} \frac{\mathsf{E}_0^L(\gamma)}{L^3} = \frac{1}{(2\pi)^3} \int_{B(0;\Lambda)} \mathrm{Tr}_{\mathbb{C}^4}\left(D^0(p)\gamma(p)\right) \mathrm{d}p. \tag{3.5}$$

Theorem 3.2. *Assume that $\Lambda > 0$. Then $\mathcal{T}$ possesses a unique minimizer $\gamma^0 = P^0 - I_\Lambda/2$ on $\mathcal{A}_\Lambda$ defined by*

$$P^0 := \chi_{(-\infty;0)}(D^0). \tag{3.6}$$

This minimizer is called the free vacuum. *It is a translation-invariant operator with vanishing density of charge: $\rho_{\gamma^0} \equiv 0$.*

Proof. The proof is just an application of the lemma A.1. Indeed, for each $p \in B(0;\Lambda)$ the unique minimizer of $\Gamma \mapsto \mathrm{Tr}_{\mathbb{C}^4}\left(D^0(p)\Gamma\right)$ is

$$\Gamma = -\frac{D^0(p)}{2\|D^0(p)\|}.$$

Hence, γ^0 is the unique global minimizer of $\mathcal{T}$ over $\mathcal{A}_\Lambda$. The same argument as in the theorem in the box applies to prove that $\rho_{\gamma^0} \equiv 0$. □

Remark 3.2. *We can see here the importance of taking commutators in formula (2.3). With these commutators, the free vacuum is not charged and is translation-invariant, which fits to the idea of Dirac. That is also why these commutators act as a kind of renormalization.*

Remark 3.3. *In the model with exchange term, we can do the same remark as in the box and obtain the free vacuum γ^0 which satisfies the self consistent equation*

$$\begin{cases} \gamma^0 = -\frac{\mathrm{sgn}(\mathcal{D}^0)}{2} \\ \mathcal{D}^0 = D^0 - \alpha \frac{\gamma^0(x,y)}{|x-y|}. \end{cases}$$

We have again the modified Dirac operator $\mathcal{D}^0$ which is the sum of the usual Dirac operator and a term of Coulombian potential induced by the vacuum.

3.3 The thermodynamic limit

The thermodynamic limit is stated both to justify and to reinforce the choice of γ^0 as the unique free vacuum.

Theorem 3.3. *Assume that $\Lambda > 0$. Then we have*

$$\lim_{L\to\infty} \frac{\mathsf{E}_0^L(\gamma_0^L)}{L^3} = \min_{\mathcal{A}_\Lambda} \mathcal{T} = \mathcal{T}(\gamma^0).$$

In words, the energy per unit volume of the free vacuum in a box converges towards the energy per unit volume of the free vacuum in the whole space. Moreover, γ_0^L converges towards γ^0 in the following sense:

$$\lim_{L\to\infty} \|\gamma_0^L - \gamma^0\|_{\mathfrak{S}_\infty(\mathfrak{H}_\Lambda^L)} = \lim_{L\to\infty} \sup_{k\in\Gamma_\Lambda^L} |\gamma_0^L(k) - \gamma^0(k)| = 0.$$

Proof. Both limits are true because we have for all $k \in \Gamma_\Lambda^L$,

$$\gamma_0^L(k) = \gamma^0(k).$$

The second limit is then obvious while the first one is proved by the same limit as formula (3.5). □

Remark 3.4. *In this case, the thermodynamic limit is trivial because we know explicitly the minimizer of the energy per unit volume. In the HF case with exchange term, this minimizer satisfies a self-consistent equation so that the thermodynamic limit becomes non-trivial. However, it was shown in [HLS07] that the free vacuum is indeed unique.*

We have now built our reference operator, the free vacuum γ^0. We are thus able to derive the QED energy in the Hartree-Fock approximation.

4 Bogoliubov-Dirac-Fock energy

4.1 A formal computation

We want to measure the energy of any state γ on the whole space relatively to the one of the free vacuum γ^0. The formula (2.17) gives the energy in a box. We can deduce from this expression

the formula for the reduced HF energy in the whole space $\mathsf{E}_\nu^{\mathrm{rHF}}$ by taking a formal limit $L \to \infty$. It leads to

$$\mathsf{E}_\nu^{\mathrm{rHF}}(\gamma) = \mathrm{tr}(D^0\gamma) - \alpha \iint \frac{\rho_\gamma(x)\nu(y)}{|x-y|}\,\mathrm{d}x\mathrm{d}y + \frac{\alpha}{2}\iint \frac{\rho_\gamma(x)\rho_\gamma(y)}{|x-y|}\,\mathrm{d}x\mathrm{d}y. \tag{4.1}$$

We have already said that this energy does not make sense. The so-called Bogoliubov-Dirac-Fock (BDF) energy introduced in [HLS05a, HLS05b, HLS09, HLS07] measures the energy $\mathsf{E}_\nu^{\mathrm{BDF}}$ of a state γ relatively to the (infinite) one of γ^0. It depends on the variable $Q = \gamma - \gamma^0$ and can be derived formally as

$$\begin{aligned} \text{“}\mathsf{E}_\nu^{\mathrm{BDF}}(Q) &= \mathsf{E}_\nu^{\mathrm{rHF}}(\gamma) - \mathsf{E}_\nu^{\mathrm{rHF}}(\gamma^0) &(4.2)\\ &= \mathrm{tr}(D^0 Q) - \alpha \iint \frac{\rho_Q(x)\nu(y)}{|x-y|}\,\mathrm{d}x\mathrm{d}y + \frac{\alpha}{2}\iint \frac{\rho_Q(x)\rho_Q(y)}{|x-y|}\,\mathrm{d}x\mathrm{d}y\text{”}. &(4.3)\end{aligned}$$

Remark 4.1. *The expression of this energy can be rigorously justified by a thermodynamic limit. This formal computation enables us to understand better the issues raised by this energy.*

The only difference between this energy and the reduced HF energy (4.1) is the variable which now is $Q = \gamma - \gamma^0$. The issue is to find the right space where Q is supposed to live. One of the problems we had with the reduced HF energy was that the main variable γ was never compact. Here, Q can (and will) be compact. Moreover, the Fourier cutoff Λ allows the last terms of (4.3) to be well-defined if Q is regular enough.

However, there is a crucial subtility in the choice of the functional setting for $\mathsf{E}_\nu^{\mathrm{BDF}}$. One may be tempted to choose Q in the trace-class. Indeed, the BDF energy is completely well-defined on the trace-class. The issue is that its minimizers are *never* trace-class [GLS09, Theorem 1] and this fact is the origin of the well-known **charge renormalization** in QED.

We thus have to find a larger class of compact operators where the BDF energy is well-defined.

4.2 Functional setting for the BDF energy

In this section we introduce mathematical tools useful to define the right functional space for $\mathsf{E}_\nu^{\mathrm{BDF}}$.

4.2.1 The P^0-trace class

We said that the trace-class $\mathfrak{S}_1(\mathfrak{H}_\Lambda)$ was not the right set of compact operators for the minimisation of the BDF energy. The right space is actually a subspace of the Hilbert-Schmidt operators space $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$, which is larger than $\mathfrak{S}_1(\mathfrak{H}_\Lambda)$. Recall that these spaces are defined by, following for instance [RS72, VI.6]:

$$\mathfrak{S}_p(\mathfrak{H}_\Lambda) = \left\{A \in \mathcal{L}(\mathfrak{H}_\Lambda), \quad \mathrm{tr}(|A|^p) < \infty\right\}, \quad |A| = \sqrt{A^*A},$$

where $\mathcal{L}(\mathfrak{H}_\Lambda)$ denotes the space of all linear operators on $\mathfrak{H}_\Lambda$.

Definition 4.1. *Let A be an Hilbert-Schmidt operator on $\mathfrak{H}_\Lambda$. We say that A is P^0-*trace class*, where P^0 is defined on (3.6), if $A^{++} := (1-P^0)A(1-P^0)$ and $A^{--} := P^0AP^0$ are both trace-class. The set of all P^0-trace class operators on $\mathfrak{H}_\Lambda$ is denoted by $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$. We define the P^0-*trace *of A by*

$$\mathrm{tr}_{P^0}(A) := \mathrm{tr}(A^{++}) + \mathrm{tr}(A^{--}). \tag{4.4}$$

It is a Banach space endowed with the norm

$$\|A\|_{1;P^0} := \|A^{++}\|_{\mathfrak{S}_1(\mathfrak{H}_\Lambda)} + \|A^{--}\|_{\mathfrak{S}_1(\mathfrak{H}_\Lambda)} + \|A^{+-}\|_{\mathfrak{S}_2(\mathfrak{H}_\Lambda)} + \|A^{-+}\|_{\mathfrak{S}_2(\mathfrak{H}_\Lambda)}, \tag{4.5}$$

where $A^{+-} := (1-P^0)AP^0$ and $A^{-+} := P^0A(1-P^0)$.

Remark 4.2. *The P^0-trace actually measures the charge of a state Ω with density matrix P. verifying $Q := P - P^0 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ in the Fock space built upon P^0 (see for instance [HLS05b]). If we denote by $\mathcal{Q}$ the charge operator, defined for instance in [HLS05a, HLS05b], we have*

$$\Omega(\mathcal{Q}) = \mathrm{tr}_{P^0}(Q),$$

so that the choice of the P^0-trace is not arbitrary.

Remark 4.3. *If A is trace-class, then A is P^0-trace class and $\mathrm{tr}(A) = \mathrm{tr}_{P^0}(A)$.*

We also define a weak topology on $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$ such that

$$Q_n \rightharpoonup Q \, (\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)) \Leftrightarrow \left\{ \begin{array}{ll} Q_n \rightharpoonup Q & (\mathfrak{S}_2) \\ Q_n^{++} \rightharpoonup Q^{++} & (\mathfrak{S}_1) \\ Q_n^{--} \rightharpoonup Q^{--} & (\mathfrak{S}_1) \end{array} \right. , \tag{4.6}$$

where the weak topology on $\mathfrak{S}_1$ is defined as $A_n \rightharpoonup A$ if $\mathrm{tr}(A_n K) \to \mathrm{tr}(AK)$ for all $K \in \mathfrak{S}_\infty(\mathfrak{H}_\Lambda)$ the set of compact operators. We have used the notation $A_n \rightharpoonup A$ for the weak convergence.

4.2.2 The Coulomb space

While the P^0-trace class will be used to define the kinetic energy of a state, the other terms of the energy will be defined with the Coulomb space.

Definition 4.2. *Let $f \in \mathcal{S}' : \mathbb{R}^3 \to \mathbb{R}$ a function such that $\widehat{f}$ is measurable. We define its* Coulomb energy *by*

$$D(f,f) := 4\pi \int_{\mathbb{R}^3} \frac{|\widehat{f}(k)|^2}{|k|^2} \, dk. \tag{4.7}$$

We then define the Coulomb space $\mathcal{C}$ as

$$\mathcal{C} := \{ f, \quad D(f,f) < \infty \}.$$

It is a Hilbert space endowed with the scalar product

$$D(f,g) = 4\pi \int_{\mathbb{R}^3} \frac{\overline{\widehat{f}(k)}\widehat{g}(k)}{|k|^2} \, dk.$$

We denote

$$\|f\|_{\mathcal{C}} := D(f,f)^{1/2}.$$

Remark 4.4. *Notice that if f,g are smooth enough (in $H^1(\mathbb{R}^3)$ for instance) we find the usual physical definition of the Coulomb energy between two charge distributions f and g*

$$D(f,g) = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(x)g(y)}{|x-y|} \, dx\, dy.$$

Any operator $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ has an integral kernel operator [RS72, Theorem VI.23] denoted by $Q(x,y)$. Its Fourier transform $\widehat{Q}(p,q)$ being supported in $B(0;\Lambda) \times B(0;\Lambda)$, the function $Q(x,y)$ is smooth so that the density ρ_Q of Q is well-defined as

$$\rho_Q(x) := \mathrm{Tr}_{\mathbb{C}^4}(Q(x,x)).$$

In the Fourier domain one has the formula

$$\widehat{\rho_Q}(k) = (2\pi)^{-3/2} \int_{\substack{|p+k/2|\leqslant\Lambda \\ |p-k/2|\leqslant\Lambda}} \mathrm{Tr}_{\mathbb{C}^4} \left(\widehat{Q}(p+k/2, p-k/2) \right) \mathrm{d}p.$$

This last formula actually shows that $\widehat{\rho_Q}$ is in $L^2(B(0;2\Lambda))$, so that ρ_Q is in $L^2(\mathbb{R}^3)$ as well.

We now have the useful result proved in [HLS09]:

Lemma 4.1. *The map $Q \in \mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda) \mapsto \rho_Q \in \mathcal{C} \cap L^2$ is continuous. More precisely, there exists a constant $C(\Lambda)$ so that*

$$\forall Q \in \mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda), \quad \|\rho_Q\|_{L^2} + D(\rho_Q, \rho_Q)^{1/2} \leqslant C(\Lambda) \|Q\|_{1;P^0}.$$

4.3 Properties of the BDF energy

We are now able to write rigorously the expression of the BDF energy

$$\boxed{\mathcal{E}^\nu(Q) := \mathsf{E}_\nu^{\mathrm{BDF}}(Q) = \mathrm{tr}_{P^0}(D^0 Q) - \alpha D(\rho_Q, \nu) + \frac{\alpha}{2} D(\rho_Q, \rho_Q),} \tag{4.8}$$

with Q belonging to the variational set

$$\mathcal{K} := \left\{ Q \in \mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda), \quad Q^* = Q, \quad -P^0 \leqslant Q \leqslant 1 - P^0 \right\}. \tag{4.9}$$

Using lemma 4.1 and the boundedness of D^0 on $\mathfrak{H}_\Lambda$, we see that $\mathcal{E}^\nu$ is well-defined on $\mathcal{K}$.

Proposition 4.1. *The application $\mathcal{E}^\nu$ is coercive and weakly lower semi-continuous (wlsc) on $\mathcal{K}$.*

Proof. To prove that $\mathcal{E}^\nu$ is coercive on $\mathcal{K}$ we just remark that for any $Q \in \mathcal{K}$,

$$-\alpha D(\rho_Q, \nu) + \frac{\alpha}{2} D(\rho_Q, \rho_Q) = \frac{\alpha}{2} D(\rho_Q - \nu, \rho_Q - \nu) - \frac{\alpha}{2} D(\nu, \nu) \geqslant -\frac{\alpha}{2} D(\nu, \nu),$$

so that

$$\mathcal{E}^\nu(Q) \geqslant \mathrm{tr}_{P^0}(D^0 Q) - \frac{\alpha}{2} D(\nu, \nu). \tag{4.10}$$

We then have the following lemma

Lemma 4.2. *The application $Q \in \mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda) \mapsto \mathrm{tr}_{P^0}(D^0 Q)$ is coercive.*

Proof. Let (Q_n) be a sequence in $\mathcal{K}$ such that $\|Q_n\|_{1;P^0} \to \infty$. According to the definition of the norm $\|\cdot\|_{1;P^0}$, it means that either $\|Q_n^{--}\|_{\mathfrak{S}_1}$,$\|Q_n^{++}\|_{\mathfrak{S}_1}$,$\|Q_n^{+-}\|_{\mathfrak{S}_2}$, or $\|Q_n^{-+}\|_{\mathfrak{S}_2}$ tend to ∞. If $\|Q_n^{--}\|_{\mathfrak{S}_1} \to \infty$ or $\|Q_n^{++}\|_{\mathfrak{S}_1} \to \infty$, since

$$\mathrm{tr}_{P^0}(D^0 Q_n) = \mathrm{tr}(|D^0|(Q_n^{++} - Q_n^{--})),$$

and $|D^0| \geqslant \mathrm{Id}$, $Q_n^{++} \geqslant 0 \geqslant Q_n^{--}$ because of the condition $-P^0 \leqslant Q \leqslant 1 - P^0$, we have

$$\mathrm{tr}_{P^0}(D^0 Q_n) \geqslant \|Q_n^{--}\|_{\mathfrak{S}_1} + \|Q_n^{++}\|_{\mathfrak{S}_1} \to \infty.$$

If $\|Q_n^{+-}\|_{\mathfrak{S}_2}$ or $\|Q_n^{-+}\|_{\mathfrak{S}_2} \to \infty$, we remark that

$$\begin{aligned} \|Q_n^{+-}\|_{\mathfrak{S}_2}^2 + \|Q_n^{--}\|_{\mathfrak{S}_2}^2 &= \|(Q_n^2)^{--}\|_{\mathfrak{S}_1} \\ \|Q_n^{-+}\|_{\mathfrak{S}_2}^2 + \|Q_n^{++}\|_{\mathfrak{S}_2}^2 &= \|(Q_n^2)^{++}\|_{\mathfrak{S}_1}, \end{aligned}$$

and that

$$\|Q_n^2\|_{\mathfrak{S}_1} = \|(Q_n^2)^{++}\|_{\mathfrak{S}_1} + \|(Q_n^2)^{--}\|_{\mathfrak{S}_1},$$

so that $\|Q_n^{+-}\|_{\mathfrak{S}_2}$ or $\|Q_n^{-+}\|_{\mathfrak{S}_2} \to \infty \Rightarrow \|Q_n^2\|_{\mathfrak{S}_1} \to \infty$. Finally,

$$\mathrm{tr}_{P^0}(D^0 Q_n) = \mathrm{tr}(|D^0|(Q_n^{++} - Q_n^{--})) \geqslant \mathrm{tr}(|D^0|Q_n^2) \geqslant \|Q_n^2\|_{\mathfrak{S}_1} \to \infty.$$

We thus have proved the lemma. □

The lemma and the inequality (4.10) imply the coercivity of $\mathcal{E}^\nu$.

