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Ground State Energy of Atoms for Coulomb-Dirac operators

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Introduction

Let us consider a non-negative finite Borel measure μ on $\mathbb{R}^3$ and the corresponding linear Schrödinger operator

$$-\frac{\Delta}{2} - \mu * \frac{1}{|x|}$$

which describes a non-relativistic electron moving in the Coulomb potential generated by the charge distribution μ. It is well-known in the literature that the lowest eigenvalue of this operator is given by the variational principle [LL01]

$$\lambda_1\left(-\frac{\Delta}{2} - \mu * \frac{1}{|x|}\right) = \inf_{\substack{\varphi \in H^1(\mathbb{R}^3) \\ \int_{\mathbb{R}} |\varphi|^2 = 1}} \left\{ \frac{1}{2}\int_{\mathbb{R}^3} |\nabla\varphi(x)|^2 dx - \int_{\mathbb{R}^3} \left(\mu * \frac{1}{|\cdot|}\right)(x)|\varphi(x)|^2 dx \right\}.$$

Since it is an infimum over affine functions of μ, it is a concave function of μ. Therefore, on the convex set of non-negative Borel measures with fixed mass $\mu(\mathbb{R}^3) = \nu$, it is minimized when μ is proportional to a delta and we have

$$\lambda_1\left(-\frac{\Delta}{2} - \mu * \frac{1}{|x|}\right) \geqslant \lambda_1\left(-\frac{\Delta}{2} - \frac{\mu(\mathbb{R}^3)}{|x|}\right) = -\frac{\mu(\mathbb{R}^3)^2}{2}$$

for every $\mu \geqslant 0$. The interpretation is that the lowest possible electronic energy is reached by taking the most concentrated charge distribution, at fixed total charge $\mu(\mathbb{R}^3)$.

In the presence of molecules containing heavy nuclei, relativistic effects play an important role in the description of quantum electrons, since they will naturally attain high velocities, of the order of the speed of light. A proper description should then involve the Dirac operator D_0, derived in 1928 by Dirac himself [Tha13]. The Schrödinger operator is then replaced by $D_0 - \mu * |x|^{-1} = -i\alpha \cdot \nabla + \beta - \mu * |x|^{-1}$ (α and β are defined in the first chapter). One important difference with the Schrödinger case is that the essential spectrum of this operator is $(-\infty, -1] \cup [1, +\infty)$, hence is unbounded from below (and from above). The eigenvalues in the gap $(-1, 1)$ physically correspond to stationary states of the relativistic electrons. Therefore it seems natural to expect that the lowest eigenvalue in $(-1, 1)$ will again be minimized for the Dirac measure $\mu(\mathbb{R}^3)\,\delta_0$, like in the Schrödinger case. The aim of this thesis is to study this conjecture following the work done in the papers [ELS21a, ELS21b] by Maria J. Esteban, Mathieu Lewin and Éric Séré. In particular, I will study the following minimization problem

$$\lambda_1(\nu) := \inf_{\substack{\mu \geqslant 0 \\ \mu(\mathbb{R}^3) \leqslant \nu}} \lambda_1\left(D_0 - \mu * \frac{1}{|x|}\right). \tag{1}$$

Compared with nonrelativistic theories in which the Schrödinger operator $-\Delta/2$ appears instead of D_0, the unboundedness of the spectrum leads to important physical, mathematical and numerical difficulties. Indeed, if one simply replaces $-\Delta/2$ by D_0 in the energies of operators that are commonly used in the nonrelativistic case, one obtains energies which are not bounded from below.

Although there is no observable electron of negative energy, the negative spectrum plays an important role in physics. Dirac himself suspected that the negative spectrum of his operator could generate new interesting physical phenomena, and in the 1930's he proposed the following interpretation [Dir34]:

> We make the assumption that, in the world as we know it, nearly all the states of negative energy for the electrons are occupied, with just one electron in each state, and that a uniform filling of all the negative-energy states is completely unobservable to us.

Physically, one therefore has to imagine that the vacuum (called the *Dirac sea*) is filled with infinitely many virtual particles occupying the negative energy states. With this conjecture, a real free electron cannot be in a negative state due to the Pauli principle which forbids it to be in the same state as a virtual electron of the Dirac sea. With this interpretation, Dirac was able to conjecture the existence of "holes" in the vacuum, interpreted as "anti-electrons" or positrons, having a positive charge and a positive energy (a better explanation of this fact will be given in Section 1.3). The positron was discovered in 1932 by Anderson. Dirac also predicted the phenomenon of vacuum polarization: In the presence of an electric field, the virtual electrons are displaced, and the vacuum acquires a nonconstant density of charge. All these phenomena are now well known and well established in physics. They are direct consequences of the existence of the negative spectrum of D_0, showing the crucial role played by Dirac's discovery.

Another difficulty with the models, in addition to the unboundedness of the spectrum, is the lack of compactness: The Palais–Smale condition is not satisfied due to the unboundedness of the domain $\mathbb{R}^3$.

The combination of the above two types of difficulties poses a challenge in the Calculus of Variations.

In the first chapter of this thesis I define the (free) Dirac operator and study its properties, like self-adjointness and spectrum.

Then we add the potential $\mu * |x|^{-1}$. The difficulty here is that, for a singular measure μ, the operator $D_0 - \mu * |x|^{-1}$ can have several self-adjoint extensions, all with a different point spectrum. Even in the simple case $\mu = \nu\delta_0$, the Dirac-Coulomb operator $D_0 - \nu|x|^{-1}$ has infinitely many self-adjoint extensions when $\nu > \sqrt{3}/2$ [Tha13]. This is due to the fact that the Coulomb potential has a critical scaling with regard to the one-order differential operator D_0. This problem does not arise for the Schrödinger operator $-\Delta/2 - \mu * |x|^{-1}$ which is essentially self-adjoint for every finite measure μ, by Hardy's inequality. The solution to this problem has been found many years ago (see [ELS19] for a complete list of references).

The second chapter of the thesis, following the article [ELS21a], is dedicated to prove the existence of a similar distinguished self-adjoint extension for $D_0 - \mu * |x|^{-1}$ with domain in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, under the sole assumptions that

$$|\mu|\left(\mathbb{R}^3\right) < \infty \quad \text{and} \quad |\mu(\{R\})| < 1 \quad \text{for all } R \in \mathbb{R}^3.$$

This is done using Nenciu's method ([Nen76], Corollary 2.1).

Then, considering the particular case of positive measures, I characterize the domain using a method introduced in [EL07, EL08] and recently generalized in [SST20]. This characterization of the domain allows us to provide min-max formulas for the eigenvalues in the gap $(-1, 1)$, following for example [DES00, DES06, ELS19, SST20].

In the third and last chapter, following now [ELS21b], I investigate the detailed properties of the lowest possible eigenvalue among all possible measures μ with a fixed maximal charge ν; that is, the minimization problem (1). This problem is indeed the main motivation for studying Dirac operators with general measures μ.

The difficulty here is that the lowest Dirac eigenvalue in the gap $(-1, 1)$ depends in a non trivial way on the measure, not like in the Schrödinger case. The main result of this thesis will be Theorem 5 in [ELS21b]. It states that for any $0 \leqslant \nu < \nu_1$, where ν_1 will be defined as the critical mass for which we have $\lambda_1(D_0 - \mu * |x|^{-1}) > -1$ for all $\mu(\mathbb{R}^3) < \nu_1$, there exists at least one minimizing measure for $\lambda_1(\nu)$ and any minimizer concentrate on a compact set of Lebesgue measure zero. Thus, although the full conjecture remains open so far, we already know that an optimal measure should be singular.

The existence of the optimal measure is proved by a rather delicate adaptation of techniques from nonlinear analysis to the context of Dirac operators. The first eigenvalue is a highly nonlinear function of the measure μ, even if the operator only depends linearly on μ. The main enemy here is the action of the non-compact group of space translations and this will be controlled using Lions' concentration-compactness method [Lio84a, Lio84b, Lio85a, Lio85b, Lew10].

Chapter 1

The Free Dirac Operator

1.1 Notation

Dirac derived in 1928 his operator to describe the relativistic motion of a spin-1/2 particle in $\mathbb{R}^3$ [Tha13]. For simplicity, we will work in a system of units for which $m = c = \hbar = 1$ (the electron mass, the speed of light and the Planck constant, respectively). The free Dirac operator is then given by

$$D_0 := -i\boldsymbol{\alpha} \cdot \nabla + \beta = -i \sum_{k=1}^{3} \alpha_k \partial_{x_k} + \beta \tag{1.1}$$

where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ is a triplet of matrices and $\alpha_1, \alpha_2, \alpha_3, \beta$ are 4×4 Hermitian matrices which satisfy the following anticommutation relations:

$$\begin{cases} \alpha_k \alpha_l + \alpha_l \alpha_k = 2\delta_{kl} \mathbb{1}, \\ \alpha_k \beta + \beta \alpha_k = 0, \\ \beta^2 = \mathbb{1}. \end{cases}$$

The usual representation in 2×2 block matrices is given by

$$\beta = \begin{pmatrix} \mathbb{1}_2 & \mathbb{0}_2 \\ \mathbb{0}_2 & -\mathbb{1}_2 \end{pmatrix}, \qquad \alpha_k = \begin{pmatrix} \mathbb{0}_2 & \sigma_k \\ \sigma_k & \mathbb{0}_2 \end{pmatrix} \qquad \text{for } k = 1, 2, 3,$$

where the Pauli matrices are defined by

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

The important property of the Dirac operator is that $D_0^2 = -\Delta + \mathbb{1}$, where Δ is the usual Laplacian.

The operator D_0 is then given explicitly by the matrix-valued differential expression

$$D_0 = \begin{pmatrix} \mathbb{1}_2 & -i\boldsymbol{\sigma}\cdot\nabla \\ -i\boldsymbol{\sigma}\cdot\nabla & -\mathbb{1}_2 \end{pmatrix}, \tag{1.2}$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$. Therefore, D_0 acts on vector-valued wave-functions

$$\varphi(x) = \begin{pmatrix} \varphi_1(x) \\ \vdots \\ \varphi_4(x) \end{pmatrix} \in \mathbb{C}_4.$$

In particular, D_0 is defined on the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \equiv L^2(\mathbb{R}^3)^4 \equiv L^2(\mathbb{R}^3, \mathbb{C}^4)$. It consists of 4-components column vectors $\varphi = (\varphi_1, \varphi_2, \varphi_3, \varphi_4)^\perp$ where each component φ_i is a complex-valued L^2 function of the space variable $x \in \mathbb{R}^3$. In $\mathscr{H}$, the scalar product is given by

$$(\varphi, \psi) = \int_{\mathbb{R}^3} \sum_{k=1}^{4} \overline{\varphi_k(x)}\psi_k(x)\, d^3x.$$

We want to define the free Dirac operator

$$D_0\varphi = -i\boldsymbol{\alpha}\cdot\nabla\varphi + \beta\varphi, \qquad \text{for every } \varphi \in \mathcal{D}(D_0)$$

on a suitable domain $\mathcal{D}(D_0)$ of this Hilbert space. In the next section, we will prove that D_0 is self-adjoint on $\mathcal{D}(D_0) = H^1(\mathbb{R}^3)^4 \subset \mathscr{H}$, which is a natural domain for first-order differential operators.