The map $Q \in \mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda) \mapsto \frac{\alpha}{2} D(\rho_Q - \nu, \rho_Q - \nu) - \frac{\alpha}{2} D(\nu, \nu)$ is clearly convex and strongly continuous by lemma 4.1 so that it is weakly lower semi-continuous on $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$.

We just have to prove that $\liminf \mathrm{tr}_{P^0}(D^0 Q_n) \geqslant \mathrm{tr}_{P^0}(D^0 Q)$ when $Q_n \rightharpoonup Q$.

Lemma 4.3. *Let (A_n) be a sequence of positive trace-class operators converging weakly towards A in the trace-class. Then $\liminf \mathrm{tr}(A_n) \geqslant \mathrm{tr}(A)$, that is the trace is weakly lower semi-continuous over the set of positive trace-class operators.*

Proof. Since A_n is compact we can write $\mathrm{tr}(A_n) = \sum_i \lambda_i^n$, where the (λ_i^n) are the positive eigenvalues of A_n. Since they are all positive, we can choose that $\lambda_1^n \geqslant \lambda_2^n \geqslant \ldots$. We have thus the formula

$$\lambda_1^n = \sup_\varphi \langle A_n \varphi, \varphi \rangle.$$

Let φ be such that $\langle A\varphi, \varphi \rangle = \lambda_1$. Then we have

$$\lambda_1^n \geqslant \langle A_n \varphi, \varphi \rangle = \mathrm{tr}(A_n \underbrace{|\varphi\rangle\langle\varphi|}_{\text{compact}}) \to \mathrm{tr}(A|\varphi\rangle\langle\varphi|) = \lambda_1,$$

by definition of the weak convergence (4.6). Consequently,

$$\liminf \lambda_1^n \geqslant \lambda_1,$$

and we have the same formula for each λ_i^n by the min-max formula. Then,

$$\liminf \mathrm{tr}(A_n) \geqslant \mathrm{tr}(A),$$

and the lemma is proved. □

We apply the lemma to the sequences $(|D^0|^{1/2} Q_n^{++} |D^0|^{1/2})$ and $(-|D^0|^{1/2} Q_n^{--} |D^0|^{1/2})$ which are both sequences of positive operators which verify

$$\mathrm{tr}_{P^0}(D^0 Q_n) = \mathrm{tr}(|D^0|^{1/2} Q_n^{++} |D^0|^{1/2}) + \mathrm{tr}(-|D^0|^{1/2} Q_n^{--} |D^0|^{1/2}).$$

By the definition of weak convergence, $Q_n \rightharpoonup Q$ implies that $Q_n^{++} \rightharpoonup Q^{++}$ in $\mathfrak{S}_1(\mathfrak{H}_\Lambda)$, and since $|D^0|$ is bounded, $|D^0|^{1/2} Q_n^{++} |D^0|^{1/2} \rightharpoonup |D^0|^{1/2} Q^{++} |D^0|^{1/2}$ as well. Applying the lemma we find that

$$\begin{aligned}\liminf \mathrm{tr}_{P^0}(D^0 Q_n) &= \liminf \Big(\mathrm{tr}(|D^0|^{1/2} Q_n^{++} |D^0|^{1/2}) + \mathrm{tr}(-|D^0|^{1/2} Q_n^{--} |D^0|^{1/2}) \Big) \\ &\geqslant \mathrm{tr}(|D^0|^{1/2} Q^{++} |D^0|^{1/2}) + \mathrm{tr}(-|D^0|^{1/2} Q^{--} |D^0|^{1/2}) = \mathrm{tr}_{P^0}(D^0 Q),\end{aligned}$$

and $\mathcal{E}^\nu$ is thus weakly lower semi-continuous. □

Corollary 4.1. *The energy $\mathcal{E}^\nu$ is bounded from below since we have*

$$\mathcal{E}^\nu(Q) + \frac{\alpha}{2} D(\nu, \nu) \geqslant 0, \tag{4.11}$$

from the equation (4.10).

Remark 4.5. *This corollary is exactly what we were looking for: a bounded-below energy, which was not trivial to find in QED.*

Remark 4.6. *If $\nu = 0$, we remark that $\mathcal{E}^0 \geqslant 0$ so that $Q = 0$, that is $P = P^0$, is the unique minimizer of $\mathcal{E}^0$. In this sense, we can also justify the choice of P^0 as the free vacuum.*

Corollary 4.2. *The functional $\mathcal{E}^\nu$ has a minimizer over $\mathcal{K}$, called the* polarized vacuum.

Proof. The energy $\mathcal{E}^\nu$ being wlsc and the set $\mathcal{K}$ being convex and strongly closed hence weakly closed, the existence of such a minimizer is completely straghtforward. □

Remark 4.7. *In the full HF model with the exchange term, the existence of a polarized vacuum still holds by proving that the energy is also wlsc. However, the exchange term being not convex, the proof is much more complicated and uses concentration-compactness methods to prove that any charge escaping to infinity has a positive energy. It relies on the fact that the exchange term can actually be controlled by the kinetic energy.*

5 Existence of atoms and molecules for the reduced model

The study of the existence of atoms and molecules consists in minimizing the energy $\mathcal{E}^\nu$ on charge sectors. We have already seen that the charge of a $Q \in \mathcal{K}$ is given by $\mathrm{tr}_{P^0}(Q)$. So that when one wants to study a system with a charge $-eN$, one has to minimize $\mathcal{E}^\nu$ over the N-charge sector

$$\mathcal{K}(N) := \{Q \in \mathcal{K}, \quad \mathrm{tr}_{P^0}(Q) = N\}. \tag{5.1}$$

We note

$$E^\nu(N) := \inf_{Q \in \mathcal{K}(N)} \mathcal{E}^\nu(Q) \tag{5.2}$$

The main problem occuring with this model is that $\mathcal{K}(N)$ is not weakly closed (or else a minimizer would exist for any N, but the contrary has been proved in [GLS09]). Indeed, a minimizing sequence may gain or lose charge at the limit. Plus, even if the reduced model is not physical, one can argue that an atom cannot have an arbitrary charge because of the limited binding forces of a nucleus. Thus, the existence of a minimizer in a certain charge domain will depend on a binding condition as we will see.

This work has been done in [HLS09] for the full-model. In this study we will do the same for the reduced model but we will moreover prove the thermodynamic limit for this model, which has not been done yet.

5.1 The existence theorem

We prove the existence theorem as it is done in [HLS09, Theorem 1] because some key tools for the proof will be useful for the thermodynamic limit.

Theorem 5.1. *Let $\Lambda > 0$, $\nu \in \mathcal{C}$, and $q \in \mathbb{R}$. The following statements are equivalent:*

(i) $\forall k \in \mathbb{R} \setminus \{0\}, \quad E^\nu(q) < E^\nu(q-k) + E^0(k)$

(ii) *Any minimizing sequence $(Q_n)_{n\geqslant 1}$ for $E^\nu(q)$ is precompact in $\mathcal{K}$ and converges up to a subsequence towards a minimizer of $E^\nu(q)$.*

Remark 5.1. *This type of condition is usual in the study of atoms and molecules. In non-relativistic theory, there is the same kind of result which is the famous Hunziker-Von Winter-Zhislin (HVZ) theorem [Hun66, Van64, Zhi60]. The HVZ condition* (i) *basically says that an atom is stable if it is energically more favorable to have all the electrons bound to the nucleus than to have a charge k fleeing to infinity while a charge $q-k$ stays near the nucleus.*

Remark 5.2. *The concentration-compactness inequality*

$$E^\nu(q) \leqslant E^\nu(q-k) + E^0(k)$$

is always true, as proved in [HLS09, Prop. 8]. This kind of inequality is usual in concentration-compactness methods developped by P.L. Lions [Lio84].

Proof. We only prove (i)⇒(ii), the other implication (proved in [HLS09, Prop. 8]) being usual in concentration-compactness methods with a problem at infinity which is translation-invariant. We first prove a criterium for the strong convergence of minimizing sequences.

Lemma 5.1. *Let (Q_n) be a minimizing sequence for $E^\nu(q)$ such that $Q_n \rightharpoonup Q$ weakly in $\mathcal{K}$. Then $Q_n \to Q$ strongly in $\mathcal{K}$ if and only if $\mathrm{tr}_{P^0}(Q) = q$.*

Proof. By definition of a minimizing sequence we have $\lim \mathcal{E}^\nu(Q_n) = E^\nu(q)$. If $\mathrm{tr}_{P^0}(Q) = q$ then Q becomes eligible for $E^\nu(q)$ and since $\mathcal{E}^\nu$ is wlsc on $\mathcal{K}$ we have

$$E^\nu(q) \leqslant \mathcal{E}^\nu(Q) \leqslant \liminf \mathcal{E}^\nu(Q_n) \leqslant \limsup \mathcal{E}^\nu(Q_n) = \lim \mathcal{E}^\nu(Q_n) = E^\nu(q),$$

so that Q is a minimizer of $E^\nu(q)$ and all these inequalities are equalities. By the proof of the wls-continuity of $\mathcal{E}^\nu$ it implies that

$$\mathrm{tr}_{P^0}(D^0 Q_n) \to \mathrm{tr}_{P^0}(D^0 Q) \tag{5.3}$$

because each of the terms of the energy is wlsc. First, let us show that $Q_n \to Q$ in $\mathfrak{S}_2$, that is $\mathrm{tr}(Q_n^2) \to \mathrm{tr}(Q^2)$ (because we already have $Q_n \rightharpoonup Q$ in $\mathfrak{S}_2$).

The energy being coercive, the sequence (Q_n) is bounded in $\mathfrak{S}_2$ so that its kernel $(Q_n(x,y))$ is bounded in $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$. Thanks to the cutoff in the Fourier domain, it is also bounded in $H^1(\mathbb{R}^3 \times \mathbb{R}^3)$ so that we can suppose that, at least up to a subsequence, $Q_n(x,y) \to Q(x,y)$ strongly in $L^2_{\mathrm{loc}}(\mathbb{R}^3 \times \mathbb{R}^3)$.

We now introduce two smooth functions $\chi, \xi \in C^\infty([0;\infty);[0;1])$ such that $\chi^2 + \xi^2 = 1$ which will be used to "localize" the sequence (Q_n) to exploit its local convergence. We define them as $\chi(x) = 1$ when $x \in [0;1]$ and $\chi(x) = 0$ when $x \geqslant 2$. We then define $\chi_R(x) := \chi(|x|/R)$ and $\xi_R(x) := \xi(|x|/R)$ for $x \in \mathbb{R}^3$. We note χ_R, ξ_R the multiplication operators by χ_R, ξ_R acting on $\mathfrak{H}_\Lambda$. We have

$$\mathrm{tr}(Q_n^2) = \mathrm{tr}(\chi_R Q_n^2 \chi_R) + \mathrm{tr}(\xi_R Q_n^2 \xi_R)$$

and

$$\lim_{n\to\infty} \mathrm{tr}(\chi_R Q_n^2 \chi_R) = \mathrm{tr}(\chi_R Q^2 \chi_R)$$

by the local strong convergence of $(Q_n(x,y))$. We also have

$$\lim_{R\to\infty} \mathrm{tr}(\chi_R Q^2 \chi_R) = \mathrm{tr}(Q^2)$$

by the dominated convergence theorem. It thus remains to prove that $\mathrm{tr}(\xi_R Q_n^2 \xi_R) \to 0$ to have $\mathrm{tr}(Q_n^2) \to \mathrm{tr}(Q^2)$. That is where the convergence (5.3) is useful. Indeed, we have

$$\mathrm{tr}_{P^0}(D^0 Q_n) = \mathrm{tr}(|D^0|(Q_n^{++} - Q_n^{--}))$$

and

$$\mathrm{tr}(|D^0|Q_n^{++}) = \mathrm{tr}(\chi_R|D^0|Q_n^{++}\chi_R) + \mathrm{tr}(|D^0|\xi_R Q_n^{++}\xi_R) + \mathrm{tr}([\xi_R, |D^0|]Q_n^{++}\xi_R).$$

Since (Q_n^{++}) is bounded in $\mathfrak{S}_1$, we have

$$\left|\mathrm{tr}([\xi_R, |D^0|]Q_n^{++}\xi_R)\right| \leqslant C\|[\xi_R, |D^0|]\|_{\mathcal{B}(\mathfrak{H}_\Lambda)}.$$

It has been proven in [HLS05b, Lemma 1] that

$$\|[\xi_R, |D^0|]\|_{\mathcal{B}(\mathfrak{H}_\Lambda)} \leqslant \frac{C'}{R}.$$

We have

$$\mathrm{tr}_{P^0}(D^0 Q_n) = \mathrm{tr}(\chi_R|D^0|(Q_n^{++} - Q_n^{--})\chi_R) + \mathrm{tr}(|D^0|\xi_R(Q_n^{++} - Q_n^{--})\xi_R) + \mathrm{tr}([\xi_R, |D^0|](Q_n^{++} - Q_n^{--})\xi_R),$$

so that

$$\underbrace{|\,\mathrm{tr}([\xi_R, |D^0|](Q_n^{++} - Q_n^{--})\xi_R)|}_{\leqslant C''/R} + |\,\mathrm{tr}_{P^0}(D^0 Q_n) - \mathrm{tr}(\chi_R|D^0|(Q_n^{++} - Q_n^{--})\chi_R)| \geqslant |\,\mathrm{tr}(|D^0|\xi_R(Q_n^{++} - Q_n^{--})\xi_R)|$$

and

$$|\,\mathrm{tr}(|D^0|\xi_R(Q_n^{++} - Q_n^{--})\xi_R)| \geqslant \mathrm{tr}(|D^0|\xi_R Q_n^2 \xi_R) \geqslant \mathrm{tr}(\xi_R Q_n^2 \xi_R) \geqslant 0,$$

by the Bach inequality (A.1) and the fact that $|D^0| \geqslant 1$. Taking now the limit $n \to \infty$ in this inequality, where we have already seen that

$$\lim_{n\to\infty} \mathrm{tr}(\chi_R|D^0|(Q_n^{++} - Q_n^{--})\chi_R) = \mathrm{tr}(\chi_R|D^0|(Q^{++} - Q^{--})\chi_R),$$

we have

$$C''/R + |\,\mathrm{tr}_{P^0}(D^0 Q) - \mathrm{tr}(\chi_R|D^0|(Q^{++} - Q^{--})\chi_R)| \geqslant \limsup_{n\to\infty} \mathrm{tr}(\xi_R Q_n^2 \xi_R) \geqslant 0.$$

Taking now the limit $R \to \infty$ we finally find that

$$\lim_{R\to\infty} \limsup_{n\to\infty} \mathrm{tr}(\xi_R Q_n^2 \xi_R) = 0.$$

The sequence (Q_n) thus converges towards Q in $\mathfrak{S}_2$. We now have to prove that $Q_n^{++} \to Q^{++}$ and $Q_n^{--} \to Q^{--}$ strongly in $\mathfrak{S}_1$. We just remark that the limit (5.3) follows from the weakly lower semi-continuity of the map $A \mapsto \mathrm{tr}(A)$ for positive operators. The proof of this fact in lemma 4.3 implies that actually, if we denote by $\lambda_i(A)$ the i-th greatest eigenvalue of the trace-class positive operator A,

$$\lambda_i(|D^0|^{1/2}Q_n^{++}|D^0|^{1/2}) \to \lambda_i(|D^0|^{1/2}Q^{++}|D^0|^{1/2}) \quad (n \to \infty) \tag{5.4}$$

$$\lambda_i(|D^0|^{1/2}Q_n^{--}|D^0|^{1/2}) \to \lambda_i(|D^0|^{1/2}Q^{--}|D^0|^{1/2}) \quad (n \to \infty) \tag{5.5}$$

We now use the following lemma proved in [Sim79, Theorem 2.19]

Lemma 5.2 (Grümm's convergence theorem)**.** *Fix $p < \infty$. Suppose that $A_n \to A$ and $A_n^* \to A^*$ in the strong operator topology and $\|A_n\|_{\mathfrak{S}_p} \to \|A\|_{\mathfrak{S}_p}$. Then $\|A_n - A\|_{\mathfrak{S}_p} \to 0$.*

We apply this lemma to the sequences $(|D^0|^{1/2}Q_n^{++}|D^0|^{1/2})$ and $(|D^0|^{1/2}Q_n^{--}|D^0|^{1/2})$ which are sequences of positive self-adjoint operators. Since $Q_n \to Q$ in $\mathfrak{S}_2$ we also have

$$|D^0|^{1/2}Q_n^{++}|D^0|^{1/2} \to |D^0|^{1/2}Q^{++}|D^0|^{1/2}$$

in $\mathfrak{S}_2$ and since the imbedding $\mathfrak{S}_2 \hookrightarrow \mathfrak{S}_\infty$ is continuous, we also have the convergence in $\mathfrak{S}_\infty$, and the first hypothesis of Grümm's lemma is verified. Moreover, the limit (5.4) implies that

$$\||D^0|^{1/2}Q_n^{++}|D^0|^{1/2}\|_{\mathfrak{S}_1} \to \||D^0|^{1/2}Q^{++}|D^0|^{1/2}\|_{\mathfrak{S}_1}$$

since all the eigenvalues are positive. Hence, we have by Grümm's lemma

$$\||D^0|^{1/2}(Q_n^{++} - Q^{++})|D^0|^{1/2}\|_{\mathfrak{S}_1} \to 0.$$

Finally, by the continuity of the map $A \in \mathfrak{S}_1 \mapsto KA \in \mathfrak{S}_1$ for K bounded operator,

$$\|Q_n^{++} - Q^{++}\|_{\mathfrak{S}_1} \leqslant \||D^0|^{-1/2}\|_{\mathrm{op}}^2 \||D^0|^{1/2}(Q_n^{++} - Q^{++})|D^0|^{1/2}\|_{\mathfrak{S}_1} \to 0.$$

We do the same for Q_n^{--} and we finally have $Q_n \to Q$ in $\mathfrak{S}_1^{P^0}$.

The other implication is trivial since the strong convergence implies the conservation of the charge. □

We end the proof by contradiction. We assume that there exists a minimizing sequence (Q_n) for $E^\nu(q)$ which not precompact in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$. Since $\mathcal{E}^\nu(Q_n) \to E^\nu(q)$ and $\mathcal{E}^\nu$ is coercive, the sequence (Q_n) is bounded in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$ so that we can assume that $Q_n \rightharpoonup Q$ weakly and that $Q_n \nrightarrow Q$ strongly. According to lemma 5.1, it is equivalent to the fact that $\mathrm{tr}_{P^0}(Q) \neq q$. We set $\mathrm{tr}_{P^0}(Q) = q - k$ with $k \in \mathbb{R} \setminus \{0\}$ and then prove that this implies

$$E^\nu(q) \geqslant E^\nu(q-k) + E^0(k),$$

which contradicts (i).

The idea is to show that the sequence (Q_n) splits into a compact part and a part that goes to infinity, as usual for concentration-compactness methods. However, the issue about this splitting of (Q_n) is to keep the constraint given by the definition of $\mathcal{K}$. We cannot just localize Q_n by taking the operator $\chi_R Q_n \chi_R$ since it does not respect the constraint $-P^0 \leqslant \chi_R Q_n \chi_R \leqslant 1 - P^0$ for $Q_n \in \mathcal{K}$. We thus have to define adapted localization operators.

Localization operators. From now on we use the notation $P_+^0 := 1 - P^0$. We define

$$X_R := P^0 \chi_R P^0 + P_+^0 \chi_R P_+^0. \tag{5.6}$$

We obviously have $0 \leqslant X_R \leqslant 1$ so that we can define Y_R as the unique non-negative operator verifying $X_R^2 + Y_R^2 = 1$. The important property satisfied by X_R, Y_R is that they commute with P^0. They also verify the following properties

Lemma 5.3. *The localization operators X_R, Y_R are continuous on $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$, that is there exists $C > 0$ independent of Λ, R such that*

$$\forall Q \in \mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda), \quad \|X_R Q X_R\|_{1;P^0} + \|Y_R Q Y_R\|_{1;P^0} \leqslant C\|Q\|_{1:P^0}.$$

Moreover, if Q belongs to $\mathcal{K}$, $X_R Q X_R$ and $Y_R Q Y_R$ also do.

Proof. Since $0 \leqslant \chi_R \leqslant 1$, one can see that $\|X_R\|_{\mathfrak{S}_\infty}, \|Y_R\|_{\mathfrak{S}_\infty} \leqslant 1$ so that

$$\|X_R Q X_R\|_{\mathfrak{S}_2} \leqslant \|X_R\|^2_{\mathfrak{S}_\infty} \|Q\|_{\mathfrak{S}_2} \leqslant \|Q\|_{\mathfrak{S}_2},$$

because the map $A \in \mathfrak{S}_2 \mapsto AK \in \mathfrak{S}_2$ is continuous for $K \in \mathfrak{S}_\infty$. Moreover,

$$[X_R, P^0] = 0 \Rightarrow \|(X_R Q X_R)^{--}\|_{\mathfrak{S}_1} = \|X_R Q^{--} X_R\|_{\mathfrak{S}_1} \leqslant \|Q^{--}\|_{\mathfrak{S}_1}.$$

The same result holds for Y_R. Finally, since $-P^0 \leqslant Q \leqslant P^0_+$, we have

$$X_R Q X_R \leqslant X_R P^0_+ X_R = (P^0_+ \chi_R P^0_+)^2 \leqslant P^0_+ \chi_R^2 P^0_+ \leqslant P^0_+.$$

We show that $X_R Q X_R \geqslant -P^0$ by the same argument.

For Y_R we just remark that if we have $0 \leqslant Q + P^0 \leqslant 1$, then

$$\begin{array}{rccl} 0 \leqslant & Y_R(Q+P^0)Y_R & \leqslant Y_R^2 = 1 - X_R^2 & (Y_R^* = Y_R) \\ 0 \leqslant & Y_R Q Y_R + P^0 - X_R^2 P^0 & \leqslant 1 - X_R^2 & \\ \underbrace{X_R P^0 X_R}_{\geqslant 0} \leqslant & Y_R Q Y_R + P^0 & \leqslant 1 - \underbrace{P^0_+ X_R^2}_{= X_R P^0_+ X_R} & (P^0 - 1 = -P^0_+), \end{array}$$

since X_R commutes with P^0_+. We just remark that $0 \leqslant X_R P^0_+ X_R \leqslant 1$ because X_R is selfadjoint and $A \leqslant B \Rightarrow CAC^* \leqslant CBC^*$. Finally we have

$$0 \leqslant Y_R Q Y_R + P^0 \leqslant 1,$$

hence $Y_R Q Y_R \in \mathcal{K}$.

□

Lemma 5.4. *We have the following limits*

$$\lim_{R\to\infty} \|X_R - \chi_R\|_{\mathfrak{S}_\infty} = 0, \quad \lim_{R\to\infty} \|Y_R - \xi_R\| = 0. \tag{5.7}$$

For $Q \in \mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$, one has

$$\lim_{R\to\infty} \|X_R Q X_R - Q\|_{1;P^0} = 0, \quad \lim_{R\to\infty} \|Y_R Q Y_R\|_{1;P^0} = 0. \tag{5.8}$$

Proof. We have $X_R - \chi_R = [P^0, \chi_R]P^0 + [P^0_+, \chi_R]P^0_+$. In the Fourier domain, P^0 is a multiplication operator since for any $p \in \mathbb{R}^3$, in a diagonalization basis of $D^0(p)$, it multiplies by a matrix of the form

$$\left[\begin{array}{cc} 0 & 0 \\ 0 & I_2 \end{array}\right].$$

The transformation matrix to a diagonalization basis of $D^0(p)$ is given explicitly in [Tha92] and depends smoothly on the variable p, so that P^0 is a multiplication operator by the matrices $f(p)$ in the Fourier domain with f smooth on $\mathbb{R}^3$. Now let $\varphi, \psi \in \mathfrak{H}_\Lambda$. We compute

$$\begin{array}{rcl} \langle \psi, [P^0, \chi_R]\varphi \rangle & = & \displaystyle\iint_{\mathbb{R}^6} \widehat{\chi_R}(p-q)\overline{\widehat{\psi}(p)}\widehat{\varphi}(q)\,(f(p) - f(q))\,\mathrm{d}p\mathrm{d}q \\ & = & \displaystyle\iint_{B(0;\Lambda)^2} \widehat{\chi_R}(r)\overline{\widehat{\psi}(s+\frac{r}{2})}\widehat{\varphi}(s-\frac{r}{2})\left(f(s+\frac{r}{2}) - f(s-\frac{r}{2})\right)\mathrm{d}r\mathrm{d}s. \end{array}$$

Since f is smooth and $B(0;\Lambda)$ is compact we have $|f(s+r/2)-f(s-r/2)| \leqslant |r|M$ for some $M>0$ on $B(0;\Lambda)^2$. Hence

$$|\langle\psi,[P^0,\chi_R]\varphi\rangle| \leqslant M\left(\int_{B(0;\Lambda)}|r\widehat{\chi_R}(r)|\,\mathrm{d}r\right)\|\widehat{\psi}\|_{L^2}\|\widehat{\varphi}\|_{L^2},$$

so that

$$\|[P^0,\chi_R]\|_{\mathfrak{S}_\infty} \leqslant \int_{B(0;\Lambda)}|r\widehat{\chi_R}(r)|\,\mathrm{d}r = \frac{C}{R}\int_{B(0;\Lambda)}|r\widehat{\chi_1}(r)|\,\mathrm{d}r = O(1/R).$$

This also proves that $\lim_{R\to\infty}\|X_R^2-\chi_R^2\|=0$ since $\|X_R\|,\|\chi_R\|\leqslant 1$ and

$$X_R^2-\chi_R^2 = X_R(X_R-\chi_R)+(X_R-\chi_R)\chi_R.$$

The square root being a monotone operator we have the following theorem from [Bha97, Theorem X.1.1]:

Theorem 5.2. *Let f be an operator monotone function on $\mathbb{R}_+$ such that $f(0)=0$. Then for all positive operators A,B,*

$$\|f(A)-f(B)\| \leqslant f(\|A-B\|).$$

Applying this theorem we obtain

$$\|Y_R-\xi_R\| \leqslant \|Y_R^2-\xi_R^2\|^{1/2} = \|X_R^2-\chi_R^2\|^{1/2} \to 0 \quad (R\to\infty).$$

We now want to prove that $\|X_RQX_R-Q\|_{1;P^0}\to 0$ for any $Q\in\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$. It is enough to prove it for Q of the form $|\varphi\rangle\langle\varphi|$ by density of the finite rank operators in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$ and by the uniform boundedness of $(X_R)_R$. It is enough to show that $\chi_R|\varphi\rangle\langle\varphi|\chi_R-|\varphi\rangle\langle\varphi|\to 0$ in $\mathfrak{S}_1$ by (5.7). But this is obvious since $\chi_R\varphi\to\varphi$ in $\mathfrak{H}_\Lambda$ by dominated convergence. We can use the exact same argument for Y_R, using again (5.7). □

Lemma 5.5. *For any R, X_R and $1-Y_R$ are in $\mathfrak{S}_1(\mathfrak{H}_\Lambda)$ and in particular are compact. The map $Q\mapsto X_RQX_R$ is also compact: if $Q_n\rightharpoonup Q$ in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$, then $X_RQ_nX_R\to X_RQX_R$ in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$. It is also true when we replace X_R by $1-Y_R$.*

Proof. We use the Kato-Seiler-Simon inequality [Sim79, Theorem 4.1]

$$\|f(-i\nabla)g(x)\|_{\mathfrak{S}_2} \leqslant C\|f\|_{L^2}\|g\|_{L^2},$$

where $f(-i\nabla)$ denotes a translation-invariant operator acting by the multiplication by $f(p)$ in the Fourier domain, and $g(x)$ denotes a multiplication operator acting on L^2. We thus obtain

$$\|X_R\|_{\mathfrak{S}_1} = \|P^0\sqrt{\chi_R}\|_{\mathfrak{S}_2}^2+\|P_+^0\sqrt{\chi_R}\|_{\mathfrak{S}_2}^2 \leqslant 2C|B(0;\Lambda)|R\int_{\mathbb{R}^3}\chi,$$

which proves that X_R is trace-class for any fixed R. We then have

$$0\leqslant 1-Y_R\leqslant 1-Y_R^2=X_R^2\leqslant X_R,$$

so that $1-Y_R\in\mathfrak{S}_1$. Now let $Q_n\rightharpoonup Q$ in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$. The compactness of the map $Q\mapsto X_RQX_R$ can actually be shown for any $A\in\mathfrak{S}_1$ instead of X_R. Indeed, by density of the finite rank operators in $\mathfrak{S}_1$ it is sufficient to prove that

$$|\varphi\rangle\langle\varphi|Q_n|\varphi\rangle\langle\varphi|\to|\varphi\rangle\langle\varphi|Q|\varphi\rangle\langle\varphi|.$$

We just remark that

$$|\varphi\rangle\langle\varphi|Q_n|\varphi\rangle\langle\varphi| = \underbrace{\mathrm{tr}(Q_n|\varphi\rangle\langle\varphi|)}_{\to \mathrm{tr}(Q|\varphi\rangle\langle\varphi|)}|\varphi\rangle\langle\varphi|,$$

by definition of $Q_n \rightharpoonup Q$. We do the exact same thing for $1 - Y_R \in \mathfrak{S}_1$. □

We are now nearly able to conclude. Let us consider our minimizing sequence (Q_n) which converges weakly towards Q in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$. We can write

$$\begin{aligned}\mathrm{tr}_{P^0}(D^0 Q_n) = \mathrm{tr}_{P^0}(D^0 X_R Q_n X_R) + \mathrm{tr}_{P^0}(D^0 Y_R Q_n Y_R) + \mathrm{tr}([X_R, |D^0|](Q_n^{++} - Q_n^{--})X_R) \\ + \mathrm{tr}([Y_R, |D^0|](Q_n^{++} - Q_n^{--})Y_R). \quad (5.9)\end{aligned}$$

Notice that we have used the fact that X_R, Y_R commute with P^0, P_+^0 in the computation of the last two terms. We have

$$|\,\mathrm{tr}([X_R, |D^0|](Q_n^{++} - Q_n^{--}X_R))| \leqslant C\|[X_R, |D^0|]\|_{\mathfrak{S}_\infty},$$

since $(Q_n^{++}), (Q_n^{--})$ are bounded in $\mathfrak{S}_1$ and $\|X_R\| \leqslant 1$. Hence

$$\begin{aligned}\mathrm{tr}_{P^0}(D^0 Q_n) \geqslant \mathrm{tr}_{P^0}(D^0 Q) + \mathrm{tr}_{P^0}(D^0 Y_R Q_n Y_R) + \mathrm{tr}_{P^0}(D^0 X_R (Q_n - Q) X_R) \\ + \mathrm{tr}_{P^0}(D^0(X_R Q X_R - Q)) - C(\|X_R, |D^0|\|_{\mathfrak{S}_\infty} + \|[Y_R, |D^0|]\|_{\mathfrak{S}_\infty}). \quad (5.10)\end{aligned}$$