1.2 Self-adjointness and Spectrum

The free Dirac operator is easily analyzed in the Fourier space. The Fourier transformation $\mathcal{F}$ maps $L^2(\mathbb{R}^3, d^3x)^4$ into itself (sometimes to distinguish between the variables we shall write $\mathcal{F}L^2(\mathbb{R}^3, d^3x)^4 = L^2(\mathbb{R}^3, d^3\boldsymbol{p})^4$). Any matrix differential operator in $L^2(\mathbb{R}^3, d^3x)^4$ is mapped via $\mathcal{F}$ into a matrix multiplication operator in $L^2(\mathbb{R}^3, d^3\boldsymbol{p})^4$. For the Dirac operator (1.2), using the fact that $\mathcal{F}(-i\nabla) = \boldsymbol{p}$, one obtains the matrix multiplication operator $h(\boldsymbol{p})$, given by :

$$h(\boldsymbol{p}) := (\mathcal{F}D_0\mathcal{F}^{-1})(\boldsymbol{p}) = \begin{pmatrix} \mathbb{1}_2 & \boldsymbol{\sigma}\cdot\boldsymbol{p} \\ \boldsymbol{\sigma}\cdot\boldsymbol{p} & -\mathbb{1}_2 \end{pmatrix} = \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta. \tag{1.3}$$

For each $\boldsymbol{p}$, this is a 4×4 Hermitian matrix with eigenvalues

$$\lambda_1(p) = \lambda_2(p) = -\lambda_3(p) = -\lambda_4(p) = \sqrt{p^2+1} =: \lambda(p), \quad \text{where } p = |\boldsymbol{p}|.$$

The unitary transformation $u(\boldsymbol{p})$ which brings $h(\boldsymbol{p})$ to its diagonal form is given explicitly by

$$u(\boldsymbol{p}) = \frac{(1+\lambda(p))\mathbb{1} + \beta\boldsymbol{\alpha}\cdot\boldsymbol{p}}{\sqrt{2\lambda(p)(1+\lambda(p))}} = a_+(p)\mathbb{1} + a_-(p)\beta\frac{\boldsymbol{\alpha}\cdot\boldsymbol{p}}{p},$$

where

$$a_\pm(p) = \sqrt{\frac{1\pm 1/\lambda(p)}{2}}.$$

It is easy to check that $u(\boldsymbol{p})h(\boldsymbol{p})u(\boldsymbol{p})^{-1} = \beta\lambda(p)$ where $u(\boldsymbol{p})^{-1} = a_+(p)\mathbb{1} - a_-(p)\beta\frac{\boldsymbol{\alpha}\cdot\boldsymbol{p}}{p}$. From this latter equation and (1.3), we see that the unitary transformation $\mathcal{W} := u\mathcal{F}$ converts D_0 into a multiplication operator by the diagonal matrix $(\mathcal{W}D_0\mathcal{W}^{-1})(\boldsymbol{p}) = (u\mathcal{F}D_0\mathcal{F}^{-1}u^{-1})(\boldsymbol{p}) = (uhu^{-1})(\boldsymbol{p}) = \beta\lambda(p)$ in the Hilbert space $L^2(\mathbb{R}^3, d^3\boldsymbol{p})^4$.

Thanks to the spectral theorem, we conclude that D_0 is self-adjoint on $\mathcal{D}(D_0) = \mathcal{W}^{-1}\mathcal{D}(\beta\lambda(\cdot)) = \mathcal{F}^{-1}u^{-1}\mathcal{D}(\lambda(\cdot)) = \mathcal{F}^{-1}\mathcal{D}(\lambda(\cdot))$, since it is unitarily equivalent to the multiplication by a diagonal matrix-valued function of $\boldsymbol{p}$. Here we used the fact that the multiplication by a unitary matrix does not change the domain of any multiplication operator. Moreover, $H^1(\mathbb{R}^3)^4$ is defined by

$$H^1(\mathbb{R}^3)^4 := \{f \in L^2(\mathbb{R}^3, d^3\boldsymbol{p})^4 | (1+|\boldsymbol{p}|^2)^{1/2} f \in L^2(\mathbb{R}^3, d^3\boldsymbol{p})^4\}.$$

By definition of λ this set is equal to $\mathcal{D}(\lambda(\cdot))$.

The spectrum of D_0 equals the spectrum of the multiplication operator $\beta\lambda$ which is simply the image of the functions $p \mapsto \lambda_i(p)$ for $i = 1, ..., 4$; that is, $\sigma(D_0) = (-\infty, -1] \cup [1, +\infty)$.

Along this manuscript, we will use the notation abuse $D_0 = \alpha\cdot p + \beta$ by which we mean that D_0 acts in the following way:

$$(D_0\varphi)(x) = \mathcal{F}^{-1}\left((\alpha\cdot p+\beta)\mathcal{F}(\varphi)(p)\right)(x) \quad \forall\varphi \in H^1(\mathbb{R}^3, \mathbb{C}^4).$$

1.3 Charge conjugation

The free Dirac operator represents the energy of the system described by the time-dependent Dirac equation $i\frac{\partial}{\partial t}\varphi(t,x) = D_0\varphi(t,x)$. Since the spectrum of the Dirac operator has a negative part, the system can be in a state with negative energy, but the occurrence of negative energies for an electron is a peculiar fact. A better understanding of the negative energy solutions can be obtained if we consider the Dirac equation in an external field, and the operation of charge conjugation. The Dirac operator for a charge e in an external electromagnetic field (φ_{el}, A) is given by

$$H(e) = \alpha\cdot(p - eA(t,x)) + \beta + e\varphi_{\text{el}}(t,x).$$

Now, we will consider the antiunitary transformation

$$C\psi := U_C\overline{\psi},$$

where U_C is a unitary 4×4 matrix such that $\beta U_C = -U_C\beta$ and $\alpha_k U_C = U_C\overline{\alpha_k}$, for $k = 1, 2, 3$. In our notation, we take $U_C = i\beta\alpha_2$. It is easy to see that, when $\psi(t)$ is a solution of the Dirac equation with Hamiltonian $H(e)$, $C\psi(t)$ is a solution of the Dirac equation with Hamiltonian $H(-e)$. This motivates the name *charge conjugation* for the operator C. Moreover, we have

$$CH(e)C^{-1} = -H(-e).$$

Thus, the negative energy subspace of $H(e)$ is connected via a symmetry transformation to the positive energy subspace of the Dirac operator $H(-e)$ for a particle with opposite charge (antiparticle, positron).

Going back to the free Dirac operator, since $D_0 = H(0)$, we get

$$CD_0C^{-1} = -D_0.$$

(The same holds for $\alpha \cdot p + \varepsilon\beta$ and $(\alpha \cdot p + \varepsilon\beta)^{-1}$ in place of D_0.) This gives the symmetry of the spectrum of these operators. Indeed, let us denote by A any of them and by $\rho(A)$ the resolvent of A. Then,

$$\begin{aligned}
\lambda \in \rho(A) \cap \mathbb{R} &\Leftrightarrow A - \lambda \quad \text{is invertible with bounded inverse} \\
&\Leftrightarrow C(A - \lambda)C^{-1} \quad \text{is invertible with bounded inverse} \\
&\Leftrightarrow -A - \lambda \quad \text{is invertible with bounded inverse} \\
&\Leftrightarrow -\lambda \in \rho(A) \cap \mathbb{R}.
\end{aligned}$$

We conclude since the spectrum is the complementary in $\mathbb{R}$ of the resolvent ρ.

The symmetry of the spectrum for a bounded self-adjoint operator gives us an other important property that will be useful along the thesis: The maximum of the spectrum equals the norm of the operaror A. Indeed, for bounded operators Gelfand's formula tells us that the spectral radius $r(A)$, defined as the max of the norm of the eigenvalues, is given by

$$r(A) = \lim_{n\to\infty} \|A^n\|^{1/n}.$$

By the symmetry of the spectrum, it is clear that $r(A) = \max \sigma(A)$. On the other hand, for any self-adjoint operator the right-hand side is exactly the norm, since the identity $\|A^2\| = \|AA^*\| = \|A\|^2$ implies by induction $\|A^{2n}\| = \|A\|^{2n}$. Hence, $\lim \|A^n\|^{1/n} = \lim \|A^{2n}\|^{1/2n} = \lim \|A\| = \|A\|$. Finally,

$$\max \sigma(A) = r(A) = \|A\|. \tag{1.4}$$

Chapter 2

Distinguished extension and min-max formulas

We now add to the free Dirac operator the potential generated by a charge distribution μ ; that is

$$V_\mu := \mu * \frac{1}{|x|}.$$

We want to study the properties of $D_0 - V_\mu$ in order to arrive at a min-max formulation of the eigenvalues, that is necessary to study the first, namely the smallest, eigenvalue. All the theorems and their proofs of this chapter can be found in [ELS21a].

2.1 Distinguished self-adjoint extension for a general charge

The aim of this section is to give a meaning to the operator $D_0 - V_\mu$ for the largest possible class of bounded measure μ.

Theorem 2.1 (Distinguished self-adjoint extension)**.** *Let μ be any finite signed Borel measure on $\mathbb{R}^3$, such that*

$$|\mu(\{R\})| < 1 \quad \forall R \in \mathbb{R}^3.$$

Then the operator $D_0 - V_\mu$ defined first on $H^1(\mathbb{R}^3, \mathbb{C}^4)$ or on $C_c^\infty(\mathbb{R}^3, \mathbb{C}^4)$ has a unique self-adjoint extension whose domain is included in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$.

The functions in the domain of the extension $\mathcal{D}(D_0 - V_\mu)$ have a square integrable gradient in $\mathbb{R}^3 \setminus \cup_{j=1}^k B_r(R_j)$ for all $r > 0$, where $R_1, ..., R_k \in \mathbb{R}^3$ are all the points such that $|\mu(R_j)| \geqslant \frac{1}{2}$.

The operator $D_0 - V_\mu$ is the norm resolvent limit of $D_0 - V_\mu \mathbb{1}_{\{|V_\mu|\leqslant n\}}$ when $n \to \infty$. Moreover, its essential spectrum is $\sigma_{\mathrm{ess}}(D_0 - V_\mu) = (-\infty, -1] \cup [1, +\infty)$.

The proof relies on the following lemmas.

Lemma 2.1 (Compactness for disjoint supports)**.** *Let $f \in L^2(\mathbb{R}^n)$ and $B \subset \mathbb{R}^n$ a compact set with* $\operatorname{supp}(f) \subset B$*. Moreover, let $g \in L^2_{loc}(\mathbb{R}^n)$ with* $\operatorname{supp}(g) \subset \Omega \subset \mathbb{R}^n$*, where Ω is such that $d(\Omega, B) > 0$. Finally, let us assume that $\int_\Omega \frac{|g(x)|^2}{(1+|x|^2)^{2(n-s)}} dx < \infty$, where $0 < s < n$. Then, the operator $K = g(x)\frac{1}{|p|^s} f(x)$, which formally is $\varphi \mapsto K\varphi(x) = g(x)\mathcal{F}^{-1}\left(\frac{1}{|p|^s}\mathcal{F}(f\,\varphi)(p)\right)(x)$, is compact and its norm can be estimated by*

$$\|K\| \leqslant C\|f\|_{L^2(B)} \left(\int_\Omega \frac{|g(x)|^2}{(1+|x|^2)^{2(n-s)}} dx\right)^{1/2},$$

where C depends only on $s, n, d(B, \Omega)$ and $\sup_{x\in B}|x|$*.*

Proof. The kernel of K is

$$\mathcal{K}(x,y) = k\frac{\mathbb{1}_\Omega(x) g(x) f(y)}{|x-y|^{n-s}},$$

for a positive constant k, i.e. $Kh(x) = \int_{\mathbb{R}^n} \mathcal{K}(x,y)dy = \int_{\mathbb{R}^n} k\frac{\mathbb{1}_\Omega(x)g(x)f(y)}{|x-y|^{n-s}}dy = k\mathbb{1}_\Omega(x)g(x)\int_{\mathbb{R}^n}\frac{f(y)h(y)}{|x-y|^{n-s}}dy \quad \forall h \in \mathcal{D}(K)$. This comes from the fact that $\mathcal{F}(\frac{1}{|x|^s})(p) = \frac{1}{|p|^{n-s}}$ (up to a multiplicative constant).

In addition, we have $|x-y| \geqslant c(|x|+1)$ $\forall x \in \Omega$ and $y \in B$. Indeed, the function $\psi(x,y) := \frac{|x-y|}{|x|+1}$ is bounded from below by a positive constant c. Let $R := \sup_{y\in B}|y|$. Then,

- If $x \in B(0,2R)$, then $\psi(x,y) \geqslant \frac{d(B,\Omega)}{2R+1} =: c_1$;
- If $x \notin B(0,2R)$ then $\psi(x,y) \geqslant \frac{|x|-R}{|x|+1} \geqslant \frac{R}{2R+1} =: c_2$, where in the last inequality we used the fact that the function $z \mapsto \phi(z) := \frac{y-R}{y+1}$ is increasing for $z \geqslant 0$, thus $\phi(|x|) \geqslant \phi(2R)$ when $|x| \geqslant 2R$.

Finally, take $c = \min\{c_1, c_2\}$. Therefore, we have the following estimate for the kernel:

$$|\mathcal{K}(x,y)| \leqslant \frac{k}{c^{n-s}}\frac{|g(x)|}{(1+|x|)^{n-s}}|f(y)|,$$

and we can estimate the norm:

$$\begin{aligned}
\|Kh\|_2^2 &= C\int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^n}\frac{f(y)h(y)}{|x-y|^{n-s}}dy\,\mathbb{1}_\Omega(x)g(x)\right)^2 dx\\
&\leqslant C\left(\int_\Omega \frac{|g(x)|^2}{(1+|x|)^{2(n-s)}}dx\right)\left(\int_{\mathbb{R}^n} f(y)h(y)dy\right)^2\\
&\overset{\text{Hölder}}{\leqslant} C\left(\int_\Omega \frac{|g(x)|^2}{(1+|x|^2)^{2(n-s)}}dx\right)\|f\|_{L^2(B)}^2\|h\|_2^2,
\end{aligned}$$

$$\Longrightarrow \|K\|\leqslant C\|f\|_{L^2(B)}\left(\int_\Omega \frac{|g(x)|^2}{(1+|x|^2)^{2(n-s)}}dx\right)^{1/2} < \infty \quad \text{by assumption.}$$

For simplicity, when the domain is clear, we denote by $\|\cdot\|_p$ the L^p-norm on that domain. We now conclude the proof by proving the compactness. Let $u_n \rightharpoonup 0$ be any sequence converging weakly to 0 in L^2 such that $\|u_n\|_2 = 1$ for every n. The sequence $(Ku_n)(x) = kg(x)\int_B \frac{f(y)u_n(y)}{|x-y|^{n-s}}dy$ converges to 0 a.e. since the function $y\in B\mapsto \frac{f(y)}{|x-y|^{n-s}}$ is in L^2 $\forall x\in\Omega$ ($f\in L^2$ and $|x-y|\geqslant c(|x|+1)\geqslant c$) and $u_n \overset{L^2}{\rightharpoonup} 0$. In addition, we have

$$\begin{aligned}
|(Ku_n)(x)| \leqslant \frac{k}{c^{n-s}}\frac{|g(x)|}{(|x|+1)^{n-s}}\int_{\mathbb{R}^n}|fu_n| &\overset{\text{Hölder}}{\leqslant} \frac{k}{c^{n-s}}\frac{|g(x)|}{(1+|x|)^{n-s}}\|f\|_2\|u_n\|_2\\
&= \frac{k\|f\|_2}{c^{n-s}}\frac{|g(x)|}{(1+|x|)^{n-s}},
\end{aligned}$$

which is an L^2 function by assumption. Hence $\|Ku_n\|_2 \underset{n\to\infty}{\longrightarrow} 0$ by the dominated convergence theorem. □

Lemma 2.2 (Local compactness in the absence of atoms)**.** *Let $\mu'\geqslant 0$ be a finite Radon measure on $\mathbb{R}^3$, with no atom. Then the operator*

$$\mathbb{1}_{B_R}\sqrt{\mu' * \frac{1}{|x|}}\frac{1}{|p|^{1/2}}$$

is compact for every finite $R>0$.

Proof. We write $\mu' = \mu'\mathbb{1}_{B_N} + \mu'\mathbb{1}_{B_N^c} =: \mu_1' + \mu_2'$, so that $V_{\mu'} = V_{\mu_1'} + V_{\mu_2'}$. Hence, using the fact that $\sqrt{a+b}\leqslant\sqrt{a}+\sqrt{b}$, we obtain that $0\leq \sqrt{V_{\mu'}} - \sqrt{V_{\mu_1'}} \leqslant \sqrt{V_{\mu_2'}}$ pointwisely. This implies immediately that $\|(\sqrt{V_{\mu'}} - \sqrt{V_{\mu_1'}})\frac{1}{|p|^{1/2}}\| \leqslant \|\sqrt{V_{\mu_2'}}\frac{1}{|p|^{1/2}}\|$. Now, from Theorem A.2 in Appendix A, which is based on Kato's inequality $\frac{1}{|x|}\leqslant\frac{\pi}{2}|p|$ (A.1), one has

$$\frac{1}{|p|}\leqslant \frac{\pi}{2}\mu'(\mathbb{R}^3)\frac{1}{V_{\mu'}}.$$

This implies that

$$\left\|\frac{1}{|p|^{\frac{1}{2}}}\sqrt{V_{\mu'}}\varphi\right\|_2^2 = (\sqrt{V_{\mu'}}\varphi, \frac{1}{|p|}\sqrt{V_{\mu'}}\varphi)$$
$$\leqslant \frac{\pi}{2}\mu'(\mathbb{R}^3)(\sqrt{V_{\mu'}}\varphi, \frac{1}{V_{\mu'}}\sqrt{V_{\mu'}}\varphi) = \frac{\pi}{2}\mu'(\mathbb{R}^3)\|\varphi\|_2^2.$$

In particular,

$$\left\|\sqrt{V_{\mu'}}\frac{1}{|p|^{\frac{1}{2}}}\right\| = \left\|\frac{1}{|p|^{\frac{1}{2}}}\sqrt{V_{\mu'}}\right\| \leqslant \sqrt{\frac{\pi}{2}\mu'(\mathbb{R}^3)}, \tag{2.1}$$

(where we used the fact that $\|AB\| = \|(AB)^*\| = \|B^*A^*\| = \|BA\|$ since both operators are self-adjoint). Note also that for these estimates the measure does not necessarily have to be atom-free.

Going back to our case, we have proved

$$\left\|\left(\sqrt{V_{\mu'}} - \sqrt{V_{\mu'_1}}\right)\frac{1}{|p|^{1/2}}\right\| \leqslant \sqrt{\frac{\pi}{2}\mu'(B_N^c)} \xrightarrow{N\to\infty} 0.$$

Hence we may assume that μ' has compact support, and then use the fact that the norm-limit of a sequence of compact operators is compact (see [Kat13], Theorem III.4.7).

Now for $r > 0$, let us consider two tilings of $\mathbb{R}^3$ with cubes:

$$C_j = 3r\left(j + [-1/2, 1/2)^3\right) \text{ and } C'_k = r\left(k + [-1/2, 1/2)^3\right), \text{for } j, k \in \mathbb{Z}^3,$$

of side $3r$ and r respectively. For every k, we call j_k the index of the large cube C_{j_k} of which C'_k is exactly at the center.

Let $\varepsilon > 0$. Then, by compactness of the support of μ' and the fact that μ' has no atom, we can find $r > 0$ s.t. $\mu'(C_j) \leqslant \varepsilon\ \forall j$. We then write

$$\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R}\left(\mu' * \frac{1}{|x|}\right)\frac{1}{|p|^{1/2}} = \sum_k \frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C'_k}\left(\mu'(\mathbb{1}_{C_{j_k}} + \mathbb{1}_{C^c_{j_k}}) * \frac{1}{|x|}\right)\frac{1}{|p|^{1/2}}.$$

Notice that the sum is finite. The sets C'_k and $C^c_{j_k}$ are at least at a distance r from each other, so we have

$$\left|\mathbb{1}_{C'_k}\left(\mu'\mathbb{1}_{C^c_{j_k}} * \frac{1}{|x|}\right)\right| = \left|\mathbb{1}_{C'_k}\int_{C^c_{j_k}}\frac{d\mu'(y)}{|x-y|}\right| \overset{|x-y|\geqslant r}{\leqslant} \left|\frac{\mu'(C^c_{j_k})}{r}\right| =: \frac{C}{r}.$$

Hence

$$f(x) := \mathbb{1}_{C'_k}\left(\mu'\mathbb{1}_{C^c_{j_k}} * \frac{1}{|x|}\right) \in L^p(C'_k) \quad \forall 1 \leqslant p \leqslant \infty.$$

In particular, $|f|^{1/2} \in L^6(\mathbb{R}^3)$ and $g(p) := \frac{1}{|p|^{1/2}} \in L^{6,\infty}_\omega(\mathbb{R}^3)$, where the notation $L^{6,\infty}$ stands for the weak L^6 space that is embedded with the norm

$$
\begin{aligned}
\|g\|_{L^{6,\infty}} &:= \sup_{t>0} t\mathscr{L}\left(\{x \in \mathbb{R}^3 : |g(x)| > t\}\right)^{1/6} = \sup_{t>0} t\mathscr{L}\left(\left\{\frac{1}{|x|^{1/2}} > t\right\}\right)^{\frac{1}{6}} \\
&= \sup_{t>0} t(\mathscr{L}(B_{\frac{1}{t^2}}))^{\frac{1}{6}} = \sup_{t>0} t\left(\frac{k}{t^6}\right)^{\frac{1}{6}} = k < \infty,
\end{aligned}
$$

where $\mathscr{L}$ is the Lebegue measure and k is a positive constant. Then, the operator $R := |f|^{1/2}\frac{1}{|p|^{1/2}}$ is compact by Cwikel's theorem ([Sim05], Theorem 4.2). Therefore $\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C'_k}\left(\mu'\mathbb{1}_{C^c_{j_k}} * \frac{1}{|x|}\right)\frac{1}{|p|^{1/2}} = \frac{1}{|p|^{1/2}}|f|^{1/2}|f|^{1/2}\frac{1}{|p|^{1/2}}$ $(= R^*R)$ is also compact (for every k).

Finally, we have obtained that

$$
\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R}\left(\mu' * \frac{1}{|x|}\right)\frac{1}{|p|^{1/2}} = \sum_k \frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C'_k}\left(\mu'\mathbb{1}_{C_{j_k}} * \frac{1}{|x|}\right)\frac{1}{|p|^{1/2}} + K_1,
$$

where K_1 is compact. Moreover, we can write

$$
\frac{1}{|p|^{\frac{1}{2}}}\mathbb{1}_{B_R\cap C'_k}V_{\mu'\mathbb{1}_{C_{j_k}}}\frac{1}{|p|^{\frac{1}{2}}} = (\mathbb{1}_{C_{j_k}} + \mathbb{1}_{C^c_{j_k}})\frac{1}{|p|^{\frac{1}{2}}}\mathbb{1}_{B_R\cap C'_k}V_{\mu'\mathbb{1}_{C_{j_k}}}\frac{1}{|p|^{\frac{1}{2}}}(\mathbb{1}_{C_{j_k}} + \mathbb{1}_{C^c_{j_k}}).
$$

The operator $T_k := \mathbb{1}_{C^c_{j_k}}\frac{1}{|p|^{\frac{1}{2}}}\mathbb{1}_{C'_k\cap B_R}\sqrt{\mu'\mathbb{1}_{C_{j_k}} * \frac{1}{|x|}}$ is compact by Lemma 2.1 with

$$
g(x) = \mathbb{1}_{C^c_{j_k}}, \quad f(x) = \mathbb{1}_{C'_k\cap B_R}\sqrt{\mu'\mathbb{1}_{C_{j_k}} * \frac{1}{|x|}}, \quad n = 3, \quad s = 1/2.
$$

Therefore

$$
\begin{aligned}
\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R}\left(\mu' * \frac{1}{|x|}\right)\frac{1}{|p|^{1/2}} &= \sum_k \mathbb{1}_{C_{j_k}}\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C'_k}\left(\mu'\mathbb{1}_{C_{j_k}} * \frac{1}{|x|}\right)\frac{1}{|p|^{1/2}}\mathbb{1}_{C_{j_k}} \\
&\quad + \sum_k \mathbb{1}_{C_{j_k}}\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C'_k}\left(\mu'\mathbb{1}_{C_{j_k}} * \frac{1}{|x|}\right)\frac{1}{|p|^{1/2}}\mathbb{1}_{C^c_{j_k}} \\
&\quad + \sum_k \mathbb{1}_{C^c_{j_k}}\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C'_k}\left(\mu'\mathbb{1}_{C_{j_k}} * \frac{1}{|x|}\right)\frac{1}{|p|^{1/2}}\mathbb{1}_{C_{j_k}} + K_1 \\
&=: S + \sum_k \mathbb{1}_{C_{j_k}}\frac{1}{|p|^{1/2}}\sqrt{\mu'\mathbb{1}_{C_{j_k}} * \frac{1}{|x|}}T^*_k \\
&\qquad + \sum_k T_k\sqrt{\mu'\mathbb{1}_{C_{j_k}} * \frac{1}{|x|}}\frac{1}{|p|^{1/2}}\mathbb{1}_{C_{j_k}} + K_1 =: S + K_2,
\end{aligned}
$$

where K_2 is compact because T_k is compact ($\Rightarrow T_k^*$ too) and $\frac{1}{|p|^{1/2}}\sqrt{\mu'\mathbb{1}_{C_{j_k}} * \frac{1}{|x|}}$ abd $\sqrt{\mu'\mathbb{1}_{C_{j_k}} * \frac{1}{|x|}}\frac{1}{|p|^{1/2}}$ are bounded by (2.1). At the end, S can be bounded as follows:

$$\begin{aligned}
&\left(\varphi, \mathbb{1}_{C_{j_k}}\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C_k'}V_{\mu'\mathbb{1}_{C_{j_k}}}\frac{1}{|p|^{1/2}}\mathbb{1}_{C_{j_k}}\varphi\right)\\
&= \left(\mathbb{1}_{C_{j_k}}\varphi, \frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C_k'}\sqrt{V_{\mu'\mathbb{1}_{C_{j_k}}}}\left(\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C_k'}\sqrt{V_{\mu'\mathbb{1}_{C_{j_k}}}}\right)^*\mathbb{1}_{C_{j_k}}\varphi\right)\\
&= \left\|\left(\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C_k'}\sqrt{V_{\mu'\mathbb{1}_{C_{j_k}}}}\right)^*\mathbb{1}_{C_{j_k}}\varphi\right\|_2^2\\
&\leqslant \left\|\mathbb{1}_{B_R\cap C_k'}\sqrt{V_{\mu'\mathbb{1}_{C_{j_k}}}}\frac{1}{|p|^{1/2}}\right\|^2\|\mathbb{1}_{C_{j_k}}\varphi\|_2^2\\
&\overset{2.1}{\leqslant} \frac{\pi}{2}\mu'(C_{j_k})(\varphi, \mathbb{1}_{C_{j_k}}\varphi) \quad \forall\varphi\in L^2(\mathbb{R}^3,\mathbb{C}^4).
\end{aligned}$$