To treat the direct term we use

Lemma 5.6. *Let (R_n) be a sequence in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$ such that $R_n \rightharpoonup 0$. Then for a fixed R,*

$$\lim_{n\to\infty} \|\rho_{R_n} - \rho_{Y_R R_n Y_R}\|_{\mathcal{C}} = 0.$$

Proof. We have

$$R_n - Y_R R_n Y_R = -(1 - Y_R)R_n(1 - Y_R) + R_n(1 - Y_R) + (1 - Y_R)R_n.$$

By lemma 5.5, $(1 - Y_R)R_n(1 - Y_R) \to 0$. Then, $1 - Y_R \in \mathfrak{S}_1$ so that we can approach it by finite-rank operators. It is then sufficient to prove that, denoting by $S_n := R_n|\varphi\rangle\langle\varphi|$,

$$\rho_{S_n} \to 0, \quad \varphi \in \mathfrak{H}_\Lambda \cap L^1.$$

It is easy to see that the integral kernel of S_n is

$$S_n(x, y) = \int_{\mathbb{R}^3} R_n(x, z)\varphi(z)\varphi(y)^* \,\mathrm{d}z,$$

so that

$$\rho_{S_n}(x) = \mathrm{Tr}_{\mathbb{C}^4}(S_n(x, x)) = \int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^4}(R_n(x, y)\varphi(y)\varphi(x)^*) \,\mathrm{d}x.$$

Hence

$$\|\rho_{S_n}\|_{L^1} \leqslant \iint_{\mathbb{R}^6} \|R_n(x, y)\||\varphi(y)||\varphi(x)| \,\mathrm{d}x\mathrm{d}y.$$

Since $R_n \rightharpoonup 0$, we can assume that the convergence is also in L^2_{loc} thanks to the cutoff in the Fourier domains which guarantees that (R_n) is actually bounded in every H^s. For any $K \subset \mathbb{R}^6$ a compact set, $R_n \to 0$ in $L^2(K)$ and, again thanks to the Fourier cutoff, in any $H^s(K)$ so that for s large enough, $R_n \to 0$ in $C^0(K)$. We can thus assume that $R_n \to 0$ uniformly on every

compact set of $\mathbb{R}^6$. Since $\varphi \in L^1$, $\|\rho_{S_n}\|_{L^1} \to 0$ by dominated convergence, hence $\|\widehat{\rho_{S_n}}\|_{L^\infty} \to 0$ and also $\|\rho_{S_n}\|_{\mathcal{C}} \to 0$ since

$$\int_{B(0;\Lambda)} \frac{|\widehat{\rho_{S_n}}(k)|^2}{|k|^2}\,\mathrm{d}k \leqslant \|\widehat{\rho_{S_n}}\|_{L^\infty}^2 \int_{B(0;\Lambda)} \frac{\mathrm{d}k}{|k|^2}.$$

□

Let us now finish the proof of the theorem.

$$\begin{aligned} D(\rho_{Q_n},\rho_{Q_n}) &= D(\rho_Q,\rho_Q) + D(\rho_{Y_R(Q_n-Q)Y_R},\rho_{Y_R(Q_n-Q)Y_R}) + \varepsilon_1^R(n) \\ &\geqslant D(\rho_Q,\rho_Q) + D(\rho_{Y_RQ_nY_R},\rho_{Y_RQ_nY_R}) + \varepsilon_1^R(n) - C_1\|\rho_{Y_RQY_R}\|_{\mathcal{C}}^2, \end{aligned}$$

where we have used that the sequence (Q_n) is bounded in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$ in the last term, C_1 being a constant independent of R and n. We also have

$$D(\rho_{Q_n},\nu) = D(\rho_Q,\nu) + \varepsilon_2(n),$$

where $\varepsilon_2(n) = D(\rho_{Q_n-Q},\nu) \to 0$ as $n \to \infty$ since $Q_n \rightharpoonup Q \Rightarrow \rho_{Q_n} \rightharpoonup \rho_Q$ in $\mathcal{C}$, and

$$\begin{aligned} \varepsilon_1^R(n) &= \|\rho_{Q_n-Q}\|_{\mathcal{C}}^2 - \|\rho_{Y_R(Q_n-Q)Y_R}\|_{\mathcal{C}}^2 + 2D(\rho_{Q_n-Q},\rho_Q) \\ &= D(\underbrace{\rho_{Q_n-Q} - \rho_{Y_R(Q_n-Q)Y_R}}_{\to 0\,(n\to\infty)\text{ by lemma 5.6}}, \underbrace{\rho_{Q_n-Q} + \rho_{Y_R(Q_n-Q)Y_R}}_{\text{bounded}}) + 2\,\underbrace{D(\rho_{Q_n-Q},\rho_Q)}_{\to 0\,(Q_n\to Q)}, \end{aligned}$$

so that $\varepsilon_1^R(n) \to 0$ as $n \to \infty$. We thus have for the total energy

$$\begin{aligned} \mathcal{E}^\nu(Q_n) \geqslant \mathcal{E}^\nu(Q) + \mathcal{E}^0(Y_RQ_nY_R) + \varepsilon_1^R(n) - \varepsilon_2(n) + \mathrm{tr}_{P^0}(D^0X_R(Q_n-Q)X_R) \\ + \mathrm{tr}_{P^0}(D^0(X_RQX_R-Q)) - C(\|[Y_R,|D^0|]\|_{\mathfrak{S}_\infty} + \|[X_R,|D^0|]\|_{\mathfrak{S}_\infty}) - C_1\|\rho_{Y_RQY_R}\|_{\mathcal{C}}^2. \quad (5.11) \end{aligned}$$

Notice that

$$q = \mathrm{tr}_{P^0}(Q_n) = \mathrm{tr}_{P^0}(X_RQ_nX_R) + \mathrm{tr}_{P^0}(Y_RQ_nY_R),$$

where we have used $[P^0,X_R] = 0 = [P^0,Y_R]$. Moreover,

$$\begin{aligned} \mathcal{E}^\nu(Q) + \mathcal{E}^0(Y_RQ_nY_R) &\geqslant E^\nu(q-k) + E^0(\mathrm{tr}_{P^0}(Y_RQ_nY_R)) \\ &= E^\nu(q-k) + E^0(q - \mathrm{tr}_{P^0}(X_RQ_nX_R)). \end{aligned}$$

We now pass to the limit $n \to \infty$ in the inequality (5.11) with a fixed R, using lemma 5.5, the boundedness of D^0 and the continuity of the map $q \mapsto E^\nu(q)$ proved in [HLS09, Corollary 9]:

$$\begin{aligned} E^\nu(q) \geqslant E^\nu(q-k) + E^0(q - \mathrm{tr}_{P^0}(X_RQX_R)) + \mathrm{tr}_{P^0}(D^0(X_RQX_R-Q)) \\ - C(\|[Y_R,|D^0|]\|_{\mathfrak{S}_\infty} + \|[X_R,|D^0|]\|_{\mathfrak{S}_\infty}) - C_1\|\rho_{Y_RQY_R}\|_{\mathcal{C}}^2 \quad (5.12) \end{aligned}$$

Using now lemma 5.4 and the boundedness of $|D^0|$ we have

$$\lim_{R\to\infty} \|[X_R,|D^0|]\|_{\mathfrak{S}_\infty} = \lim_{R\to\infty} \|[\chi_R,|D^0|]\|_{\mathfrak{S}_\infty} = 0,$$

and by the same argument the same result holds for Y_R. Finally, we pass to the limit $R \to \infty$ in the inequality (5.12). Using again lemma 5.4, the continuity of the maps $Q \mapsto \rho_Q$, $q \mapsto E^\nu(q)$, and the boundedness of D^0, we get

$$E^\nu(q) \geqslant E^\nu(q-k) + E^0(k),$$

which contradicts the hypothesis (i) and proves the theorem. □

5.2 The Thermodynamic limit

We have seen that there exists minimizers of the energy with charge constraints under a binding condition. We now want to prove the convergence of the lowest energy in a box towards the lowest energy in the whole space. We recall the context in the box $C_L = [-L/2; L/2[^3$. We consider the lowest energy

$$E^{L,\nu}(q) := \inf\left\{\mathcal{E}^{L,\nu}(Q), \quad Q \in \mathcal{Q}_\Lambda^L(q)\right\},$$

where

$$\begin{aligned}
\mathcal{E}^{L,\nu}(Q) &= \mathrm{tr}(D^L Q) - \alpha D_L(\rho_Q, \nu_L) + \frac{\alpha}{2} D_L(\rho_Q, \rho_Q) \\
\mathcal{Q}_\Lambda^L(q) &:= \left\{Q \in \mathcal{Q}_\Lambda^L, \quad \mathrm{tr}(Q) = q\right\} \\
\mathcal{Q}_\Lambda^L &:= \left\{Q \in \mathcal{L}(\mathfrak{H}_\Lambda^L), \quad Q^* = Q, \quad -P_L^0 \leqslant Q \leqslant 1 - P_L^0\right\}.
\end{aligned}$$

Notice that the charge constraint is here $\mathrm{tr}(Q) = q$ while one would have expected $\mathrm{tr}_{P_L^0}(Q)$ as in the whole space. Indeed, since we work in a finite-dimensional setting thanks to the box, any operator in $\mathcal{Q}_\Lambda^L$ is trace-class (it is a matrix!), hence $\mathrm{tr}(Q) = \mathrm{tr}_{P_L^0}(Q)$. Moreover, the finite-dimensional setting also implies that the variational set $\mathcal{Q}_\Lambda^L(q)$ is compact and not empty for L large enough (because of the charge constraint), so that by the strong continuity of the energy, the existence of a minimizer for $E^{L,\nu}(q)$ is completely straightforward.

We then want to prove the following theorem.

Theorem 5.3. *Let $\Lambda > 0$, $\nu \in \mathcal{C}$ and $q \in \mathbb{R}$. Then we have the thermodynamic limit*

$$\boxed{\lim_{L\to\infty} E^{L,\nu}(q) = E^\nu(q).} \tag{5.13}$$

The proof of this theorem is split into two steps:

$$\limsup_{L\to\infty} E^{L,\nu}(q) \leqslant E^\nu(q) \tag{5.14}$$

$$\liminf_{L\to\infty} E^{L,\nu}(q) \geqslant E^\nu(q) \tag{5.15}$$

We adapt the proofs of [HLS07, Theorem 2.9] and [CDL08, Theorem 5]. The inequality (5.14) consists in establishing that the infimum on the left side of the inequality is lower than the energy of a minimizer in the whole space. In order to do so, we just have to restrain the minimizer in the whole space to the box C_L in a way that it becomes eligible for the minimization problem in a box $E^{L,\nu}(q)$ and its energy in a box stays close to its energy in the whole space, which is $E^\nu(q)$ by definition.

Restraining an operator in the whole space to the box C_L, that is for $Q \in \mathcal{L}(\mathfrak{H}_\Lambda)$ associating a $\widetilde{Q} \in \mathcal{L}(\mathfrak{H}_\Lambda^L)$, is not a trivial task. It is easier to do so for an operator which has a finite-rank, that is a finite linear combination of projectors $|\varphi\rangle\langle\varphi|$,$\varphi \in \mathfrak{H}_\Lambda$, because we just have to associate to φ a $\widetilde{\varphi} \in \mathfrak{H}_\Lambda^L$ which we can do through the Fourier transform. Furthermore, it has been proved in [HLS09, Proposition 5] that finite-rank operators are dense in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$ and since the energy is strongly continuous for this topology, there exists a minimizing sequence for $E^\nu(q)$ which consists of finite-rank operators.

Moreover, one can choose explicitly this minimizing sequence according to [HLS09, Proposition 5] and [HLS09, Theorem 5]. They indeed prove that there exists an orthonormal basis

$(v_i)_{i\geqslant -N}$ of $\mathfrak{H}_\Lambda^+ := (1-P^0)\mathfrak{H}_\Lambda$, an orthonormal basis $(u_i)_{i\geqslant -M}$ of $\mathfrak{H}_\Lambda^- := P^0\mathfrak{H}_\Lambda$, a sequence $(\lambda_i)_{i\geqslant 0} \in \ell^2(\mathbb{R}^+)$, and a finite-rank γ with $0 \leqslant \gamma \leqslant 1$, such that the sequence $(Q_K) \in \mathcal{Q}_\Lambda(q)$ defined by

$$Q_K = \sum_{i=-N}^{-1} |v_i\rangle\langle v_i| - \sum_{i=-M}^{-1} |u_i\rangle\langle u_i| + \sum_{i=0}^{K} \frac{\lambda_i^2}{1+\lambda_i^2}(|v_i\rangle\langle v_i| - |u_i\rangle\langle u_i|) + \sum_{i=0}^{K} \frac{\lambda_i}{1+\lambda_i^2}(|u_i\rangle\langle v_i| + |v_i\rangle\langle u_i|) + \gamma, \quad (5.16)$$

is a minimizing sequence for $E^\nu(q)$. Moreover, we have

$$\gamma(Q_K - \gamma + P^0) = (Q_K - \gamma + P^0)\gamma = 0. \quad (5.17)$$

We now explain how to confine this operator in a box. We define an operator

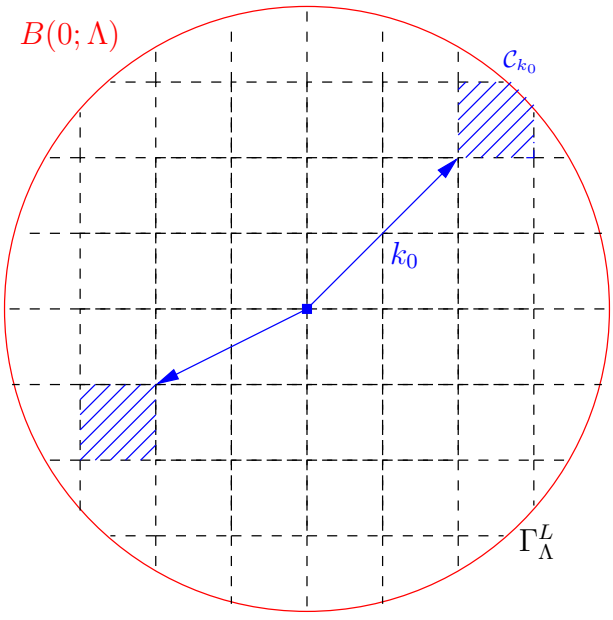
$$i_L : \mathfrak{H}_\Lambda^L \longrightarrow \mathfrak{H}_\Lambda,$$

by defining its action on the Fourier domain. Recall that in the Fourier domain, functions in $\mathfrak{H}_\Lambda^L$ are only defined on the lattice

$$\Gamma_\Lambda^L = \frac{2\pi}{L}\mathbb{Z}^3 \cap B(0;\Lambda),$$

while functions in $\mathfrak{H}_\Lambda$ are defined on the whole ball $B(0;\Lambda)$. Hence, defining i_L is the same as defining an application $\Gamma_\Lambda^L \to B(0;\Lambda)$. Before doing so, let us define a 4×4 matrix $U(k)$ for each $k \in B(0;\Lambda)$. For such a k, let $k_0 = (k_0^1, k_0^2, k_0^3)$ be the unique element of Γ_Λ^L such that k belongs to the "cube"

$$\mathcal{C}_{k_0} := \left(k_0 + \left(\frac{2\pi}{L}\right)\left[0; \frac{k_0^1}{|k_0^1|}\right[\times \left[0; \frac{k_0^2}{|k_0^2|}\right[\times \left[0; \frac{k_0^3}{|k_0^3|}\right[\right) \cap B(0;\Lambda).$$



Such a choice for $\mathcal{C}_{k_0}$ ensures that $|k| \geqslant |k_0|$ for all $k \in \mathcal{C}_{k_0}$, which will have its importance later. We now recall that $D^0(k_0)$ is a self-adjoint 4×4 matrix with two eigenvalues of multiplicity 2: $\lambda(k_0) := \sqrt{1+k_0^2}$ and $-\lambda(k_0)$. Hence, there exists a unitary matrix $V(k_0)$ such that (see [Tha92])

$$V^*(k_0)D^0(k_0)V(k_0) = \begin{bmatrix} \lambda(k_0)I_2 & 0 \\ 0 & -\lambda(k_0)I_2 \end{bmatrix}.$$

We thus define U by the formula

$$U(k) = V(k)V^*(k_0). \tag{5.18}$$

The action of $U(k)$ over $\mathbb{C}^4$ is to map the eigenspace of $D^0(k_0)$ linked to the eigenvalue $\lambda(k_0)$ (resp. $-\lambda(k_0)$), which we denote by $\mathfrak{H}_\Lambda^+(k_0)$ (resp. $\mathfrak{H}_\Lambda^-(k_0)$), to the eigenspace of $D^0(k)$ linked to the eigenvalue $\lambda(k)$ (resp. $-\lambda(k)$), that is $\mathfrak{H}_\Lambda^+(k)$ (resp. $\mathfrak{H}_\Lambda^-(k)$). Actually, $U(k)$ is an isometry

$$U(k) : \mathfrak{H}_\Lambda^\pm(k_0) \longrightarrow \mathfrak{H}_\Lambda^\pm(k).$$

Let us now define for any $k_0 \in \Gamma_\Lambda^L$ a function

$$\chi_{k_0} : B(0;\Lambda) \longrightarrow \mathbb{R}$$

such that

$$\mathrm{supp}\chi_{k_0} \subset \mathcal{C}_{k_0}, \quad \int \chi_{k_0}^2 = 1.$$

Typically, one can consider $\chi_{k_0} = (2\pi/L)^{-3/2}\mathbf{1}_{\mathcal{C}_{k_0}}$, the characteristic function of the cube $\mathcal{C}_{k_0}$. We are now able to define the operator i_L. Let $f \in \mathfrak{H}_\Lambda^L$, then $i_L(f) \in \mathfrak{H}_\Lambda$ is defined by

$$\forall k \in B(0;\Lambda), \qquad \widehat{i_L(f)}(k) = \left(\frac{2\pi}{L}\right)^{3/2} \sum_{k_0 \in \Gamma_\Lambda^L} U(k)\widehat{f}(k_0)\chi_{k_0}(k). \tag{5.19}$$

In words, the Fourier transform of $i_L(f)$ in k is defined by the value of the Fourier transform of f in k_0 where k_0 is the unique element of the lattice Γ_Λ^L such that $k \in \mathcal{C}_{k_0}$. Let us now detail the properties satisfied by the operator i_L.