This exactly means that

$$\mathbb{1}_{C_{j_k}}\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R\cap C_k'}V_{\mu'\mathbb{1}_{C_{j_k}}}\frac{1}{|p|^{1/2}}\mathbb{1}_{C_{j_k}} \leqslant \frac{\pi}{2}\mu'(C_{j_k})\mathbb{1}_{C_{j_k}} \quad \forall k.$$

Hence

$$0 \leqslant S \leqslant \frac{\pi}{2}\sum_k \mu'(C_{j_k})\mathbb{1}_{C_{j_k}} \leqslant \varepsilon\frac{\pi}{2}\sum_k \mathbb{1}_{C_{j_k}} \leqslant \frac{27\pi}{2}\varepsilon,$$

where we used the fact that $\mu'(C_j) \leqslant \varepsilon$ by our choice of r and that every point touches at most 27 C_{j_k}. Letting ε go to 0, we obtain that $\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R}\left(\mu' * \frac{1}{|x|}\right)\frac{1}{|p|^{1/2}} = \left(\mathbb{1}_{B_R}\sqrt{\mu' * \frac{1}{|x|}}\frac{1}{|p|^{1/2}}\right)^*\left(\mathbb{1}_{B_R}\sqrt{\mu' * \frac{1}{|x|}}\frac{1}{|p|^{1/2}}\right)$ is compact, being norm-limit of compact operators. Therefore, $\mathbb{1}_{B_R}\sqrt{\mu' * \frac{1}{|x|}}\frac{1}{|p|^{1/2}}$ also is compact, and this concludes the proof. □

We are now ready to prove the main theorem.

Proof of Theorem 2.1. Our goal is to show that

$$\limsup_{|s|\to\infty}\left\|\sqrt{|V_\mu|}\frac{1}{D_0+is}\sqrt{|V_\mu|}\right\| \leqslant \max_{R\in\mathbb{R}^3}|\mu(\{R\})|, \tag{2.2}$$

which is strictly less then 1 since $\mu(\{R\}) < 1\,\forall R\in\mathbb{R}^3$ and μ is finite.

Let us write now μ in the following way:

$$\mu = \sum_{m=1}^{\infty}\nu_m\delta_{R_m} + \mu',$$

where R_m are all distinct, $\max_m |\nu_m| < 1$ (by assumption) and μ' has no atom. Then, we can write

$$\mu = \left(\sum_{m=1}^{K} \nu_m \delta_{R_m} + \mu' \mathbb{1}_{B_N}\right) + \left(\sum_{m>K} \nu_m \delta_{R_m} + \mu' \mathbb{1}_{B_N^c}\right) =: \mu_1 + \mu_2.$$

Notice that $|\mu_2|(\mathbb{R}^3)$ tends to 0 as $K, N \to \infty$. Using this fact and Kato's inequality, it suffices to show (2.2) for μ with finitely many atoms and for μ' with compact support. Indeed:

$$\begin{aligned}\left\|\sqrt{|V_\mu|}\frac{1}{D_0+is}\sqrt{|V_\mu|}\right\| &\leqslant \left\|\left(\sqrt{|V_{\mu_1}|}+\sqrt{|V_{\mu_2}|}\right)\frac{1}{D_0+is}\left(\sqrt{|V_{\mu_1}|}+\sqrt{|V_{\mu_2}|}\right)\right\| \\ &\leqslant \sum_{i,j=1}^{2}\left\|\sqrt{|V_{\mu_i}|}\frac{1}{D_0+is}\sqrt{|V_{\mu_j}|}\right\|,\end{aligned}$$

since $\sqrt{|V_\mu|} = \sqrt{|V_{\mu_1}+V_{\mu_2}|} \leqslant \sqrt{|V_{\mu_1}|} + \sqrt{|V_{\mu_2}|}$ and $\|fAf\| = \|fg^{-1}gAgg^{-1}f\| \leqslant \|fg^{-1}\|^2\|gAg\| \leqslant \|gAg\|$ if $0 \leqslant f \leqslant g$ because $\|fg^{-1}\| = \|fg^{-1}\|_\infty \leqslant 1$. But all the terms with $i = 2$ or $j = 2$ tend to 0:

$$\begin{aligned}\left\|\sqrt{|V_{\mu_i}|}\frac{1}{D_0+is}\sqrt{|V_{\mu_j}|}\right\| &= \left\|\sqrt{|V_{\mu_i}|}\frac{1}{|p|^{1/2}}\frac{|p|}{D_0+is}\frac{1}{|p|^{1/2}}\sqrt{|V_{\mu_j}|}\right\| \\ &\overset{2.1}{\leqslant} \frac{\pi}{2}\sqrt{|\mu_i|(\mathbb{R}^3)|\mu_j|(\mathbb{R}^3)}\left\|\frac{|p|}{D_0+is}\right\| \overset{K,N\to\infty}{\longrightarrow} 0,\end{aligned}$$

because $\frac{|p|}{|D_0+is|} = \frac{|p|}{\sqrt{(D_0-is)(D_0+is)}} = \frac{|p|}{\sqrt{|p|^2+1+s^2}}\mathbb{1}_4$ implies that

$$\left\|\frac{|p|}{D_0+is}\right\| = \sup_{p\in\mathbb{R}^3}\frac{|p|}{\sqrt{|p|^2+1+s^2}} = 1 \tag{2.3}$$

by Theorem A.4 in Appendix A. Therefore, we can assume this property of μ for the rest of the proof, and we have

$$|V_\mu(x)| = \left|\int \frac{d\mu(y)}{|x-y|}\right| \leqslant \frac{|\mu|(\mathbb{R}^3)}{||x|-N|},$$

whenever $\mathrm{supp}(\mu) \subset B_N$. Let now $R > N$ and $\eta < \min_{1\leqslant m\neq l\leqslant K}\frac{|R_m-R_l|}{2}$. We write

$$V_\mu = \sum_{m=1}^{K}\frac{\nu_m \mathbb{1}_{B_\eta(R_m)}}{|x-R_m|} + \mathbb{1}_{B_R}V_{\mu'} + \sum_{m=1}^{K}\frac{\nu_m \mathbb{1}_{B_\eta(R_m)^c}}{|x-R_m|} + \mathbb{1}_{B_R^c}V_{\mu'}$$

$$\Rightarrow \sqrt{|V_\mu|} \leqslant \sum_{m=1}^{K} \frac{\sqrt{\nu_m}\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}} + \mathbb{1}_{B_R}\sqrt{V_{|\mu'|}} + \sqrt{\sum_{m=1}^{K}\frac{\nu_m}{\eta}} + \sqrt{\frac{|\mu'|(\mathbb{R}^3)}{R-N}},$$

where we used the two facts that $|x-R_m| \geqslant \eta$ in $B^c_\eta(R_m)$ and that $\left|\int \frac{d\mu'(y)}{|x-y|}\right| \leqslant \left|\int_{B_N} \frac{d\mu'(y)}{||x|-|y||}\right| \leqslant \frac{|\mu'|(\mathbb{R}^3)}{R-N}$ in B^c_R.

Then we can replace it in $\left\|\sqrt{|V_\mu|}\frac{1}{D_0+is}\sqrt{|V_\mu|}\right\|$ and obtain the following terms:

- $\displaystyle\sum_{m=1}^{K} |\nu_m| \frac{\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}} \frac{1}{D_0+is} \frac{\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}} =: \sum_{m=1}^{K} |\nu_m| \mathbb{1}_{\Omega_m} A_m \mathbb{1}_{\Omega_m}$

  For Coulomb potential we have (see [ADV13, Kat83, Kla81, Nen76, Wüs77]):

$$\begin{aligned}
&\sigma\left(\frac{1}{|x|^{1/2}}\frac{1}{\alpha\cdot p+\beta}\frac{1}{|x|^{1/2}}\right) = \sigma_{\text{ess}}\left(\frac{1}{|x|^{1/2}}\frac{1}{\alpha\cdot p+\beta}\frac{1}{|x|^{1/2}}\right) \\
&= \sigma\left(\frac{1}{|x|^{1/2}}\frac{1}{\alpha\cdot p}\frac{1}{|x|^{1/2}}\right) = \sigma_{\text{ess}}\left(\frac{1}{|x|^{1/2}}\frac{1}{\alpha\cdot p}\frac{1}{|x|^{1/2}}\right) = [-1,1],
\end{aligned} \tag{2.4}$$

  and

$$\left\|\frac{1}{|x|^{1/2}}\frac{1}{\alpha\cdot p+is}\frac{1}{|x|^{1/2}}\right\| = \left\|\frac{1}{|x|^{1/2}}\frac{1}{\alpha\cdot p+\beta+is}\frac{1}{|x|^{1/2}}\right\| = 1. \tag{2.5}$$

  Since $\frac{1}{D_0+is}$ commutes with translations we also have $\|A_m\| = 1$. This is useful to have a bound on the norm of the operator:

$$\begin{aligned}
&\left\|\sum_{m=1}^{K}|\nu_m|\mathbb{1}_{\Omega_m}A_m\mathbb{1}_{\Omega_m}\varphi\right\|_2^2 = \int |\sum_{m=1}^{K}|\nu_m|\mathbb{1}_{\Omega_m}A_m\mathbb{1}_{\Omega_m}\varphi|^2 \\
&= \int\sum_{m=1}^{K}|\nu_m|^2\,|\mathbb{1}_{\Omega_m}A_m\mathbb{1}_{\Omega_m}\varphi|^2 \leqslant (\max_m|\nu_m|)^2\sum_{m=1}^{K}\int|\mathbb{1}_{\Omega_m}A_m\mathbb{1}_{\Omega_m}\varphi|^2 \\
&\leqslant (\max_m|\nu_m|)^2\sum_{m=1}^{K}\|A_m\mathbb{1}_{\Omega_m}\varphi\|_2^2 \overset{\|A_m\|=1}{\leqslant} (\max_m|\nu_m|)^2\sum_{m=1}^{K}\|\mathbb{1}_{\Omega_m}\varphi\|_2^2 \\
&= (\max_m|\nu_m|)^2\int\sum_{m=1}^{K}\mathbb{1}_{\Omega_m}|\varphi|^2 = (\max_m|\nu_m|)^2\int|\sum_{m=1}^{K}\mathbb{1}_{\Omega_m}\varphi|^2 \\
&= (\max_m|\nu_m|)^2\left\|\sum_{m=1}^{K}\mathbb{1}_{\Omega_m}\varphi\right\|_2^2 \leqslant (\max_m|\nu_m|)^2\left\|\sum_{m=1}^{K}\mathbb{1}_{\Omega_m}\right\|^2\|\varphi\|_2^2, \\
&\Rightarrow \left\|\sum_{m=1}^{K}|\nu_m|\mathbb{1}_{\Omega_m}A_m\mathbb{1}_{\Omega_m}\right\| \leqslant (\max_m|\nu_m|)\left\|\sum_{m=1}^{K}\mathbb{1}_{\Omega_m}\right\| = \max_m|\nu_m| < 1.
\end{aligned}$$

Note that the estimate does not depend on K but requires η to be small enough to guarantee that the balls do not overlap. The choice of η depends on the smallest distance between the nuclei. All the other terms are small for s large enough.

- $$\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}}\frac{1}{D_0+is}\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}} = \underbrace{\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}}\frac{1}{|p|^{1/2}}}_{B}\underbrace{\frac{|p|}{D_0+is}}_{A_s}\underbrace{\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}}}_{K}$$

  is of the form BA_sK, where B is bounded by Kato's inequality (2.1), K is compact by Lemma 2.2 and $A_s \underset{s\to\infty}{\to} 0$ strongly. Indeed $\int |\frac{|p|}{\alpha\cdot p+\beta+is}\widehat{\varphi}|^2 = \int |\frac{|p|}{\sqrt{|p|^2+1+s^2}}\widehat{\varphi}|^2 \to 0$ by dominated convergence, with $\|A_s\| \leqslant C$ uniformly in s (see 2.3). Then, by Theorem A.5, one has $\|BA_sK\| \to 0$.

- $$\left(\sqrt{\sum_{m=1}^{K}\frac{\nu_m}{\eta}}+\sqrt{\frac{|\mu'|(\mathbb{R}^3)}{R-N}}\right)\frac{1}{D_0+is}\left(\sqrt{\sum_{m=1}^{K}\frac{\nu_m}{\eta}}+\sqrt{\frac{|\mu'|(\mathbb{R}^3)}{R-N}}\right)$$
  $$=: C^2\frac{1}{D_0+is}$$

  and $\|\frac{1}{D_0+is}\| \overset{A.4}{=} \|\frac{1}{|D_0+is|}\| = \sup_{p\in\mathbb{R}^3}\frac{1}{\sqrt{|p|^2+1+s^2}} \leqslant \frac{1}{|s|} \underset{s\to\infty}{\to} 0.$

- $$\left(\sum_{m=1}^{K}\frac{\sqrt{\nu_m}\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}}\right)\frac{1}{D_0+is}\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}} =$$
  $$=\underbrace{\left(\sum_{m=1}^{K}\frac{\sqrt{\nu_m}\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}}\right)\frac{1}{|p|^{1/2}}}_{B}\underbrace{\frac{|p|}{D_0+is}}_{A_s}\underbrace{\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}}}_{K}$$

  is again of the form BA_sK. Note that $B = \sum_{m=1}^{K}\sqrt{V_{|\nu_m|\delta_{R_m}}}\mathbb{1}_{B_\eta(R_m)}\frac{1}{|p|^{1/2}}$ is a finite sum of bounded operators by Kato's inequality.

- $$\underbrace{\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}}}_{A}\underbrace{\frac{1}{D_0+is}}_{B}\underbrace{\left(\sum_{m=1}^{K}\frac{\sqrt{\nu_m}\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}}\right)}_{C}$$

Since $\|ABC\| = \|C^*B^*A^*\|$ we can look instead at

$$\begin{aligned}&\left(\sum_{m=1}^{K} \frac{\sqrt{\nu_m}\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}}\right) \frac{1}{D_0 - is}\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}} \\ &= \underbrace{\left(\sum_{m=1}^{K} \frac{\sqrt{\nu_m}\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}}\right) \frac{1}{|p|^{1/2}}}_{B} \underbrace{\frac{|p|}{D_0 - is}}_{A_s} \underbrace{\frac{1}{|p|^{1/2}}\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}}}_{K},\end{aligned}$$

which is again of the form BA_sK and hence, its norm tends to 0.

- $$\begin{aligned}&\left(\sum_{m=1}^{K} \frac{\sqrt{\nu_m}\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}}\right) \frac{1}{D_0 + is}\left(\sqrt{\sum_{m=1}^{K}\frac{\nu_m}{\eta}} + \sqrt{\frac{|\mu'|(\mathbb{R}^3)}{R-N}}\right), \\ &\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}}\frac{1}{D_0 + is}\left(\sqrt{\sum_{m=1}^{K}\frac{\nu_m}{\eta}} + \sqrt{\frac{|\mu'|(\mathbb{R}^3)}{R-N}}\right), \\ &\left(\sqrt{\sum_{m=1}^{K}\frac{\nu_m}{\eta}} + \sqrt{\frac{|\mu'|(\mathbb{R}^3)}{R-N}}\right)\frac{1}{D_0 + is}\left(\sum_{m=1}^{K} \frac{\sqrt{\nu_m}\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}}\right), \\ &\left(\sqrt{\sum_{m=1}^{K}\frac{\nu_m}{\eta}} + \sqrt{\frac{|\mu'|(\mathbb{R}^3)}{R-N}}\right)\frac{1}{D_0 + is}\mathbb{1}_{B_R}\sqrt{V_{|\mu'|}}\end{aligned}$$

  can all be seen, multiplying and dividing by $|p|^{1/2}$, as a composition of a bounded operator (by Kato's inequality) and $\frac{|p|^{1/2}}{D_0+is}$, whose norm tends to 0: $\|A_s\| \overset{A.4}{=} \|\frac{|p|^{1/2}}{|D_0+is|}\| = \sup_{p\in\mathbb{R}^3} \frac{|p|^{1/2}}{\sqrt{|p|^2+1+s^2}} \leqslant \frac{1}{\sqrt{2|s|}} \to 0.$

- We are left with

  $$\frac{\mathbb{1}_{B_\eta(R_k)}}{|x-R_k|^{1/2}}\frac{1}{D_0+is}\frac{\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}} \quad \text{with } k \neq m.$$

  We can write

  $$\frac{1}{D_0+is} = \frac{\alpha\cdot p}{|p|^2+1+s^2} + \frac{\beta}{|p|^2+1+s^2} - i\frac{s}{|p|^2+1+s^2}.$$

  So we get three terms:

*

$$\frac{\mathbb{1}_{B_\eta(R_k)}}{|x-R_k|^{1/2}}\frac{\beta}{|p|^2+1+s^2}\frac{\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}} =$$

$$= \underbrace{\sqrt{V_{\delta_{R_k}}}\mathbb{1}_{B_\eta(R_k)}\frac{1}{|p|^{1/2}}}_{B_1}\underbrace{\frac{\beta|p|}{|p|^2+1+s^2}}_{A_s}\underbrace{\frac{1}{|p|^{1/2}}\sqrt{V_{\delta_{R_m}}}\mathbb{1}_{B_\eta(R_m)}}_{B_2}$$

where B_1, B_2 are bounded by Kato's inequality and

$$\|A_s\| = \sup_{p\in\mathbb{R}^3}\frac{|p|}{|p|^2+1+s^2} \leqslant \frac{1}{2|s|} \underset{s\to\infty}{\longrightarrow} 0;$$

*

$$\frac{\mathbb{1}_{B_\eta(R_k)}}{|x-R_k|^{1/2}}\frac{\alpha\cdot p}{|p|^2+1+s^2}\frac{\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}} =: A_s,$$

The kernel of the operator $\frac{\alpha\cdot p}{|p|^2+1+s^2}$ is the function

$$a(x,y) = i\frac{\alpha\cdot(x-y)}{4\pi|x-y|^3}e^{-\sqrt{1+s^2}|x-y|} + i\sqrt{1+s^2}\frac{\alpha\cdot(x-y)}{4\pi|x-y|^2}e^{-\sqrt{1+s^2}|x-y|},$$

since

$$\mathcal{F}(\frac{\alpha\cdot p}{|p|^2+1+s^2})(x) = i\frac{\alpha\cdot(x)}{4\pi|x|^3}e^{-\sqrt{1+s^2}|x|} + i\sqrt{1+s^2}\frac{\alpha\cdot(x)}{4\pi|x|^2}e^{-\sqrt{1+s^2}|x|}.$$

Therefore, $a(x,y)$ can be bounded by

$$\begin{aligned}|a(x,y)| &\leqslant \frac{e^{-\sqrt{1+s^2}|x-y|}}{4\pi|x-y|^2} + \sqrt{1+s^2}\frac{e^{-\sqrt{1+s^2}|x-y|}}{4\pi|x-y|} \\ &\leqslant \frac{1}{4\pi\sqrt{|1+s|^{1/2}|x-y|^5}} + \frac{\sqrt{1+s^2}}{4\pi\sqrt{|1+s^2|^{3/2}|x-y|^5}} \\ &\leqslant \frac{C}{|s|^{1/2}|x-y|^{5/2}}.\end{aligned}$$

The kernel of A_s is then bounded by

$$\begin{aligned}|A_s(x,y)| &= \left|\frac{\mathbb{1}_{B_\eta(R_k)}(x)}{|x-R_k|^{1/2}}a(x,y)\frac{\mathbb{1}_{B_\eta(R_m)}(y)}{|y-R_m|^{1/2}}\right| \\ &\leqslant \frac{C}{|s|^{1/2}}\left|\frac{\mathbb{1}_{B_\eta(R_k)}(x)}{|x-R_k|^{1/2}}\frac{1}{|x-y|^{5/2}}\frac{\mathbb{1}_{B_\eta(R_m)}(y)}{|y-R_m|^{1/2}}\right| = \frac{C}{|s|^{1/2}}B(x,y),\end{aligned}$$

where $B(x,y)$ is the kernel of the operator $B = \frac{\mathbb{1}_{B_\eta(R_k)}}{|x-R_k|^{1/2}}\frac{1}{|p|^{1/2}}\frac{\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}}$ since $\mathcal{F}(\frac{1}{|p|^{1/2}})(x) = c\frac{1}{|x|^{5/2}}$. Recalling now that $|A(x,y)| \leqslant B(x,y)$ implies $\|A\| \leqslant \|B\|$, we obtain $\|A_s\| \leqslant \frac{C}{|s|^{1/2}}\|\frac{\mathbb{1}_{B_\eta(R_k)}}{|x-R_k|^{1/2}}\frac{1}{|p|^{1/2}}\frac{\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}}\|$. The norm on the right-hand side is finite by Lemma 2.1 whose hypotheses are clearly satisfied: the supports are disjoint and $\int \frac{\mathbb{1}_{B_\eta(R_k)}}{|x-R_k|(1+|x|^2)^5} < \infty$). Hence the norm of A_s tends to 0 as s goes to infinity.

*
$$\frac{\mathbb{1}_{B_\eta(R_k)}}{|x-R_k|^{1/2}} \frac{-is}{|p|^2+i+s^2} \frac{\mathbb{1}_{B_\eta(R_m)}}{|x-R_m|^{1/2}} =: B_s$$

is completely similar to the previous case since the kernel of $\frac{-is}{|p|^2+i+s^2}$ is bounded by

$$|b(x,y)| = \frac{|s|e^{-\sqrt{i+s^2}|x-y|}}{4\pi|x-y|} \leqslant \frac{|s|}{4\pi\sqrt{|1+s^2|^{3/2}|x-y|^{5/2}}} \leqslant \frac{C}{|s|^{1/2}|x-y|^{5/2}}.$$

This concludes the proof of (2.2), i.e. $\limsup_{|s|\to\infty} \left\| \sqrt{|V_\mu|}\frac{1}{D_0+is}\sqrt{|V_\mu|} \right\| < 1$. This allows us to use Nenciu's method ([Nen76], Corollary 2.1), which is based on the resolvent expansion [Nen76, KW79, Kla81]

$$(D_0+V-z)^{-1} = (D_0-z)^{-1} - (D_0-z)^{-1}\sqrt{|V|}(1+SK_z)^{-1}S\sqrt{|V|}(D_0-z)^{-1}, \quad (2.6)$$

where $K_z = \sqrt{|V|}(D_0-z)^{-1}\sqrt{|V|}$ and $S = \operatorname{sgn}(V)$. In the notation of Corollary 2.1 in [Nen76], we have $A = D_0$, $V_1 = -V_\mu$ and $V_2 = 0$. All the hypothesis are satisfied:

1. $|D_0| \geqslant 1 > 0$;

2. $-V_\mu$ is D_0 form bounded:

$$\int |V_\mu\varphi|^2 \overset{\text{Kato}}{\leqslant} C\int |p||\widehat{\varphi}|^2 \leqslant C\int \sqrt{1+|p|^2}|\widehat{\varphi}|^2 = \||D_0|\varphi\|_2^2.$$

   Moreover, we have just proved that there exists $is \in \sigma(D_0)$ such that

$$\left\| S\left(\sqrt{|V_\mu|}\frac{1}{D_0+is}\sqrt{|V_\mu|}\right)\right\| \leqslant \left\|\sqrt{|V_\mu|}\frac{1}{D_0+is}\sqrt{|V_\mu|}\right\| < 1,$$

   which implies that $\mathbb{1} + S(\sqrt{|V_\mu|}\frac{1}{D_0+is}\sqrt{|V_\mu|})$ is invertible;

3. $V_2|D_0|^{1/2}$ is obviously compact since $V_2 = 0$;

4. $\underbrace{\sqrt{|V_\mu|}\frac{1}{D_0+is}}_{A}\underbrace{\frac{1}{D_0-z}\sqrt{|V_\mu|}}_{B}$ is compact for $z \notin \sigma(D_0)$ since A bounded, as already seen, and B is compact. Let us prove this latter claim. Firstly,

$(D_0 - z)^{-1}$ is continuous from L^2 to H^1. Indeed, for every $z \notin \sigma(D_0)$ there exists C_z s.t. $\|\frac{1}{\alpha\cdot p+\beta-z}\| \leqslant \frac{C_z}{\sqrt{|p|^2+1}}$ (seen as a 4×4 matrix for fixed p), which implies

$$\int_{\mathbb{R}^3}(|p|^2+1)\left|\frac{1}{\alpha\cdot p+\beta-z}\widehat{\varphi}\right|^3 dp \leqslant C_z^2\int_{\mathbb{R}^3}|\widehat{\varphi}|^2 dp.$$