Proposition 5.1. *1. The operator $i_L : \mathfrak{H}_\Lambda^L \to \mathfrak{H}_\Lambda$ is an isometry;*

2. The adjoint $i_L^* : \mathfrak{H}_\Lambda \to \mathfrak{H}_\Lambda^L$ of i_L is defined by

$$\forall g \in \mathfrak{H}_\Lambda, \quad \forall k_0 \in \Gamma_\Lambda^L, \quad \widehat{i_L^* g}(k_0) = \left(\frac{2\pi}{L}\right)^{-3/2} \int_{B(0;\Lambda)} U^*(k)\widehat{g}(k)\chi_{k_0}(k)\, dk;$$

3. $i_L^* i_L = Id_{\mathfrak{H}_\Lambda^L}$ but for any $f \in \mathfrak{H}_\Lambda$ we only have

$$i_L i_L^* f \to f \quad (L \to \infty);$$

4. (Intertwinning property) $i_L P_L^0 = P^0 i_L$ and $i_L^* P^0 = P_L^0 i_L^*$;

5. (Kinetic energy)

$$\|i_L^* D^0 i_L - D_L^0\|_{\mathcal{L}(\mathfrak{H}_\Lambda^L)} = O(1/L).$$

Proof. 1. Let $f \in \mathfrak{H}^L_\Lambda$. Then

$$\begin{aligned}
\int_{\mathbb{R}^3} |i_L f(x)|^2 \,\mathrm{d}x &= \int_{B(0;\Lambda)} |\widehat{i_L f}(k)|^2 \,\mathrm{d}k \\
&= \left(\frac{2\pi}{L}\right)^3 \sum_{k_0,k_0' \in \Gamma^L_\Lambda} \int_{B(0;\Lambda)} \langle U(k)\widehat{f}(k_0), U(k)\widehat{f}(k_0')\rangle_{\mathbb{C}^4} \chi_{k_0}(k)\chi_{k_0'}(k) \,\mathrm{d}k \\
&= \left(\frac{2\pi}{L}\right)^3 \sum_{k_0 \in \Gamma^L_\Lambda} \int_{B(0;\Lambda)} |U(k)\widehat{f}(k_0)|^2 \chi^2_{k_0}(k) \,\mathrm{d}k \qquad (k_0 \neq k_0' \Rightarrow \chi_{k_0}\chi_{k_0'} = 0) \\
&= \left(\frac{2\pi}{L}\right)^3 \sum_{k_0 \in \Gamma^L_\Lambda} \int_{B(0;\Lambda)} |\widehat{f}(k_0)|^2 \chi^2_{k_0}(k) \,\mathrm{d}k \qquad (U \text{ isometry}) \\
&= \left(\frac{2\pi}{L}\right)^3 \sum_{k_0 \in \Gamma^L_\Lambda} |\widehat{f}(k_0)|^2 = \int_{\mathbb{T}_L} |f|^2 \qquad \left(\int \chi^2_{k_0} = 1\right).
\end{aligned}$$

Hence i_L is an isometry.

2. Let $f \in \mathfrak{H}^L_\Lambda$ and $g \in \mathfrak{H}_\Lambda$. Then

$$\begin{aligned}
\langle i_L f, g\rangle_{\mathfrak{H}_\Lambda} &= \int_{B(0;\Lambda)} \langle \widehat{i_L f}(k), \widehat{g}(k)\rangle_{\mathbb{C}^4} \,\mathrm{d}k \\
&= \left(\frac{2\pi}{L}\right)^{3/2} \sum_{k_0 \in \Gamma^L_\Lambda} \langle \widehat{f}(k_0), \int_{B(0;\Lambda)} U^*(k)\widehat{g}(k)\chi_{k_0}(k) \,\mathrm{d}k\rangle_{\mathbb{C}^4} \\
&= \langle f, i_L^* g\rangle_{\mathfrak{H}^L_\Lambda},
\end{aligned}$$

with $\widehat{i_L^* g}(k_0)$ given by the formula in the proposition.

3. Let $f \in \mathfrak{H}^L_\Lambda$. Then for any $k_0 \in \Gamma^L_\Lambda$ we have

$$\begin{aligned}
\widehat{i_L^* i_L f}(k_0) &= \left(\frac{2\pi}{L}\right)^{-3/2} \int_{B(0;\Lambda)} U^*(k)\widehat{i_L f}(k)\chi_{k_0}(k) \,\mathrm{d}k \\
&= \sum_{k' \in \Gamma^L_\Lambda} \int_{B(0;\Lambda)} U^*(k)U(k)\widehat{f}(k')\chi_{k'}(k)\chi_{k_0}(k) \,\mathrm{d}k \\
&= \widehat{f}(k_0) \int_{B(0;\Lambda)} \chi^2_{k_0}(k) \,\mathrm{d}k = \widehat{f}(k_0).
\end{aligned}$$

Thus we have $i_L^* i_L = \mathrm{Id}_{\mathfrak{H}^L_\Lambda}$. Conversely, if $g \in \mathfrak{H}_\Lambda$, then for any $k \in B(0;\Lambda)$

$$\begin{aligned}
\widehat{i_L i_L^* g}(k) &= \left(\frac{2\pi}{L}\right)^{3/2} \sum_{k_0 \in \Gamma^L_\Lambda} U(k)\widehat{i_L^* g}(k_0)\chi_{k_0}(k) \\
&= \sum_{k_0 \in \Gamma^L_\Lambda} \int_{B(0;\Lambda)} U(k)U^*(k')\widehat{g}(k')\chi_{k_0}(k')\chi_{k_0}(k) \,\mathrm{d}k' \\
&= U(k) \int_{B(0;\Lambda)} U^*(k')\widehat{g}(k') \left[\sum_{k_0 \in \Gamma^L_\Lambda} \chi_{k_0}(k')\chi_{k_0}(k)\right] \,\mathrm{d}k'.
\end{aligned}$$

One can remark that for any $\varphi \in C^\infty(\mathbb{R}^3)$,

$$T_k\varphi := \int_{B(0;\Lambda)} \left[\sum_{k_0 \in \Gamma_\Lambda^L} \chi_{k_0}(k')\chi_{k_0}(k) \right] \varphi(k')\,\mathrm{d}k' \longrightarrow \varphi(k) \qquad (L \to \infty).$$

Indeed,

$$\begin{aligned} |T_k\varphi - \varphi(k)| &= \left| \sum_{k_0 \in \Gamma_\Lambda^L} \int_{B(0;\Lambda)} \chi_{k_0}(k')\chi_{k_0}(k)\varphi(k')\,\mathrm{d}k' - \varphi(k) \right| \\ &= \left| \sum_{k_0 \in \Gamma_\Lambda^L} \left(\frac{2\pi}{L}\right)^{-3/2} \int_{\mathcal{C}_{k_0}} \chi_{k_0}(k)\varphi(k')\,\mathrm{d}k' - \varphi(k) \right| \\ &= \left| \left(\frac{2\pi}{L}\right)^{-3} \int_{\mathcal{C}_{k_1(L)}} \varphi(k')\,\mathrm{d}k' - \varphi(k) \right|, \end{aligned}$$

where $k_1(L)$ is the unique element of Γ_Λ^L such that $k \in \mathcal{C}_{k_1(L)}$. Hence,

$$\begin{aligned} |T_k\varphi - \varphi(k)| &= \left| \left(\frac{2\pi}{L}\right)^{-3} \int_{\mathcal{C}_{k_1(L)}} (\varphi(k') - \varphi(k))\,\mathrm{d}k' \right| \\ &\leqslant \left(\frac{2\pi}{L}\right)^{-3} \int_{\mathcal{C}_{k_1(L)}} |\varphi(k') - \varphi(k)|\,\mathrm{d}k' \\ &\leqslant \sup_{k' \in \mathcal{C}_{k_1(L)}} |\varphi(k') - \varphi(k)| = O(1/L). \end{aligned}$$

We want to apply this to the map $k' \mapsto U^*(k')\widehat{g}(k')$. The map $k' \mapsto U^*(k')$ is actually C^∞ [Tha92] but we cannot say the same about $\widehat{g}$. Thus, we will assume that $g \in \mathcal{S}(\mathbb{R}^3) \cap \mathfrak{H}_\Lambda$ so that $\widehat{g} \in C^\infty$ and then

$$\widehat{i_L i_L^* g}(k) = U(k)U^*(k)\widehat{g}(k) = \widehat{g}(k).$$

So that $i_L i_L^* \to \mathrm{Id}_{\mathfrak{H}_\Lambda}$ pointwise on $\mathcal{S}(\mathbb{R}^3) \cap \mathfrak{H}_\Lambda$ which is dense in $\mathfrak{H}_\Lambda$. Since $i_L i_L^*$ is an isometry and hence is continuous, we have $i_L i_L^* \to \mathrm{Id}_{\mathfrak{H}_\Lambda}$ pointwise on $\mathfrak{H}_\Lambda$.

4. It is sufficient to prove that $P^0 i_L = i_L P_L^0 : \mathfrak{H}_\Lambda^L \to \mathfrak{H}_\Lambda$. We will prove this equality on $\mathfrak{H}_\Lambda^{L,-} := P_L^0 \mathfrak{H}_\Lambda^L$ and $\mathfrak{H}_\Lambda^{L,+} := (1 - P_L^0)\mathfrak{H}_\Lambda^L$ because

$$\mathfrak{H}_\Lambda^L = \mathfrak{H}_\Lambda^{L,-} \overset{\perp}{\oplus} \mathfrak{H}_\Lambda^{L,+}.$$

Since

$$\varphi \in \mathfrak{H}_\Lambda^{\pm} \Leftrightarrow \left(\widehat{\varphi}(k) \in \mathfrak{H}_\Lambda^{\pm}(k) \quad \forall k \in \Gamma_\Lambda^L\right),$$

for any $\varphi \in \mathfrak{H}_\Lambda^{L,\pm}$, we have on the one hand

$$i_L P_L^0 \varphi = \delta(-,\pm) i_L \varphi,$$

and on the other hand

$$\widehat{i_L\varphi}(k) = \left(\frac{2\pi}{L}\right)^{3/2} \sum_{k_0 \in \Gamma_\Lambda^L} \underbrace{U(k)\widehat{\varphi}(k_0)}_{\in \mathfrak{H}_\Lambda^{\pm}(k)} \chi_{k_0}(k),$$

so that we also have

$$P^0 i_L \varphi = \delta(-,\pm) i_L \varphi.$$

Indeed in the whole space we also have

$$f \in \mathfrak{H}_\Lambda^- := P^0 \mathfrak{H}_\Lambda \Leftrightarrow \left(\widehat{f}(k) \in \mathfrak{H}_\Lambda^-(k) \quad \forall k \in B(0;\Lambda) \right),$$

with the obvious converse equivalence for $\mathfrak{H}_\Lambda^+ := (1-P^0)\mathfrak{H}_\Lambda$. We thus have $i_L P_L^0 = P^0 i_L$ and the proposition is proved.

5. Let us consider $f \in \mathfrak{H}_\Lambda^{L,+}$ and let us compute $i_L^* D^0 i_L f$. We have for $k \in B(0;\Lambda)$

$$\begin{aligned}
\widehat{D^0 i_L f}(k) &= \left(\frac{2\pi}{L}\right)^{3/2} \sum_{k_0 \in \Gamma_\Lambda^L} D^0(k) \underbrace{U(k)\widehat{f}(k_0)}_{\in \mathfrak{H}_\Lambda^+(k)} \chi_{k_0}(k) \\
&= \left(\frac{2\pi}{L}\right)^{3/2} \sum_{k_0 \in \Gamma_\Lambda^L} \sqrt{1+k^2} U(k) \widehat{f}(k_0) \chi_{k_0}(k),
\end{aligned}$$

so that for $k' \in \Gamma_\Lambda^L$

$$\begin{aligned}
i_L^* \widehat{D^0 i_L} f(k') &= \left(\frac{2\pi}{L}\right)^{-3/2} \int_{B(0;\Lambda)} U^*(k) \widehat{D^0 i_L f}(k) \chi_{k'}(k)\, \mathrm{d}k \\
&= \int_{B(0;\Lambda)} \sum_{k_0 \in \Gamma_\Lambda^L} \sqrt{1+k^2} U^*(k) U(k) \widehat{f}(k_0) \chi_{k_0}(k) \chi_{k'}(k)\, \mathrm{d}k \\
&= \int_{B(0;\Lambda)} \sqrt{1+k^2} \widehat{f}(k') \chi_{k'}^2(k)\, \mathrm{d}k.
\end{aligned}$$

One can remark that $\chi_{k'}^2 \to \delta(\cdot - k')$ in $\mathcal{D}'(\mathbb{R}^3)$ or we can do the direct computation

$$\begin{aligned}
\left| i_L^* \widehat{D^0 i_L} f(k') - \widehat{D_L^0 f}(k') \right| &= \left| \int_{B(0;\Lambda)} \sqrt{1+k^2} \widehat{f}(k') \chi_{k'}^2(k)\, \mathrm{d}k - \sqrt{1+k'^2} \widehat{f}(k') \right| \\
&= \left| \widehat{f}(k') \left(\frac{2\pi}{L}\right)^{-3} \int_{\mathcal{C}_{k'}} \underbrace{(\sqrt{1+k^2} - \sqrt{1+k'^2})}_{| \quad | \leqslant |k-k'|}\, \mathrm{d}k \right| \\
&\leqslant |\widehat{f}(k')| \sup_{k \in \mathcal{C}_{k'}} |k-k'| = O(1/L).
\end{aligned}$$

□

We are now able to establish the inequality (5.14).