Going back to the initial space, this means that $\|(D_0-z)^{-1}\varphi\|_{H^1} \leqslant C_z\|\varphi\|_2$, as wanted. Then, it remains to prove that the multiplication operator $\sqrt{|V_\mu|}$ is compact from H^1 to L^2. By Sobolev's embedding, for every $\varepsilon > 0$, H^1 is compactly embedded in $L^{6-\varepsilon}_{\rm loc}$. For $R > 0$ fixed, let us split this operator into $\sqrt{|V_\mu|}\mathbb{1}_{|x|\leqslant R}$ and $\sqrt{|V_\mu|}\mathbb{1}_{|x|>R}$. The operator $\sqrt{|V_\mu|}\mathbb{1}_{|x|\leqslant R}$ is continuous from $L^{6-\varepsilon}_{\rm loc}$ to L^2 by Hölder inequality with $p = 6-\varepsilon$ and $q = 3+\varepsilon'$ where $\varepsilon' = \frac{2(6-\varepsilon)}{4-\varepsilon} - 3$, so that $\frac{1}{2} = \frac{1}{p}+\frac{1}{q}$ ($V_\mu\mathbb{1}_{|x|\leqslant R}$ is in $L^{6+\varepsilon'}$ for every $\varepsilon' > 0$). Then we have that $\sqrt{|V_\mu|}\mathbb{1}_{|x|\leqslant R}$ is compact from H^1 to L^2 and $\sqrt{|V_\mu|}\mathbb{1}_{|x|>R}$ can be taken small (in norm) as desired taking R large enough, so that $\sqrt{|V_\mu|}$ is compact as the norm-limit of compact operators. This ends the proof of the fact that

$$\frac{1}{D_0-z}\sqrt{|V_\mu|} \quad \text{is compact.} \tag{2.7}$$

Finally, the corollary implies that $D_0 - V_\mu$ has a unique self-adjoint extension whose domain is included in $\mathcal{D}(|D_0|^{1/2}) = H^{1/2}(\mathbb{R}^3)$. Once we have this, two consequences of the resolvent formula (2.6) and the compactness of B (2.7) are that the essential spectrum of the extension is still $\sigma_{\rm ess}(D_0) = (-\infty,-1]\cap[1,\infty)$ and $D_0 - V_\mu\mathbb{1}_{\{|V_\mu|\leqslant n\}} \underset{n\to\infty}{\longrightarrow} D_0 - V_\mu$ in the norm resolvent sense ([KW79], Theorem 1 and 2).

It remains to prove the statement about the gradient of functions in the domain. Let us denote by $R_1,\dots,R_K$ all the points such that $|\mu|(R_k) \geqslant \frac{1}{2}$. Let us fix $x' \in \mathbb{R}^3 \smallsetminus \{R_1,\dots,R_K\}$, then we have

$$\lim_{r\to 0}|\mu|(B_r(x')) < \frac{1}{2}.$$

Let $\chi \in C_c^\infty$ with support in $B_{1/2}(0)$ and let $\chi_r(x) = \chi((x-x')/r)$. Every $\Psi \in \mathcal{D}(D_0 - V_\mu)$ satisfies

$$(D_0 - V_\mu)\Psi = \Phi \in L^2(\mathbb{R}^3)$$

in $H^{-1/2}$, so that

$$D_0(\chi_r\Psi) - V_\mu\chi_r\Psi = \chi_r\Phi - i(\alpha\cdot\nabla\chi_r)\Psi \in L^2(\mathbb{R}^3).$$

We decompose $\mu = \mu\mathbb{1}_{B_r(x')} + \mu\mathbb{1}_{B_r(x')^c}$ and use that

$$\left|V_{\mu\mathbb{1}_{B_r(x')^c}}\right| = \left|\int_{B_r(x')^c}\frac{d\mu(y)}{|x-y|}\right| \overset{|x-y|\geqslant r-\frac{r}{2}}{\leqslant} \frac{2}{r}|\mu|(\mathbb{R}^3) \text{ on } B_{r/2}(x') \supset \operatorname{supp}(\chi_r\Psi).$$

This gives $V_{\mu \mathbb{1}_{B_r(x')^c}} \chi_r \Psi \in L^2$ and, hence, also $(D_0 - V_{\mu \mathbb{1}_{B_r(x')}})\chi_r\Psi = (D_0 - V_\mu)\chi_r\Psi + V_{\mu \mathbb{1}_{B_r(x')^c}}\chi_r\Psi \in L^2(\mathbb{R}^3)$. By Hardy's inequality, we have $(\varphi, \frac{\varphi}{|x|^2}) \leqslant 4(\nabla\varphi, \nabla\varphi) = 4(\varphi, -\Delta\varphi)$, i.e. $|x|^{-2} \leqslant 4(-\Delta)$, and, since $D_0^2 = -\Delta + 1 \geqslant -\Delta$ we have $|x|^{-2} \leqslant 4(D_0)^2$. By Theorem A.3, this gives

$$\|V_{\mu \mathbb{1}_{B_r(x')}}\varphi\|_2 \leqslant \underbrace{2|\mu|(B_r(x'))}_{a} \|D_0\varphi\|_2. \tag{2.8}$$

By the Rellich-Kato theorem, since for r small enough $a < 1$, $D_0 - V_{\mu \mathbb{1}_{B_r(x')}}$ is self-adjoint in H^1 and also invertible. Thus, $\chi_r\Psi \in H^1(\mathbb{R}^3)$. Taking now $\chi_R \in C_c^\infty$ such that $\chi_R = 1$ on $B_{R/2}$ and null outside B_R, we have that $V_{\mu \mathbb{1}_{B_{R/4}}}$ is bounded on $B_{R/2}^c \supset \operatorname{supp}((1-\chi_R)\Psi)$ in the same way as before. So $V_{\mu \mathbb{1}_{B_{R/4}}}(1-\chi_R)\Psi \in L^2$, which also implies $(D_0 - V_{\mu \mathbb{1}_{B_{R/4}^c}})(1-\chi_R)\Psi \in L^2$. Using that $|\mu|(B_{R/4}^c) \to 0$ when $R \to \infty$ leads again to $D_0 - V_{\mu \mathbb{1}_{B_{R/4}^c}}$ self-adjoint on H^1. Hence $(1-\chi_R)\Psi \in H^1$.

We obtain the claim by covering $\mathbb{R}^3 \setminus \cup_{j=1}^K B_r(R_j)$ with finitely many balls together with the complement of a large ball. □

2.2 Description of the domain for a positive measure

One can describe the distinguished self-adjoint extension more precisely in the case of a positive measure $\mu \geqslant 0$. Let us introduce a new space for the first two components $\varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2)$, called upper spinor, of a four-components column vector in $L^2(\mathbb{R}^3, \mathbb{C}^4)$. We define the following norm

$$\|\varphi\|_{\mathcal{V}_\mu} := \left(\int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla\varphi(x)|^2}{1 + V_\mu(x)} dx + \int_{\mathbb{R}^3} |\varphi(x)|^2 dx \right)^{1/2},$$

which is well-defined on $H^1(\mathbb{R}^3, \mathbb{C}^2)$ and which is controlled by the H^1-norm since $(1 + V_\mu)^{-1} \leqslant 1$ since $V_\mu \geqslant 0$. We need to know whether the completion $\mathcal{V}_\mu$ of $H^1(\mathbb{R}^3, \mathbb{C}^2)$ for this new norm is the same as the largest space given by the conditions

$$\varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2), \quad \frac{\sigma \cdot \nabla\varphi}{(1 + V_\mu)^{1/2}} \in L^2(\mathbb{R}^3, \mathbb{C}^2).$$

The following theorem answers this question affirmatively.

Theorem 2.2 (The upper-spinor space $\mathcal{V}_\mu$)**.** *Let $\mu \geqslant 0$ be any finite Borel measure on $\mathbb{R}^3$ such that*

$$\mu(\{R\}) < 1 \ \forall R \in \mathbb{R}^3.$$

We have

$$\frac{\|\varphi\|^2_{H^{1/2}(\mathbb{R}^3,\mathbb{C}^2)}}{\max(2,16\mu(\mathbb{R}^3))} \leqslant \|\varphi\|_{\mathcal{V}_\mu} \leqslant \|\varphi\|_{H^1(\mathbb{R}^3,\mathbb{C}^2)} \quad \forall \varphi \in H^1(\mathbb{R}^3,\mathbb{C}^2). \tag{2.9}$$

The completion of $H^1(\mathbb{R}^3,\mathbb{C}^2)$ for the norm $\|\cdot\|_{\mathcal{V}_\mu}$ is a subspace of $H^{1/2}(\mathbb{R}^3,\mathbb{C}^2)$ satisfying the continuous embeddings in (2.9). It coincides with the completion of $C_c^\infty(\mathbb{R}^3,\mathbb{C}^2)$ for the same norm and is given by

$$\mathcal{V}_\mu = \left\{\varphi \in L^2(\mathbb{R}^3,\mathbb{C}^2) : \exists g \in L^2(\mathbb{R}^3,\mathbb{C}^2), \sigma\cdot\nabla\varphi = (1+V_\mu)^{1/2} g\right\}, \tag{2.10}$$

where $\sigma\cdot\nabla\varphi$ is understood in the sense of distributions.

Proof. **Step 1 - Proof of (2.9)**
The second inequality follows from $(1+V_\mu)^{-1} \leqslant 1$. Let us prove the first one. By Theorem A.3 we have

$$\left\|V_\mu \frac{1}{D_0}\right\| \leqslant 2\mu(\mathbb{R}^3).$$

We also have $\||p|(\beta+1)\frac{1}{D_0}\| \leqslant \|\beta+1\|\|\frac{|p|}{D_0}\| = \sup_{p\in\mathbb{R}^3} \frac{2|p|}{\sqrt{1+|p|^2}} \leqslant \sqrt{2}$. By the Rellich–Kato theorem, the operator $D_0 - \frac{V_\mu}{8\mu(\mathbb{R}^3)} - |p|\frac{\beta+\mathbb{1}}{4} =: D_0 - V$ is self-adjoint on H^1. Indeed,

$$\begin{aligned}
&\left\|\left(\frac{V_\mu}{8\mu(\mathbb{R}^3)} + |p|\frac{\beta+\mathbb{1}}{4}\right)\varphi\right\| = \left\|V\frac{1}{D_0}D_0\varphi\right\| \\
&\leqslant \frac{1}{4}\|D_0\varphi\| + \frac{\sqrt{2}}{4}\|D_0\varphi\| = \underbrace{\left(\frac{1}{4}+\frac{\sqrt{2}}{4}\right)}_{a}\|D_0\varphi\|, \quad \text{with } a<1.
\end{aligned}$$

Moreover, 0 is not in the spectrum, and there is a universal estimate on the gap (see [Lew22], Theorem 4.5): since $0 \in \rho(D_0)\cap\mathbb{R}$ and $\|VD_0^{-1}\| < 1$, one has $]-\eta,\eta[\subset \rho(D_0 - V)$ for $\eta = d(0,\sigma(D_0)(1-\|VD_0^{-1}\|)) \geqslant 1-a$.

For the same reason, $\forall t \in [0,1]$, $D_0 - t\frac{V_\mu}{8\mu(\mathbb{R}^3)} - |p|\frac{\beta+\mathbb{1}}{4}$ has a gap around the origin at least as big as when $t=1$ since $a_t = \frac{t}{4} + \frac{\sqrt{2}}{4} \leqslant a$.

Note that $|p|\frac{\beta+\mathbb{1}}{4}$ acts only on the upper spinor. Restricted to the lower spinor, the quadratic form associated with this operator is just $-1 - t\frac{V_\mu}{8\mu(\mathbb{R}^3)} \leqslant -1$.

From the min-max principle and a continuation argument in t (see [DES00], Lemma 2.1 and Section 3), the fact that 0 is never in the spectrum is equivalent to say that, $\forall\varphi \in H^1(\mathbb{R}^3,\mathbb{C}^2)$,

$$\int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\varphi(x)|^2}{1+\frac{V_\mu(x)}{8\mu(\mathbb{R})}}dx \geqslant \frac{1}{8\mu(\mathbb{R})}\int_{\mathbb{R}^3} V_\mu(x)|\varphi(x)|^2 dx + \frac{1}{2}(\varphi,|p|\varphi) - \frac{1}{2}\|\varphi\|_2^2.$$

Since $\frac{1}{1+a} \geqslant \frac{1}{\max(1,b)(1+\frac{a}{b})}$ for every b, we get with $a = V_\mu, b = 8\mu(\mathbb{R}^3)$

$$\int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla\varphi(x)|^2}{1+V_\mu(x)} dx \geqslant \frac{(\varphi, |p|\varphi) - \|\varphi\|^2_{L^2(\mathbb{R}^3)}}{2\max\left(1, 8\mu\left(\mathbb{R}^3\right)\right)}, \quad \forall \varphi \in H^1(\mathbb{R}^3, \mathbb{C}^2).$$

Denoting $M = 2\max(1, 8\mu\left(\mathbb{R}^3\right)) \geqslant 2$ we have

$$M \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla\varphi(x)|^2}{1+V_\mu(x)} dx \geqslant (\varphi, |p|\varphi) - \|\varphi\|^2_{L^2(\mathbb{R}^3)} \geqslant (\varphi, |p|\varphi) - (M-1)\|\varphi\|^2_{L^2(\mathbb{R}^3)}$$

so that

$$\|\varphi\|^2_{\mathcal{V}_\mu} = \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla\varphi(x)|^2}{1+V_\mu(x)} dx + \|\varphi\|^2_{L^2} \geqslant \frac{(\varphi, |p|\varphi) + \|\varphi\|^2_{L^2}}{M} \geqslant c\|\varphi\|^2_{H^{1/2}}.$$

The operator $-\sigma\cdot\nabla\frac{1}{1+V_\mu}\sigma\cdot\nabla+1$, which is the one associated to the quadratic form $\|\cdot\|^2_{\mathcal{V}_\mu}$, is well-defined and symmetric in the domain $C_c^\infty\left(\mathbb{R}^3, \mathbb{C}^2\right)$, by Lemma 2.3 below. Then, by ([RS75], Theorem X.23), the quadratic form defined in $C_c^\infty\left(\mathbb{R}^3, \mathbb{C}^2\right)$ is closable in $L^2(\mathbb{R}^3, \mathbb{C}^2)$. Finally, the domain of the closure is automatically a subspace of $H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$ by the last inequality above.

Step 2 - $\mathcal{V}_\mu$ coincides with the maximal space

We want to prove (2.10), i.e. that $\mathcal{V}_\mu$ coincides with the maximal space in which one can give a meaning to the associated norm $\|\cdot\|_{\mathcal{V}_\mu}$. Firstly, let us prove the following lemma.

Lemma 2.3 (Regularity of $(1+V_\mu)^\alpha$)**.** *Let μ be a non-negative Radon measure over $\mathbb{R}^3$. Then $\nabla\left(1+V_\mu\right)^\alpha \in L^2\left(\mathbb{R}^3\right)$ for all $\alpha < 1/2$ and we have*

$$\int_{\mathbb{R}^3} \left|\nabla\left(1+V_\mu\right)^\alpha\right|^2 \leqslant C_\alpha \mu\left(\mathbb{R}^3\right),$$

for a constant C_α depending only on α. When $\alpha = 0$ we have the same estimate with $(1+V_\mu)^\alpha$ replaced by $\log\left(1+V_\mu\right)$.

Proof. Let us assume that $\mu \in C_c^\infty(\mathbb{R}^3)$. Let $\Omega_0 := \{V_\mu < 1\}$ and $\Omega_i := \{2^{i-1} \leqslant V_\mu < 2^i\}$ for $i \geqslant 1$. Then we have

$$\begin{aligned}\int_{\mathbb{R}^3} \left|\nabla\left(1+V_\mu\right)^\alpha\right|^2 &= \alpha^2 \int_{\mathbb{R}^3} \frac{\left|\nabla V_\mu\right|^2}{\left(1+V_\mu\right)^{2-2\alpha}} = \alpha^2 \sum_{i=0}^\infty \int_{\Omega_i} \frac{\left|\nabla V_\mu\right|^2}{\left(1+V_\mu\right)^{2-2\alpha}} \\ &\leqslant \alpha^2 \int_{\Omega_0} \left|\nabla V_\mu\right|^2 + \alpha^2 \sum_{i=1}^\infty \frac{1}{\left(1+2^{i-1}\right)^{2-2\alpha}} \int_{\Omega_i} \left|\nabla V_\mu\right|^2,\end{aligned}$$

where we used that $V\mu \geqslant 0$ and $V\mu \geqslant 2^{i-1}$ on Ω_i. Now, defining

$$v_i := \begin{cases} \mathbb{1}_{\{V_\mu \geqslant 1\}} + V_\mu \mathbb{1}_{\{V_\mu < 1\}} & \text{for } i = 0 \\ 2^{i-1}\mathbb{1}_{\{V_\mu \leqslant 2^{i-1}\}} + 2^i \mathbb{1}_{\{V_\mu \geqslant 2^i\}} + V_\mu \mathbb{1}_{\{2^{i-1} < V_\mu < 2^i\}} & \text{for } i \geqslant 1 \end{cases},$$

and since $-\Delta V\mu = 4\pi\mu$, we have $\forall i \geqslant 0$

$$\int_{\Omega_i} |\nabla V_\mu|^2 \overset{(v_i = V_\mu \text{ on } \Omega_i)}{=} \int_{\mathbb{R}^3} \nabla V_\mu \cdot \nabla v_i = 4\pi \int_{\mathbb{R}^3} v_i \, \mathrm{d}\mu \overset{v_i \leqslant 2^i}{\leqslant} 4\pi 2^i \mu\left(\mathbb{R}^3\right)$$

$$\Rightarrow \int_{\mathbb{R}^3} |\nabla (1 + V_\mu)^\alpha|^2 \leqslant 4\pi\alpha^2 \left(1 + \sum_{i=1}^{\infty} \frac{2^i}{\left(1 + 2^{i-1}\right)^{2-2\alpha}}\right) \mu\left(\mathbb{R}^3\right),$$

where the series is finite for $\alpha < \frac{1}{2}$.

Let us now go back to a general measure and use an approximation argument. We can assume μ to be a finite measure : Otherwise the inequality is trivial (see Appendix A.1 for an introduction to finite measures and the definition of tight convergence). Using convolution by a sequence of smooth functions in L^1 which tends to δ_0 tightly, one can construct a sequence $(\mu_n)_{n\in\mathbb{N}} \in C^\infty \cap L^1$ s.t. $\mu_n \rightharpoonup \mu$ tightly as well. By a density argument, for every n fixed, there exists also a sequence $(\mu_{n_k})_{k\in\mathbb{N}} \subset C_c^\infty$ s.t. $\|\mu_{n_k} - \mu\|_1 \to 0$ and in particular $\mu_{n_k} \rightharpoonup \mu_n$ tightly. Then, by a diagonal argument, one can find a sequence of C_c^∞ functions which converges tightly to our initial μ. We will prove in Lemma 3.5 that this implies that $V_{\mu_n} \to V_\mu$ in L^p_{loc} for every $1 \leqslant p \leqslant 2$. Then $(1 + V_{\mu_n})^\alpha \to (1 + V_\mu)^\alpha$ in $L^{p/\alpha}_{\mathrm{loc}}$ with $p/\alpha > 2p \geqslant 2$, thus in L^2_{loc}. By the C_c^∞ case, we have $\int_{\mathbb{R}^3} |\nabla (1 + V_{\mu_n})^\alpha|^2 \leqslant C\mu_n(\mathbb{R}^3) \leqslant C$ (where we used that $\mu_n(\mathbb{R}^3)$ are uniformly bounded by the tight convergence). Hence the sequence $\nabla (1 + V_{\mu_n})^\alpha$ is bounded in L^2 and therefore, up to subsequences, it converges weakly in L^2 to a function $\Psi \in L^2$. Let us prove that $\Psi = \nabla (1 + V_\mu)^\alpha$. Let $h \in C_c^\infty$, then

$$\left(\nabla (1 + V_{\mu_n})^\alpha, h\right) = \left((1 + V_{\mu_n})^\alpha, \nabla h\right) \to \left((1 + V_\mu)^\alpha, \nabla h\right).$$

Since the left-hand side converges also to (Ψ, h), we have that $\Psi = \nabla (1 + V_\mu)^\alpha$ in the distributions sense. By the lower semi-continuity of the L^2 norm we have finally

$$\int_{\mathbb{R}^3} |\nabla (1 + V_\mu)^\alpha|^2 \leqslant \liminf \int_{\mathbb{R}^3} |\nabla (1 + V_{\mu_n})^\alpha|^2 \leqslant C_\alpha \liminf \mu_n(\mathbb{R}^3) = C_\alpha \mu(\mathbb{R}^3).$$

When $\alpha = 0$, the ragument is exactly the same with $(1 + V_\mu)^\alpha$ replaced by $\log(1 + V_\mu)$. □

The above lemma says that for $\varphi \in L^2(\mathbb{R}^3)$, $(1+V_\mu)^{-1/2}\sigma\cdot\nabla\varphi$ makes sense as a distribution. It is equivalent to wonder whether there exists $g \in L^2(\mathbb{R}^3)$ such that $\sigma\cdot\nabla\varphi = (1+V_\mu)^{1/2}g$. We now prove that for every φ such that $g := (1+V_\mu)^{-1/2}\sigma\cdot\nabla\varphi \in L^2(\mathbb{R}^3,\mathbb{C}^2)$, there exists a sequence $(\varphi_n)_{n\in\mathbb{N}} \subset C_c^\infty$ which converges $\varphi_n \to \varphi$ in $\mathcal{V}_\mu$, i.e. $\varphi_n \to \varphi$ and $(1+V_\mu)^{-1/2}\sigma\cdot\nabla\varphi_n \to (1+V_\mu)^{-1/2}\sigma\cdot\nabla\varphi$ both in L^2.

Let us define $\varphi_n(x) := \varphi(x)\chi(\frac{x}{n})$ where $\chi \in C_c^\infty$ and $\chi(0) = 1$. By dominated convergence, $\varphi_n \to \varphi$ in L^2. In addition, we have, in the sense of distributions,

$$\begin{aligned}\sigma\cdot\nabla\varphi_n &= \chi(\cdot/n)\sigma\cdot\nabla\varphi + \varphi\frac{(\sigma\cdot\nabla\chi)(\cdot/n)}{n}\\ &= (1+V_\mu)^{\frac12}\left(\chi(\cdot/n)g + \varphi\frac{(\sigma\cdot\nabla\chi)(\cdot/n)}{n\,(1+V_\mu)^{\frac12}}\right),\end{aligned}$$

where the function in the parentheses has compact support and converges to g in $L^2(\mathbb{R}^3)$. Indeed $\chi(\cdot/n)g \xrightarrow{L^2} g$ and $\|\varphi\frac{(\sigma\cdot\nabla\chi)(\cdot/n)}{n(1+V_\mu)^{\frac12}}\|_2 \leqslant \frac{\|\nabla\chi\|_\infty}{n}\|\varphi\|_2 \to 0$. So, $\varphi_n \to \varphi$ in $\mathcal{V}_\mu$. Hence functions with compact support are dense. Therefore, in the following we can assume that both φ and g have compact support.

Next, we approximate φ by a sequence in H^1. Let $u \in \dot{H}^1(\mathbb{R}^3)$ such that $\varphi = \sigma\cdot\nabla u$. We then have in the sense of distributions $(1+V_\mu)^{\frac12}\,g = \sigma\cdot\nabla\varphi = \Delta u$. We have then

$$u = -\frac{1}{4\pi}\left((1+V_\mu)^{\frac12}\,g\right) * \frac{1}{|x|},\quad \varphi = \frac{1}{4\pi}\left((1+V_\mu)^{\frac12}\,g\right) * \sigma\cdot\frac{x}{|x|^3}.$$

Let us now define

$$u_\varepsilon = -\frac{1}{4\pi}\left((1+V_\mu)^{\frac12}\,\mathbb{1}_{\{V_\mu\leqslant\varepsilon^{-1}\}}g\right) * \frac{1}{|x|},\quad \varphi_\varepsilon = \sigma\cdot\nabla u_\varepsilon,$$

which satisfies

$$\sigma\cdot\nabla\varphi_\varepsilon = \Delta u_\varepsilon = (1+V_\mu)^{\frac12}\,g_\varepsilon,\quad \varphi_\varepsilon = \frac{1}{4\pi}\left((1+V_\mu)^{\frac12}\,g_\varepsilon\right) * \sigma\cdot\frac{x}{|x|^3},$$

where $g_\varepsilon = g\mathbb{1}_{\{V_\mu\leqslant\varepsilon^{-1}\}}$. Since $|\,(1+V_\mu)^{\frac12}\,\mathbb{1}_{\{V_\mu\leqslant\varepsilon^{-1}\}}g| \leqslant (1+\varepsilon^{-1})^{1/2}|g|$ and $g \in L^2$, we have $(1+V_\mu)^{\frac12}\,g_\varepsilon \in L^2(\mathbb{R}^3)$. Moreover, since g has compact support, we also have $(1+V_\mu)^{\frac12}\,\mathbb{1}_{\{V_\mu\leqslant\varepsilon^{-1}\}}g \in L^{6/5}(\mathbb{R}^3)$. Now, by the Hardy-Littlewood-Sobolev inequality

$$\|\varphi_\varepsilon\|_2 = \left\|\frac{1}{4\pi}\left((1+V_\mu)^{\frac12}\,g_\varepsilon\right) * \sigma\cdot\frac{x}{|x|^3}\right\|_2 \leqslant C\left\|\left((1+V_\mu)^{\frac12}\,g_\varepsilon\right)\right\|_{6/5} < \infty.$$