Proof of the inequality (5.14). Let $\varepsilon > 0$. Since $(Q_K)_{K \geqslant 1}$ is a minimizing sequence for $E^\nu(q)$, let K be such that

$$\mathcal{E}^\nu(Q_K) \leqslant E^\nu(q) + \varepsilon.$$

As γ is finite-rank, we write

$$\gamma = \sum_{j \in J} n_j |\psi_j\rangle\langle\psi_j|,$$

with J finite, $0 \leqslant n_j \leqslant 1$, and the (ψ_j) orthonormal. Let us now restrain Q_K to an operator on $\mathfrak{H}_\Lambda^L$. We define for all $i \leqslant K$

$$u_i^L := i_L^* u_i$$

and $(v_i^L)_{i\leqslant K}$,$(\psi_j^L)_{j\in J}$ in the same manner. We have

$$\langle u_i^L, u_j^L\rangle_{\mathfrak{H}_\Lambda^L} = \langle i_L^* u_i, i_L^* u_j\rangle_{\mathfrak{H}_\Lambda^L} = \langle i_L i_L^* u_i, u_j\rangle_{\mathfrak{H}_\Lambda} \to \delta_{ij} \quad (L\to\infty) \tag{5.20}$$

by the proposition 5.1 (3). Furthermore,

$$P_L^0 u_i^L = P_L^0 i_L^* u_i = i_L^* P^0 u_i = i_L^* u_i = u_i^L, \tag{5.21}$$

be the intertwinning property of i_L^*. We then build by the Gram-Schimdt orthonormalisation procedure an orthonormal set $(\widetilde{u_i}^L)_{i\leqslant K}$ of $P_L^0\mathfrak{H}_\Lambda^L$ such that $\|\widetilde{u_i}^L - u_i^L\| \to 0$ as $L\to\infty$. However, it is not obvious that the family $(u_i^L)_{i\leqslant K}$ is independent for a fixed L since for instance for low L, the dimension of $\mathfrak{H}_\Lambda^L$ is also low so that the family $(u_i^L)_{i\leqslant K}$ which is of fixed cardinal cannot be independent. Thus, let us prove the following lemma.

Lemma 5.7. *There exists $L>0$ so that for all $L'\geqslant L$, the family $(u_i^{L'})_{i\leqslant K}$ is independent.*

Proof. Let us consider for all L a relation

$$\sum_{i\leqslant K} \lambda_i^L u_i^L = 0,$$

where $\lambda_i^L \in \mathbb{C}$. We recall that K does not depend of L. We have to show that

$$\exists L>0, \quad \forall L'\geqslant L, \quad \sum_{i\leqslant K} \lambda_i^{L'} u_i^{L'} = 0 \Rightarrow \max_i |\lambda_i^L| = 0.$$

Let us thus assume that there exists a sequence $(L_n)_{n\in\mathbb{N}}$ with $L_n\to\infty$ and for each n a relation $\sum_{i\leqslant K}\lambda_i^{L_n}u_i^{L_n}=0$ such that $\max_i|\lambda_i^{L_n}|>0$. We pose

$$\lambda_i^n := \lambda_i^{L_n}, \quad u_i^n := u_i^{L_n}.$$

We can assume that the sequence $(\lambda_i^n)_{i,n}$ is bounded. Indeed, for a fixed n one can divide each λ_i^n by $\lambda_{i_0}^n$ such that $|\lambda_{i_0}^n| = \max_i|\lambda_i^n|$. We can thus assume that for all n, $\max_i|\lambda_i^n|=1$ and for a fixed i, we can assume that (λ_i^n) converges towards λ_i up to a subsequence. Moreover, as there is a finite number of i, we can also assume that up to subsequence, the maximum of $|\lambda_i^n|$ is attained for the same index i_0 for all n. In particular, we have $1=|\lambda_{i_0}^n|\to|\lambda_{i_0}|$. For all n we have

$$\sum_i \lambda_i^n u_i^n = 0 \Rightarrow 0 = \sum_i \lambda_i^n \langle u_i^n, u_{i_0}^n\rangle \to \sum_i \lambda_i \delta_{ii_0} = \lambda_{i_0},$$

by the limit (5.20). Hence $\lambda_{i_0}=0$ but $|\lambda_{i_0}|=1$, which is absurd and proves the lemma. □

We then apply the Gram-Schimdt process to this family for all L large enough by the lemma (notice that this family is finite so that there is a finite number of steps in this process):

$$\widetilde{u_1}^L := u_1^L \tag{5.22}$$

$$\widetilde{u_{i+1}}^L := u_{i+1}^L - \sum_{j=1}^{i} \frac{\langle \widetilde{u_j}^L, u_{i+1}^L\rangle}{\|\widetilde{u_j}^L\|^2}\widetilde{u_j}^L, \quad (i\geqslant 1). \tag{5.23}$$

We prove that $\|\widetilde{u_i}^L - u_i^L\| \to \infty$ by induction on the index i. The case $i = 1$ is trivial. Then we just remark that

$$\|\widetilde{u_i}^L - u_i^L\| \leqslant \sum_{j=1}^{i-1} \frac{|\langle \widetilde{u_j}^L, u_i^L\rangle|}{\|\widetilde{u_j}^L\|}.$$

Since $\|u_j^L - \widetilde{u_j}^L\| \to 0$ and $\|u_j^L\| \to 1$ by (5.20) for all $1 \leqslant j \leqslant i-1$, for L large enough the family $(\|\widetilde{u_j}^L\|)_{1\leqslant j\leqslant i-1}$ is bounded by below uniformly on L by a strictly positive constant. Finally, again by $\|u_j^L - \widetilde{u_j}^L\| \to 0$ and the limit (5.20), we have

$$\lim_{L\to\infty} |\langle \widetilde{u_j}^L, u_i^L\rangle| = 0, \quad 1 \leqslant j \leqslant i-1,$$

and thus

$$\lim_{L\to\infty} \|\widetilde{u_i}^L - u_i^L\| = 0.$$

We define in the same way $(\widetilde{v_i}^L), (\widetilde{\psi_j}^L)$. We now define the test state for $E^{L,\nu}(q)$ as

$$\widetilde{Q}^L := \sum_{i=-N}^{-1} |\widetilde{v_i}^L\rangle\langle\widetilde{v_i}^L| - \sum_{i=-M}^{-1} |\widetilde{u_i}^L\rangle\langle\widetilde{u_i}^L| + \sum_{i=0}^{K} \frac{\lambda_i^2}{1+\lambda_i^2}(|\widetilde{v_i}^L\rangle\langle\widetilde{v_i}^L| - |\widetilde{u_i}^L\rangle\langle\widetilde{u_i}^L|)$$
$$+ \sum_{i=0}^{K} \frac{\lambda_i}{1+\lambda_i^2}(|\widetilde{u_i}^L\rangle\langle\widetilde{v_i}^L| + |\widetilde{v_i}^L\rangle\langle\widetilde{u_i}^L|) + \sum_{j\in J} n_j |\widetilde{\psi_j}^L\rangle\langle\widetilde{\psi_j}^L|. \quad (5.24)$$

We still have $\mathrm{tr}(\widetilde{Q}^L) = q$ and $-P_L^0 \leqslant \widetilde{Q_L} \leqslant 1 - P_L^0$ by orthonormality of the $(\widetilde{u_i}^L)$, $(\widetilde{v_i}^L)$ and $(\widetilde{\psi_j}^L)$, and because

$$P_L^0 = \sum_{i\geqslant -M} |\widetilde{u_i}^L\rangle\langle\widetilde{u_i}^L|.$$

Hence, $\widetilde{Q}^L$ is eligible for $E^{L,\nu}(q)$ so that

$$\mathcal{E}^{L,\nu}(\widetilde{Q}^L) \geqslant E^{L,\nu}(q).$$

The energy of this state is

$$\mathcal{E}^{L,\nu}(\widetilde{Q}^L) = \mathrm{tr}(D_L^0 \widetilde{Q}^L) - \alpha D_L(\rho_{\widetilde{Q}^L}, \nu_L) + \frac{\alpha}{2} D_L(\rho_{\widetilde{Q}^L}, \rho_{\widetilde{Q}^L}).$$

We just have to show that this energy converges towards $\mathcal{E}^\nu(Q_K)$. Since the kinetic energy $Q \mapsto \mathrm{tr}(D^0 Q)$ is linear, we just have to prove

$$\mathrm{tr}(D_L^0 |\widetilde{\varphi}^L\rangle\langle\widetilde{\xi}^L|) \to \mathrm{tr}(D^0 |\varphi\rangle\langle\xi|),$$

where φ and ξ denote either a u_i, a v_i, or a ψ_i, according to the decomposition (5.24). Recall that

$$\mathrm{tr}(D_L^0 |\widetilde{\varphi}^L\rangle\langle\widetilde{\xi}^L|) = \langle D_L^0 \widetilde{\varphi}^L, \widetilde{\xi}^L\rangle.$$

We then notice that

$$\langle D_L^0 \widetilde{\varphi}^L, \widetilde{\xi}^L\rangle = \langle D_L^0 \varphi^L, \xi^L\rangle + O(1/L)$$

because $\|\widetilde{\varphi}^L - \varphi^L\| \to 0$ and $\|\widetilde{\xi}^L - \xi^L\| \to 0$. Moreover,

$$\langle D_L^0 \varphi^L, \xi^L\rangle = \left(\frac{2\pi}{L}\right)^3 \sum_{k_0\in\Gamma_\Lambda^L} \langle D^0(k_0)\widehat{\varphi^L}(k_0), \widehat{\xi^L}(k_0)\rangle_{\mathbb{C}^4} = \left(\frac{2\pi}{L}\right)^3 \sum_{k_0\in\Gamma_\Lambda^L} \langle D^0(k_0)\widehat{i_L^*\varphi}(k_0), \widehat{i_L^*\xi}(k_0)\rangle_{\mathbb{C}^4}.$$

We show that $|\widehat{i_L^*\varphi}(k_0) - \widehat{\varphi}(k_0)| = o_L(1)$. Indeed,

$$\begin{aligned}|\widehat{i_L^*\varphi}(k_0) - \widehat{\varphi}(k_0)| &= \left(\frac{2\pi}{L}\right)^{-3} \left| \int_{\mathcal{C}_{k_0}} (U^*(k)\widehat{\varphi}(k) - \underbrace{\widehat{\varphi}(k_0)}_{=U^*(k_0)\widehat{\varphi}(k_0)}) \,\mathrm{d}k \right| \\ &\leqslant \sup_{k\in\mathcal{C}_{k_0}} \underbrace{|U^*(k)\widehat{\varphi}(k) - U^*(k_0)\widehat{\varphi}(k_0)|}_{\text{continuous}} = o_L(1).\end{aligned}$$

Thus

$$\langle D_L^0\widetilde{\varphi}^L, \widetilde{\xi}^L\rangle = \left(\frac{2\pi}{L}\right)^3 \sum_{k_0\in\Gamma_\Lambda^L} \langle D^0(k_0)\widehat{\varphi}(k_0), \widehat{\xi}(k_0)\rangle_{\mathbb{C}^4} + O_L(1) \to \int_{B(0;\Lambda)} \langle D^0(k)\widehat{\varphi}(k), \widehat{\xi}(k)\rangle_{\mathbb{C}^4} \,\mathrm{d}k,$$

so that $\langle D_L^0\widetilde{\varphi}^L, \widetilde{\xi}^L\rangle \to \langle D^0\varphi, \xi\rangle$ and hence $\mathrm{tr}(D_L^0\widetilde{Q}^L) \to \mathrm{tr}(D^0 Q_K)$ as $L\to\infty$. It now remains to prove the convergence of the potential energy. We first remark that, if we define the sequence $(f_L) \subset \mathfrak{H}_\Lambda$ by

$$\widehat{f_L}(k) = \sum_{k_0\in\Gamma_\Lambda^L} \widehat{\rho_{\widetilde{Q}^L}}(k_0)\mathbf{1}_{\mathcal{C}_{k_0}}(k), \quad \forall k \in B(0;\Lambda),$$

then

$$\begin{aligned}D(f_L, f_L) &= \int_{B(0;\Lambda)} \frac{|\widehat{f_L}(k)|^2}{|k|^2}\,\mathrm{d}k \\ &= \sum_{k_0,k_0'\in\Gamma_\Lambda^L} \widehat{\rho_{\widetilde{Q}^L}}(k_0)\overline{\widehat{\rho_{\widetilde{Q}^L}}(k_0')} \int_{B(0,\Lambda)} \frac{\mathbf{1}_{\mathcal{C}_{k_0}}(k)\mathbf{1}_{\mathcal{C}_{k_0'}}(k)}{|k|^2}\,\mathrm{d}k \\ &= \sum_{k_0\in\Gamma_\Lambda^L} |\widehat{\rho_{\widetilde{Q}^L}}(k_0)|^2 \int_{\mathcal{C}_{k_0}} \frac{\mathrm{d}k}{|k|^2} \\ &= \left(\frac{2\pi}{L}\right)^3 \sum_{k_0\in\Gamma_\Lambda^L} \frac{|\widehat{\rho_{\widetilde{Q}^L}}(k_0)|^2}{|k_0|^2} + O(1/L) \\ &= D_L(\rho_{\widetilde{Q}^L}, \rho_{\widetilde{Q}^L}) + O(1/L).\end{aligned}$$

Hence, it is sufficient to show that

$$D(f_L, f_L) \underset{L\to\infty}{\longrightarrow} D(\rho_{Q_K}, \rho_{Q_K}),$$

to have the convergence of the potential energy. Indeed, if (f_L) converges strongly towards ρ_{Q_K} in $\mathcal{C}$, then it also converges weakly towards ρ_{Q_K} in $\mathcal{C}$ and we have also $D(f_L,\nu) \to D(\rho_{Q_K},\nu)$ as $L\to\infty$. In order to have the strong convergence in $\mathcal{C}$, we remark that by the Hardy-Littlewood-Sobolev inequality,

$$D(\rho,\rho) \leqslant C\|\rho\|_{L^{6/5}} \leqslant C'(\|\rho\|_{L^1} + \|\rho\|_{L^2}),$$

so that the strong convergence in L^1, L^2 implies the strong convergence in $\mathcal{C}$. But

$$f_L \overset{L^1,L^2}{\longrightarrow} \rho_{Q_K} \Leftrightarrow \widehat{f_L} \overset{L^2,L^\infty}{\longrightarrow} \widehat{\rho_{Q_K}} \Leftrightarrow \widehat{f_L} \overset{L^\infty}{\longrightarrow} \widehat{\rho_{Q_K}},$$

because the Fourier transforms have their supports in $B(0;\Lambda)$. According to the definition of $\widehat{f_L}$, the convergence of $\widehat{f_L}$ towards $\widehat{\rho_{Q_K}}$ in L^∞ is equivalent to show that

$$\forall k_0 \in \Gamma_\Lambda^L, \forall k \in \mathcal{C}_{k_0}, \quad |\widehat{\rho_{\widetilde{Q}^L}}(k) - \widehat{\rho_{Q_K}}(k)| = o_L(1),$$

where the $o_L(1)$ does not depend on k_0. In order to have this condition, one can show that it is sufficient to have the convergence of $(\mathbf{1}_{C_L}\rho_{\widetilde{Q}^L})$ towards ρ_{Q_K} in L^1. But according to the form (5.24) of $\widetilde{Q}^L$, it is then sufficient to prove that $([\mathbf{1}_{C_L}\varphi^L]^2)$ converges towards φ^2 in L^1, where φ denotes whether a u_i, a v_i, or a ψ_i. Indeed,

$$\rho_{|\varphi\rangle\langle\varphi|} = |\varphi|^2.$$

We already have

$$\lim_{L\to\infty} \|[\mathbf{1}_{C_L}\varphi^L]^2\|_{L^1} = \|\varphi^2\|_{L^1},$$

so that by the missing term in Fatou's lemma, it remains to show that $([\mathbf{1}_{C_L}\varphi^L]^2)$ converges almost everywhere towards φ^2. One already has the convergence of $i_L\varphi^L$ towards φ in L^2, hence almost everywhere up to a subsequence. Let us now show that $\forall x \in \mathbb{R}^3$, $i_L\varphi^L(x) - \varphi^L(x) \to 0$ as $L \to \infty$. Indeed,

$$\begin{aligned}
i_L\varphi^L(x) &= \frac{1}{(2\pi)^{3/2}} \int_{B(0;\Lambda)} \widehat{i_L\varphi^L}(k) e^{ik\cdot x}\,\mathrm{d}k \\
&= \frac{1}{L^{3/2}} \sum_{k_0\in\Gamma_\Lambda^L} \left(\int_{B(0;\Lambda)} \chi_{k_0}(k) U(k) e^{ik\cdot x}\,\mathrm{d}k \right) \widehat{\varphi^L}(k_0) \\
&= \frac{(2\pi)^{3/2}}{L^3} \sum_{k_0\in\Gamma_\Lambda^L} \underbrace{U(k_0)\widehat{\varphi^L}(k_0)}_{=\widehat{\varphi^L}(k_0)} e^{ik_0\cdot x} + o_L(1) \\
&= \varphi^L(x) + o_L(1).
\end{aligned}$$

Thus we have

$$D_L(\rho_{\widetilde{Q}_L}, \rho_{\widetilde{Q}_L}) \underset{L\to\infty}{\longrightarrow} D(\rho_{Q_K}, \rho_{Q_K})$$

and

$$D_L(\rho_{\widetilde{Q}_L}, \nu_L) \underset{L\to\infty}{\longrightarrow} D(\rho_{Q_K}, \nu).$$

Finally,

$$E^{L,\nu}(q) \leqslant \mathcal{E}^{L,\nu}(\widetilde{Q}_L) \underset{L\to\infty}{\longrightarrow} \mathcal{E}^{\nu}(Q_K) \leqslant E^{\nu}(q) + \varepsilon,$$

hence

$$\limsup_{L\to\infty} E^{L,\nu}(q) \leqslant E^{\nu}(q) + \varepsilon, \quad \forall \varepsilon > 0.$$

We have proved the inequality (5.14).

Proof of the inequality (5.15). The idea of the proof is the converse of the last one. Indeed, we have to find an energy greater than $E^\nu(q)$ while staying close to $E^{L,\nu}(q)$. In order to do so, we extend a ground state in a box C_L to a state in the whole space so that

1. it is eligible for $E^\nu(q)$, hence its energy is greater than $E^\nu(q)$;
2. its energy in the whole space remains close to its energy in a box, that is $E^{L,\nu}(q)$.

Let now $Q_L \in \mathcal{Q}_\Lambda^L(q)$. We want to extend this operator to an operator in $\mathcal{Q}_\Lambda(q)$. We define

$$\widetilde{Q}_L := i_L Q_L i_L^*.$$

Let us check that $\widetilde{Q}_L \in \mathcal{Q}_\Lambda(q)$. We have immediately $\widetilde{Q}_L^* = \widetilde{Q}_L$. Since $-P_L^0 \leqslant Q_L \leqslant 1 - P_L^0$ we have

$$-i_L P_L^0 i_L^* \leqslant \widetilde{Q}_L \leqslant i_L i_L^* - i_L P_L^0 i_L^*.$$

But since $i_L i_L^*$ is an isometry, $i_L i_L^* \leqslant 1$. Moreover by Proposition 5.1 (4),

$$i_L P_L^0 i_L^* = i_L P_L^0 P_L^0 i_L^* = P^0 i_L i_L^* P^0.$$

Recall that $A \leqslant B \Rightarrow CAC^* \leqslant CBC^*$ for all operators A, B, C, so that

$$i_L P_L^0 i_L^* \leqslant P^0 P^0 = P^0,$$

and we have

$$-P^0 \leqslant \widetilde{Q}_L \leqslant 1 - P^0.$$

Let us now examine the charge constraint.

$$\begin{aligned}
\mathrm{tr}_{P^0}(i_L Q_L i_L^*) &= \mathrm{tr}(P^0 i_L Q_L i_L^* P^0) + \mathrm{tr}(P_+^0 i_L Q_L i_L^* P_+^0) \\
&= \mathrm{tr}(i_L P_L^0 Q_L P_L^0 i_L^*) + \mathrm{tr}(i_L (1 - P_L^0) Q_L (1 - P_L^0) i_L^*) \quad \text{(Prop. 5.1 (4))} \\
&= \mathrm{tr}(P_L^0 Q_L P_L^0) + \mathrm{tr}((1 - P_L^0) Q_L (1 - P_L^0)) \quad (i_L^* i_L = \mathrm{Id}) \\
&= \mathrm{tr}(P_L^0 Q_L P_L^0 + (1 - P_L^0) Q_L (1 - P_L^0)) = \mathrm{tr}(Q_L) = q.
\end{aligned}$$

We thus have $\widetilde{Q}_L \in \mathcal{Q}_\Lambda(q)$. Let us choose Q_L as a minimizer for $E^{L,\nu}(q)$, that is $\mathcal{E}^{L,\nu}(Q_L) = E^{L,\nu}(q)$. By definition

$$E^{L,\nu}(q) = \mathcal{E}^{L,\nu}(Q_L) = \mathrm{tr}(D_L^0 Q_L) - \alpha D_L(\rho_{Q_L}, \nu_L) + \frac{\alpha}{2} D_L(\rho_{Q_L}, \rho_{Q_L}) \tag{5.25}$$

One also has

$$E^\nu(q) \geqslant \limsup_{L \to \infty} E^{L,\nu}(q) = \limsup_{L \to \infty} \mathcal{E}^{L,\nu}(Q_L),$$

by inequality (5.14). The energy being coercive, the sequences (Q_L) is bounded in the sense that $Q_L(x,y)\mathbf{1}_{C_L}(x)\mathbf{1}_{C_L}(y)$ is bounded in $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ and $\rho_{Q_L}(x)\mathbf{1}_{C_L}(x)$ is bounded in $L^2(\mathbb{R}^3)$. Hence, up to a subsequence and as in the proof of lemma 5.6 we can assume that

$$Q_L(x,y)\mathbf{1}_{C_L}(x)\mathbf{1}_{C_L}(y) \rightharpoonup Q(x,y)$$

in $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$, uniformly on compact subsets of $\mathbb{R}^6$ and that

$$\rho_{Q_L}(x)\mathbf{1}_{C_L}(x) \rightharpoonup \rho_Q(x)$$

in $L^2(\mathbb{R}^3)$, uniformly on compact subsets of $\mathbb{R}^3$. Let us now study the convergence of the kinetic energy.

Lemma 5.8. *The kinetic energy of $\widetilde{Q}_L$ satisfies*

$$\left| \mathrm{tr}_{P^0}(D^0 \widetilde{Q}_L) - \mathrm{tr}(D_L^0 Q_L) \right| = O\left(\frac{1}{L}\right).$$

Proof. A short computation similar to the one determining the charge of $\widetilde{Q}_L$ shows that

$$\mathrm{tr}_{P^0}(D^0 \widetilde{Q}_L) = \mathrm{tr}(i_L^* D^0 i_L P_L^0 Q_L P_L^0) + \mathrm{tr}(i_L^* D^0 i_L (1 - P_L^0) Q_L (1 - P_L^0)).$$

The sequence (Q_L) verifies that $(\mathrm{tr}(P_L^0 Q_L P_L^0))_L$ and $(\mathrm{tr}(1 - P_L^0) Q_L (1 - P_L^0))_L$ are both bounded. Hence, using the proposition 5.1 (5), the lemma is obvious. □

The kinetic energy being coercive, the sequence $(\widetilde{Q}_L)$ is bounded in $\mathfrak{S}_1^{P^0}$. We can thus assume that up to a subsequence, $\widetilde{Q}_L \rightharpoonup \overline{Q}$ in $\mathfrak{S}_1^{P^0}(\mathfrak{H}_\Lambda)$. Let us show that $Q = \overline{Q}$. Let $f, g \in C_0^\infty(\mathbb{R}^3)$. Since $i_L i_L^* g \to g$,

$$\langle \widetilde{Q}_L f, g\rangle = \langle i_L Q_L i_L^* f, i_L i_L^* g\rangle + O(1/L).$$

But since $i_L^* i_L = \mathrm{Id}$,

$$\begin{aligned}\langle i_L Q_L i_L^* f, i_L i_L^* g\rangle &= \langle Q_L i_L^* g, i_L^* g\rangle \\ &= \iint_{\mathbb{R}^3\times\mathbb{R}^3} Q_L(x,y)\mathbf{1}_{C_L}(x)\mathbf{1}_{C_L}(y) i_L^* f(x) i_L^* g(y)\,\mathrm{d}x\mathrm{d}y \to \langle Qf, g\rangle\end{aligned}$$

by weak convergence of $Q_L(x,y)\mathbf{1}_{C_L}(x)\mathbf{1}_{C_L}(y)$ and strong convergence of $\mathbf{1}_{C_L} i_L^* f$ towards f in $L^2(\mathbb{R}^3)$. We also have

$$\langle \widetilde{Q}_L f, g\rangle \to \langle \overline{Q} f, g\rangle$$

so that $Q = \overline{Q}$ and hence $\rho_Q = \rho_{\overline{Q}}$. We now study the convergence of the potential energy term. Let us prove the following lemma.

Lemma 5.9.

$$\liminf_{L\to\infty} D_L(\rho_{Q_L}, \rho_{Q_L}) \geqslant D(\rho_Q, \rho_Q). \tag{5.26}$$

Proof. We introduce an auxiliary function $\rho_L \in \mathcal{C}$ which has the same weak L^2-limit as $\rho_{\widetilde{Q}_L}$, by

$$\widehat{\rho_L}(k) := \sum_{k_0\in\Gamma_\Lambda^L} \widehat{\rho_{Q_L}}(k_0)\mathbf{1}_{\mathcal{C}_{k_0}}(k).$$

We have

$$\int_{\mathbb{R}^3} |\rho_L|^2 = \left(\frac{2\pi}{L}\right)^3 \sum_{k_0\in\Gamma_\Lambda^L} |\widehat{\rho_{Q_L}}(k_0)|^2 = \int_{\mathbb{T}_L} |\rho_{Q_L}|^2$$

and since $|k| \geqslant |k_0|, \forall k \in \mathcal{C}_{k_0}$,

$$D(\rho_L, \rho_L) = 4\pi \sum_{k_0\in\Gamma_\Lambda} |\widehat{\rho_{Q_L}}(k_0)|^2 \int_{\mathcal{C}_{k_0}} \frac{\mathrm{d}k}{|k|^2} \leqslant 4\pi \left(\frac{2\pi}{L}\right)^3 \sum_{k_0\in\Gamma_\Lambda^L} \frac{|\widehat{\rho_{Q_L}}(k_0)|^2}{|k_0|^2} = D_L(\rho_{Q_L}, \rho_{Q_L}),$$

so that (ρ_L) is bounded both in $L^2(\mathbb{R}^3)$ and in $\mathcal{C}$. Up to a subsequence, it thus converges weakly towards the same limit ρ, in $L^2(\mathbb{R}^3)$ and $\mathcal{C}$. By the weak continuity of the $\mathcal{C}$-norm, we have

$$\liminf_{L\to\infty} D(\rho_L, \rho_L) \geqslant D(\rho, \rho).$$

We just have to show that $\rho = \rho_Q$. Let us take $f \in C_0^\infty(\mathbb{R}^3)$ and L large enough such that $\mathrm{supp} f \subset C_L$. Then

$$\int_{\mathbb{R}^3} \rho_L f = \sum_{k_0\in\Gamma_\Lambda^L} \widehat{\rho_{Q_L}}(k_0) \int_{\mathcal{C}_{k_0}} \overline{\widehat{f}}(k)\,\mathrm{d}k = \left(\frac{2\pi}{L}\right)^3 \sum_{k_0\in\Gamma_\Lambda^L} \widehat{\rho_{Q_L}}(k_0)\overline{\widehat{f}}(k_0) + o_L(1) = \int_{\mathbb{T}_L} \rho_{Q_L} f + o_L(1).$$

Hence,

$$\int \rho f = \lim_{L\to\infty} \int \rho_L f = \lim_{L\to\infty} \int_{\mathbb{T}_L} \rho_{Q_L} f = \int \rho_Q f,$$

thus $\rho = \rho_Q$ and the lemma is proved. □

One verifies in the same way that

$$D_L(\rho_{Q_L}, \nu_L) = D(\rho_L, \nu) + o_L(1),$$

so that

$$D_L(\rho_{Q_L}, \nu_L) \underset{L\to\infty}{\longrightarrow} D(\rho, \nu) = D(\rho_Q, \nu),$$

by the weak convergence of (ρ_L) towards ρ in $\mathcal{C}$. Let us recall the equality (5.25) and use the localization operators X_R,Y_R introduced earlier

$$\begin{aligned}
E^{L,\nu}(q) &= \mathrm{tr}_{P^0}(D^0\widetilde{Q}_L) - \alpha D_L(\rho_{Q_L}, \nu_L) + \frac{\alpha}{2} D_L(\rho_{Q_L}, \rho_{Q_L}) + O(1/L) && (5.27)\\
&= \mathrm{tr}_{P^0}(X_R D^0 \widetilde{Q}_L X_R) + \mathrm{tr}_{P^0}(Y_R D^0 \widetilde{Q}_L Y_R) - \alpha D_L(\rho_{Q_L}, \nu_L) && (5.28)\\
&\quad + \frac{\alpha}{2} D_L(\rho_{Q_L}, \rho_{Q_L}) + O(1/L) && (5.29)\\
&= \mathrm{tr}_{P^0}(D^0 X_R \widetilde{Q}_L X_R) + \mathrm{tr}_{P^0}(D^0 Y_R \widetilde{Q}_L Y_R) - \alpha D_L(\rho_{Q_L}, \nu_L) && (5.30)\\
&\quad + \frac{\alpha}{2} D_L(\rho_{Q_L}, \rho_{Q_L}) + O(1/L) + O(1/R). && (5.31)
\end{aligned}$$

We now have the important fact, characteristic of the reduced model, that

$$\begin{aligned}
E^0(k) &= \inf\{\mathrm{tr}_{P^0}(D^0 Q) + (\alpha/2) D(\rho_Q, \rho_Q), \quad Q \in \mathcal{Q}_\Lambda(k)\}\\
&= \inf\{\mathrm{tr}_{P^0}(D^0 Q), \quad Q \in \mathcal{Q}_\Lambda(k)\},
\end{aligned}$$

so that

$$\begin{aligned}
\mathrm{tr}_{P^0}(D^0 Y_R \widetilde{Q}_L Y_R) &\geqslant E^0(\mathrm{tr}_{P^0}(Y_R \widetilde{Q}_L Y_R))\\
&\geqslant E^0(q - \mathrm{tr}_{P^0}(X_R \widetilde{Q}_L X_R)),
\end{aligned}$$

since $\mathrm{tr}_{P^0}(\widetilde{Q}_L) = q$. Taking the limit $L \to \infty$ in (5.31), using the local strong convergence of $(\widetilde{Q}_L)_L$, lemma 5.9, and the continuity of $k \mapsto E^0(k)$, we have for all R

$$\liminf_{L\to\infty} E^{L,\nu}(q) \geqslant \mathrm{tr}_{P^0}(D^0 X_R Q X_R) - \alpha D(\rho_Q, \nu) + \frac{\alpha}{2} D(\rho_Q, \rho_Q) + E^0(q - \mathrm{tr}_{P^0}(X_R Q X_R)) + O(1/R). \tag{5.32}$$

Finally, as $R \to \infty$, with $k := \mathrm{tr}_{P^0}(Q)$,

$$\begin{aligned}
\liminf_{L\to\infty} E^{L,\nu}(q) &\geqslant \mathrm{tr}_{P^0}(D^0 Q) - \alpha D(\rho_Q, \nu) + \frac{\alpha}{2} D(\rho_Q, \rho_Q) + E^0(q - \mathrm{tr}_{P^0}(Q))\\
&= \mathcal{E}^\nu(Q) + E^0(q-k) \geqslant E^\nu(k) + E^0(q-k) \geqslant E^\nu(q).
\end{aligned}$$

We thus have proved the inequality (5.15) and hence the theorem 5.3.

A A key lemma

Lemma A.1. *Let $A \in M_n(\mathbb{C})$ a self-adjoint matrix. Then the following minimization problem*

$$\inf_{\substack{0\leqslant\gamma\leqslant I\\ \gamma^*=\gamma}} \mathrm{tr}(A\gamma)$$

is attained by $\gamma = \chi_{(-\infty,0)}(A)$, the orthogonal projector on the direct sum of the eigenspaces of A linked to negative eigenvalues. The attained minimum is thus the sum of these negative eigenvalues, counted with multiplicity. If moreover A is invertible, this minimizer is unique. If its not invertible, every minimizer takes the form $\gamma = \chi_{(-\infty,0)}(A) + \delta$, where $0 \leqslant \delta \leqslant \chi_{\{0\}}(A)$, $\delta^* = \delta$.

Proof. Let $P = \chi_{(-\infty,0)}(A)$. We have $P + P^\perp = I$, where I is the identity operator of $\mathbb{C}^n$. We then show that for any γ eligible for the minimization problem, $\mathrm{tr}(A(\gamma - P)) \geqslant 0$. Indeed,

$$\begin{aligned}\mathrm{tr}(A(\gamma - P)) &= \mathrm{tr}((P + P^\perp)A(\gamma - P)(P + P^\perp)) \\ &= \mathrm{tr}(PA(\gamma - P)P + P^\perp A(\gamma - P)P^\perp),\end{aligned}$$

by expanding the product in the first line et by using the relations $\mathrm{tr}(XY) = \mathrm{tr}(YX)$ as well as $PP^\perp = 0$. Recall that the operator $|A| := \sqrt{A^*A}$ is a positive operator which is a multpile of the identity with coefficient $|\lambda|$ on $\ker(A - \lambda I)$, for $\lambda \in \mathrm{Sp}(A)$ the spectrum of A. We have $PA = -|A|P$ and $P^\perp A = |A|P$. Denoting $Q = \gamma - P$ we thus have

$$\mathrm{tr}(AQ) = \mathrm{tr}(|A|(Q^{++} - Q^{--})),$$

where $Q^{++} := P^\perp Q P^\perp$ et $Q^{--} := PQP$. Moreover, there is the

Lemma A.2 (Bach's inequality [BBHS99])**.**

$$Q^{++} - Q^{--} \geqslant Q^2. \tag{A.1}$$

Proof. Knowing that $0 \leqslant \gamma = Q + P \leqslant I$, we also have $0 \leqslant (Q+P)^2 \leqslant Q + P$. Writing now that

$$\begin{aligned}(Q+P)^2 &= Q^2 + QP + PQ + P^2 \\ &= Q^2 + PQP + P^\perp QP + PQP^\perp + PQP + P \\ Q + P &= PQP + P^\perp QP + PQP^\perp + P^\perp QP^\perp + P,\end{aligned}$$

We find the desired result. □

We also recall the following result. If $X, Y \geqslant 0$, then $\mathrm{tr}(XY) \geqslant 0$. This implies that if $X \geqslant 0, Y \geqslant Z$, then $\mathrm{tr}(XY) \geqslant \mathrm{tr}(XZ)$, So that $\mathrm{tr}(AQ) \geqslant \mathrm{tr}(\underbrace{|A|}_{\geqslant 0}\underbrace{Q^2}_{\geqslant 0}) \geqslant 0$. The equality holds when $Q = 0$, which proves that P is a minimizer.

Let us study the uniqueness. If $\ker(A) = 0$, then $|A| \geqslant \varepsilon I$, where $\varepsilon > 0$ is for instance the lowest norm of the non-zero eigenvalues of A. Hence $0 = \mathrm{tr}(|A|Q^2) \geqslant \varepsilon\,\mathrm{tr}(Q^2) = \varepsilon\,\mathrm{tr}(Q^*Q) = \varepsilon\|Q\|_{HS}^2$. We thus have $\mathrm{tr}(AQ) = 0 \Leftrightarrow Q = 0$ and we have the uniqueness of the minimzer.

If A is not invertible, let us $\pi = P_{\ker(A)} = \chi_{\{0\}}(A)$ the orthogonal projector on the kernel of A. In the same way as we did before, we have $|A| \geqslant \varepsilon\pi^\perp$ with $\varepsilon > 0$. Hence if γ is a minimizer, $\mathrm{tr}(\pi^\perp Q(\pi^\perp Q)^*) = \mathrm{tr}(\pi^\perp Q^2) = 0$, so $\pi^\perp Q = 0$. Q being self-adjoint, we deduce that $Q\pi^\perp = 0$ as well. Then, by writing $Q = \pi Q\pi + \pi^\perp Q\pi + \pi Q\pi^\perp + \pi^\perp Q\pi^\perp$, we obtain $Q = \pi Q\pi = \pi(\gamma - P)\pi = \pi\gamma\pi$. We deduce $0 \leqslant Q \leqslant I$, as well as $Q \leqslant \pi$ by noticing that $Q - \pi = \pi Q\pi - \pi \leqslant 0$. Finally, every minimizer takes the form $\gamma = P + Q$, avec $0 \leqslant Q \leqslant \pi$. □

We can generalize this lemma to the infinite dimension setting.

Lemma A.3. *Let $\mathfrak{H}$ be a separable Hilbert space, $A \in \mathfrak{S}_1(\mathfrak{H})$ a trace-class self-adjoint operator and Π a projector on $\mathfrak{H}$ such that $\Pi - P \in \mathfrak{S}_2(\mathfrak{H})$ where $P = \chi_{(-\infty,0)}(A)$. Then the following minimization problem*

$$\inf_{\substack{-\Pi \leqslant Q \leqslant I - \Pi \\ Q^* = Q}} \mathrm{tr}_\Pi(AQ)$$

is attained by $Q = P - \Pi$. If moreover $\exists \varepsilon > 0, |A| \geqslant \varepsilon I$, this minimizer is unique.

Proof. The proof is basically the same. We just write for any Q eligible for the minimization problem, $Q = Q' + P - \Pi$ with $-P \leqslant Q' \leqslant I - P$. Then we notice that

$$\mathrm{tr}_\Pi(AQ) = \mathrm{tr}_\Pi(AQ') + \mathrm{tr}_\Pi(A(P-\Pi)),$$

and since $\Pi - P \in \mathfrak{S}_2(\mathfrak{H})$, $\mathrm{tr}_\Pi(AQ') = \mathrm{tr}_P(AQ')$ [HLS05a, Lemma 1]. Finally, $\mathrm{tr}_P(AQ') = \mathrm{tr}(|A|((Q')^{++} - (Q')^{--}) \geqslant 0$, so that $Q' = 0$, hence $Q = P - \Pi$, is a minimizer and the proof of the uniqueness is the same as the finite-dimensional lemma. □

B Hartree-Fock states

B.1 Definitions

We here precise the definition of a Hartree-Fock state. We do not state it in the main study because we saw that every term in the energy could be expressed in terms of the one-particle density matrix and not in terms of the proper underlying Hartree-Fock state. We choose the same definition as in [BLS94].

Recall that a generalized state Ω is defined as a linear form on $\mathcal{B}(\mathfrak{H})$, the set of all bounded operators on the Hilbert space $\mathfrak{H}$ of the system, satisfying $\Omega(\mathrm{Id}) = 1$ and $\Omega(A^*A) \geqslant 0$ for all $A \in \mathcal{B}(\mathfrak{H})$. Recall also that in our context, $\mathfrak{H}$ is the Fock space built on $\mathfrak{H}_\Lambda$

$$\mathfrak{H} = \mathcal{F}(\mathfrak{H}_\Lambda) := \mathbb{C} \oplus \bigoplus_{N=1}^{\infty} \bigwedge_{1}^{N} \mathfrak{H}_\Lambda.$$

We have defined in definition 2.4 the creation and annihilation operators $\boldsymbol{\psi}^*_{k,\sigma}$ and $\boldsymbol{\psi}_{k,\sigma}$. Notice that we have skipped the L in the notation for these sake of readability.

Definition B.1. *A state Ω is said to be* quasi-free *if for any operators $e_1, \dots, e_{2N}$ which are either a $\boldsymbol{\psi}^*_{k,\sigma}$ or a $\boldsymbol{\psi}_{k,\sigma}$, then $\Omega(e_1 e_2 \dots e_{2N-1}) = 0$ and*

$$\Omega(e_1 e_2 \dots e_{2N}) = \sum_{\pi \in \widetilde{\mathcal{S}_{2N}}} (-1)^{\varepsilon(\pi)} \Omega(e_{\pi(1)} e_{\pi(2)}) \dots \Omega(e_{\pi(2N-1)} e_{\pi(2N)}), \tag{B.1}$$

where $\widetilde{\mathcal{S}_{2N}}$ is the set of permutations of $\{1, \dots, 2N\}$ which verify $\pi(1) < \pi(3) < \dots < \pi(2N-1)$ and $\pi(2j) < \pi(2j-1)$ for all $1 \leqslant j \leqslant N$, and $\varepsilon(\pi)$ is the parity of the permutation π.

Remark B.1. *The relation (B.1) justifies the equality (2.25) used to derive the QED energy.*

We now define define the *number operator* $\mathcal{N}$ on the Fock space by

$$\mathcal{N} := \sum_{k,\sigma} \boldsymbol{\psi}^*_{k,\sigma} \boldsymbol{\psi}_{k,\sigma}.$$

Definition B.2. *A state Ω is a* generalized Hartree-Fock state *if it is quasi-free and has a finite number of particles $\Omega(\mathcal{N})$.*

Remark B.2. *Actually one could define Hartree-Fock states with a finite* charge *instead of number of particles in a Fock space built upon a reference P^0 as in [CI89, Tha92], so that in terms of the one-body density matrix γ, it means that $\mathrm{tr}(\gamma^{++} - \gamma^{--}) < \infty$. This is exactly saying that γ is P^0-trace class.*

B.2 Equivalence between the $\psi(x)$ and the $\psi_{k,\sigma}$ representations

We reindex the families $(e_{k,\sigma})$ and $(\boldsymbol{\psi}_{k,\sigma})$ defined in section 2.2.1 as $(e_i)_{i\in I}$ and $(\boldsymbol{\psi}_i)_{i\in I}$. We then have

$$\boldsymbol{\psi}(x) = \sum_{i\in I} e_i(x)\boldsymbol{\psi}_i, \qquad \boldsymbol{\psi}_i = \int_{\mathbb{T}_L} \boldsymbol{\psi}(x)\overline{e_i(x)}\,\mathrm{d}x.$$

We want to prove that the relations

$$\Omega(\boldsymbol{\psi}_i\boldsymbol{\psi}_j\boldsymbol{\psi}_k\boldsymbol{\psi}_l) = \Omega(\boldsymbol{\psi}_i\boldsymbol{\psi}_j)\Omega(\boldsymbol{\psi}_k\boldsymbol{\psi}_l) - \Omega(\boldsymbol{\psi}_i\boldsymbol{\psi}_k)\Omega(\boldsymbol{\psi}_j\boldsymbol{\psi}_l) + \Omega(\boldsymbol{\psi}_i\boldsymbol{\psi}_l)\Omega(\boldsymbol{\psi}_j\boldsymbol{\psi}_k),$$

for all i, j, k, l and

$$\begin{aligned}\Omega(\boldsymbol{\psi}(x)\boldsymbol{\psi}(y)\boldsymbol{\psi}(z)\boldsymbol{\psi}(t)) = \Omega(\boldsymbol{\psi}(x)\boldsymbol{\psi}(y))\Omega(\boldsymbol{\psi}(z)\boldsymbol{\psi}(t)) - \Omega(\boldsymbol{\psi}(x)\boldsymbol{\psi}(z))\Omega(\boldsymbol{\psi}(y)\boldsymbol{\psi}(t))\\ + \Omega(\boldsymbol{\psi}(x)\boldsymbol{\psi}(t))\Omega(\boldsymbol{\psi}(y)\boldsymbol{\psi}(z)),\end{aligned}$$

for all x, y, z, t, are equivalent. But is obvious since we have the relations

$$\Omega(\boldsymbol{\psi}(x)\boldsymbol{\psi}(y)\boldsymbol{\psi}(z)\boldsymbol{\psi}(t)) = \sum_{ijkl} e_i(x)e_j(y)e_k(z)e_l(t)\Omega(\boldsymbol{\psi}_i\boldsymbol{\psi}_j\boldsymbol{\psi}_k\boldsymbol{\psi}_l),$$

and

$$\Omega(\boldsymbol{\psi}_i\boldsymbol{\psi}_j\boldsymbol{\psi}_k\boldsymbol{\psi}_l) = \iiiint \overline{e_i(x)e_j(y)e_k(z)e_l(t)}\Omega(\boldsymbol{\psi}(x)\boldsymbol{\psi}(y)\boldsymbol{\psi}(z)\boldsymbol{\psi}(t))\,\mathrm{d}x\mathrm{d}y\mathrm{d}z\mathrm{d}t.$$

Hence, the $(\boldsymbol{\psi}_i)_i$ representation and the $(\boldsymbol{\psi}(x))_x$ representation are equivalent.

References

[BBHS99] Volker Bach, Jean Marie Barbaroux, Bernard Helffer, and Heinz Siedentop. On the stability of the relativistic electron-positron field. *Commun. Math. Phys.*, 201:445–460, 1999.

[Bha97] R. Bhatia. *Matrix analysis*. Springer Verlag, 1997.

[BLS94] Volker Bach, Elliott H. Lieb, and Jan Philip Solovej. Generalized Hartree-Fock theory and the Hubbard model. *J. Statist. Phys.*, 76(1-2):3–89, 1994.

[CDL08] Éric Cancès, Amélie Deleurence, and Mathieu Lewin. A new approach to the modelling of local defects in crystals: the reduced Hartree-Fock case. *Commun. Math. Phys.*, 281(1):129–177, 2008.

[CI89] Patrick Chaix and Daniel Iracane. From quantum electrodynamics to mean field theory: I. The Bogoliubov-Dirac-Fock formalism. *J. Phys. B*, 22:3791–3814, 1989.

[CIL89] Patrick Chaix, Daniel Iracane, and Pierre-Louis Lions. From quantum electrodynamics to mean field theory: II. Variational stability of the vacuum of quantum electrodynamics in the mean-field approximation. *J. Phys. B*, 22:3815–3828, 1989.

[Dir34] P.A.M. Dirac. Théorie du positron. *Solvay report*, XXV:203–212, 1934.

[GLS09] Philippe Gravejat, Mathieu Lewin, and Éric Séré. Ground state and charge renormalization in a nonlinear model of relativistic atoms. *Commun. Math. Phys.*, 286(1):179–215, 2009.

[HLS05a] Christian Hainzl, Mathieu Lewin, and Éric Séré. Existence of a stable polarized vacuum in the Bogoliubov-Dirac-Fock approximation. *Commun. Math. Phys.*, 257(3):515–562, 2005.

[HLS05b] Christian Hainzl, Mathieu Lewin, and Éric Séré. Self-consistent solution for the polarized vacuum in a no-photon QED model. *J. Phys. A*, 38(20):4483–4499, 2005.

[HLS07] Christian Hainzl, Mathieu Lewin, and Jan Philip Solovej. The mean-field approximation in quantum electrodynamics: the no-photon case. *Comm. Pure Appl. Math.*, 60(4):546–596, 2007.

[HLS09] Christian Hainzl, Mathieu Lewin, and Éric Séré. Existence of atoms and molecules in the mean-field approximation of no-photon quantum electrodynamics. *Arch. Rational Mech. Anal.*, 192(3):453–499, 2009.

[Hun66] W. Hunziker. On the spectra of Schrödinger multiparticle Hamiltonians. *Helv. Phys. Acta*, 39:451–462, 1966.

[Lew09] Mathieu Lewin. Systèmes quantiques à grand nombre de particules: une perspective mathématique et numérique, June 2009. Thèse d'Habilitation à Diriger des Recherches.

[Lio84] Pierre-Louis Lions. The concentration-compactness principle in the calculus of variations. The locally compact case, Part I. *Ann. Inst. Henri Poincaré*, 1(2):109–149, 1984.

[LS77] Elliott H. Lieb and Barry Simon. The Hartree-Fock theory for Coulomb systems. *Commun. Math. Phys.*, 53(3):185–194, 1977.

[RS72] M. Reed and Barry Simon. *Methods of Modern Mathematical Physics. I. Functional Analysis*. Academic Press, 1972.

[Sch48] Julian Schwinger. Quantum electrodynamics. I. A covariant formulation. *Phys. Rev. (2)*, 74:1439–1461, 1948.

[Sim79] Barry Simon. *Trace ideals and their applications*, volume 35 of *London Mathematical Society Lecture Note Series*. Cambridge University Press, Cambridge, 1979.

[Sol07] Jan Philip Solovej. Many body quantum mechanics. Lectures notes at LMU Münich, 2007.

[Tha92] Bernd Thaller. *The Dirac equation*. Texts and Monographs in Physics. Springer-Verlag, Berlin, 1992.

[Van64] C. Van Winter. Theory of finite systems of particles. I. The Green function. *Mat.-Fys. Skr. Danske Vid. Selsk.*, 2(8), 1964.

[Zhi60] G. M. Zhislin. Discussion of the spectrum of Schrödinger operators for systems of many particles. (in Russian). *Trudy Moskovskogo matematiceskogo obscestva*, 9:81–120, 1960.