Namely, $\varphi_\varepsilon \in L^2(\mathbb{R}^3)$. We also have $\sigma \cdot \nabla\varphi_\varepsilon = (1+V_\mu)^{\frac{1}{2}} g_\varepsilon \in L^2(\mathbb{R}^3)$. Hence $\nabla\varphi_\varepsilon \in L^2(\mathbb{R}^3)$, which implies $\varphi_\varepsilon \in H^1(\mathbb{R}^3)$. From the dominated convergence theorem, $g_\varepsilon \xrightarrow{L^2} g$, and we now want to show that $\varphi_\varepsilon \xrightarrow{L^2} \varphi$ as well. Again by the Hardy-Littlewood-Sobolev inequality, we have

$$\begin{aligned}\int_{\mathbb{R}^3} |\varphi - \varphi_\varepsilon|^2 &\leqslant C \left\| (1+V_\mu)^{\frac{1}{2}} \mathbb{1}_{\{V_\mu \geqslant \varepsilon^{-1}\}} g \right\|_{6/5}^2 \\ &\leqslant C \|g\|_{L^2(B)}^2 \left(\int_B (1+V_\mu)^{\frac{3}{2}} \mathbb{1}_{\{V_\mu \geqslant \varepsilon^{-1}\}} \right)^{\frac{2}{3}}\end{aligned}$$

where $\mathrm{supp}(g) \subset B$. The right-hand side tends to zero when $\varepsilon \to 0$ by the monotone convergence theorem, and this shows that $\varphi_\varepsilon \to \varphi$ for the norm $\|\cdot\|_{\mathcal{V}_\mu}$. The density of C_c^∞ is then proved using the fact that $\|\cdot\|_{\mathcal{V}_\mu}$ is dominated by the H^1 norm. For $\varphi \in L^2$ there exists $(\varphi_n)_{n\in\mathbb{N}} \subset H^1$ s.t. $\varphi_n \to \varphi$ in $\mathcal{V}_\mu$, but for every n there exists $(\varphi_{n_k})_{k\in\mathbb{N}} \subset C_c^\infty$ s.t. $\varphi_{n_k} \to \varphi_k$ in H^1, and hence also in $\mathcal{V}_\mu$. Then by a diagonal argument one finds the desired sequence in C_c^∞ which converges to φ in $\mathcal{V}_\mu$.

□

Using the space $\mathcal{V}_\mu$, we can now describe the domain of the distinguished self-adjoint extension.

Theorem 2.3 (Domain of the distinguished self-adjoint extension for $\mu \geqslant 0$)**.** *Let $\mu \geqslant 0$ be any finite Radon measure on $\mathbb{R}^3$ such that*

$$\mu(\{R\}) < 1 \ \forall R \in \mathbb{R}^3.$$

Then the domain of the self-adjoint extension defined in Theorem 2.1 is explicitly given by

$$\mathcal{D}(D_0 - V_\mu) = \left\{ \Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^2) : \varphi \in \mathcal{V}_\mu, (D_0 - V_\mu)\Psi \in L^2(\mathbb{R}^3, \mathbb{C}^4) \right\} \tag{2.11}$$

where, in the last condition, $D_0\Psi$ and $V_\mu\Psi$ are understood in the sense of distributions. Moreover, this extension is the unique one that is included in $\mathcal{V}_\mu \times L^2(\mathbb{R}^3, \mathbb{C}^2)$. We have

$$\mathcal{D}(D_0 - V_\mu) \subset \mathcal{V}_\mu \times \mathcal{V}_\mu \subset H^{1/2}(\mathbb{R}^3, \mathbb{C}^4).$$

In addition, the Birman-Schwinger principle holds: $\lambda \in (-1, 1)$ is an eigenvalue of $D_0 - V_\mu$ if and only if 1 is an eigenvalue of the bounded self-adjoint operator

$$K_\lambda = \sqrt{V_\mu} \frac{1}{D_0 - \lambda} \sqrt{V_\mu}.$$

Proof. Let us consider the quadratic form

$$q_\lambda(\varphi) := \int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\varphi|^2}{1+\lambda+V_\mu}dx + \int_{\mathbb{R}^3}(1-\lambda-V_\mu)\,|\varphi|^2\,dx$$

defined on $H^1(\mathbb{R}^3)$. We show that it is coercive for the norm of $\mathcal{V}_\mu$, after adding $C\|\varphi\|^2_{L^2(\mathbb{R}^3)}$ for an appropriate constant C. Our proof will be based on Theorem 2.1, where we have shown that for s large enough

$$\left\|\sqrt{V_\mu}\frac{1}{D_0+is}\sqrt{V_\mu}\right\| < 1.$$

Step 1 - Equivalence of quadratic forms

Let us start with the following lemma.

Lemma 2.4 (Relating resolvent)**.** *For every $0\leqslant\varepsilon\leqslant 1$ and $C\geqslant 0$, we have the operator bound*

$$\frac{1}{D_0+\frac{C-\varepsilon|p|}{2}(\beta+1)} \leqslant \frac{1}{2}\left(\frac{1}{\alpha\cdot p+\beta+i\sqrt{C}}+\frac{1}{\alpha\cdot p+\beta-i\sqrt{C}}\right)+\frac{8\varepsilon(1+C)}{|p|}.$$

Proof. First, let us assume $\varepsilon=0$. We have

$$D_0+\frac{C}{2}(\beta+1)=\alpha\cdot p+\left(1+\frac{C}{2}\right)\beta+\frac{C}{2},$$

whose spectrum is given by the values of the functions

$$\pm\sqrt{|p|^2+\left(1+\frac{C}{2}\right)^2}+\frac{C}{2},$$

(as done in Section 1.2 for D_0). The upper function is clearly bounded from below by $1+C$, whereas the lower function is bounded above by -1 . So the gap is $(-1,1+C)$. This allows us to compute the resolvent, which we express in the form

$$\begin{aligned}\frac{1}{D_0+\frac{C}{2}(\beta+1)} &= \frac{1}{D_0+\frac{C}{2}(\beta+1)}\frac{D_0+\frac{C}{2}(\beta-1)}{D_0+\frac{C}{2}(\beta-1)} = \frac{\alpha\cdot p+\left(1+\frac{C}{2}\right)\beta-\frac{C}{2}}{|p|^2+\left(1+\frac{C}{2}\right)^2-\frac{C^2}{4}} \\ &= \frac{\alpha\cdot p}{|p|^2+1+C}+\frac{\beta}{|p|^2+1+C}+\frac{C}{2}\frac{\beta-1}{|p|^2+1+C}.\end{aligned} \tag{2.12}$$

Inserting

$$\frac{1}{2}\left(\frac{1}{\alpha\cdot p+\beta+i\sqrt{C}}+\frac{1}{\alpha\cdot p+\beta-i\sqrt{C}}\right)-\frac{\beta}{|p|^2+1+C}$$
$$=\frac{1}{2}\left(\frac{\alpha\cdot p+\beta-i\sqrt{C}}{|p|^2+1+C}+\frac{\alpha\cdot p+\beta+i\sqrt{C}}{|p|^2+1+C}\right)-\frac{\beta}{|p|^2+1+C}=\frac{\alpha\cdot p}{|p|^2+C+1},$$

we obtain the relation

$$\frac{1}{D_0+\frac{C}{2}(\beta+1)}=\frac{1}{2}\left(\frac{1}{\alpha\cdot p+\beta+i\sqrt{C}}+\frac{1}{\alpha\cdot p+\beta-i\sqrt{C}}\right)+\frac{C}{2}\frac{\beta-1}{|p|^2+1+C}.$$

Since $\beta\leqslant 1$, the last term is non-positive, hence we find the simple inequality

$$\frac{1}{D_0+\frac{C}{2}(\beta+1)}\leqslant\frac{1}{2}\left(\frac{1}{\alpha\cdot p+\beta+i\sqrt{C}}+\frac{1}{\alpha\cdot p+\beta-i\sqrt{C}}\right).$$

Let us now consider the case $0<\varepsilon\leqslant 1$. Note first that the spectrum of

$$D_0+\frac{C-\varepsilon|p|}{2}(\beta+1)=\alpha\cdot p+\left(1+\frac{C-\varepsilon|p|}{2}\right)\beta+\frac{C-\varepsilon|p|}{2}$$

is given by the values of the functions

$$\pm\sqrt{|p|^2+\left(1+\frac{C-\varepsilon|p|}{2}\right)^2}+\frac{C-\varepsilon|p|}{2}$$
$$=\pm\sqrt{|p|^2+1+C-\varepsilon|p|+\left(\frac{C-\varepsilon|p|}{2}\right)^2}+\frac{C-\varepsilon|p|}{2}.$$

Noticing that

$$|p|^2+1+C-\varepsilon|p|\geqslant|p|^2+1+C-|p|\geqslant\frac{|p|^2}{2}+\frac{1}{2}+C>0,$$

we see that the two eigenvalues do not approach the origin. Hence the operator is invertible. We can next estimate the difference by

$$\left\|\frac{1}{D_0+\frac{C-\varepsilon|p|}{2}(\beta+1)}-\frac{1}{D_0+\frac{C}{2}(\beta+1)}\right\|$$
$$=\frac{\varepsilon|p|}{2}\left\|\frac{1}{D_0+\frac{C-\varepsilon|p|}{2}(\beta+1)}(\beta+1)\frac{1}{D_0+\frac{C}{2}(\beta+1)}\right\|$$
$$\leqslant\varepsilon|p|\left\|\frac{1}{D_0+\frac{C-\varepsilon|p|}{2}(\beta+1)}\right\|\left\|\frac{1}{D_0+\frac{C}{2}(\beta+1)}\right\|.$$

Using (2.12) we have

$$\left\| \frac{1}{D_0 + \frac{C}{2}(\beta+1)} \right\| \leqslant \frac{|p|+1+C}{|p|^2+1+C} \leqslant \frac{1+\frac{\sqrt{1+C}}{2}}{|p|} \leqslant \frac{3\sqrt{1+C}}{2|p|}.$$

On the other hand, using again (2.12) with C replaced by $C - \varepsilon|p|$ we obtain

$$\begin{aligned} \left\| \frac{1}{D_0 + \frac{C-\varepsilon|p|}{2}(\beta+1)} \right\| &\leqslant \frac{|p|+1+C+\varepsilon|p|}{|p|^2+1+C-\varepsilon|p|} \\ &\leqslant \frac{2|p|+1+C}{\frac{|p|^2}{2}+\frac{1}{2}+C} \leqslant \frac{4+\sqrt{1+C}}{|p|} \leqslant \frac{5\sqrt{1+C}}{|p|}, \end{aligned}$$

so that

$$\left\| \frac{1}{D_0 + \frac{C-\varepsilon|p|}{2}(\beta+1)} - \frac{1}{D_0 + \frac{C}{2}(\beta+1)} \right\| \leqslant \frac{8\varepsilon(1+C)}{|p|}.$$

This gives also the same inequality without the operator norm:

$$\begin{aligned} &\left(\varphi, \frac{1}{D_0 + \frac{C-\varepsilon|p|}{2}(\beta+1)} - \frac{1}{D_0 + \frac{C}{2}(\beta+1)} \varphi \right) \\ &= \int \overline{\widehat{\varphi}} \cdot \left(\frac{1}{D_0 + \frac{C-\varepsilon|p|}{2}(\beta+1)} - \frac{1}{D_0 + \frac{C}{2}(\beta+1)} \right) \widehat{\varphi} \\ &\overset{C-S}{\leqslant} \int \left\| \frac{1}{D_0 + \frac{C-\varepsilon|p|}{2}(\beta+1)} - \frac{1}{D_0 + \frac{C}{2}(\beta+1)} \right\| |\widehat{\varphi}|^2 \\ &\leqslant \int \frac{8\varepsilon(1+C)}{|p|} |\widehat{\varphi}|^2 = \left(\varphi, \frac{8\varepsilon(1+C)}{|p|} \varphi \right). \end{aligned}$$

This, together with the case $\varepsilon = 0$, gives the claim. $\square$

Let us truncate V_μ into $W_n = V_\mu \mathbb{1}_{\{V_\mu \leqslant n\}}$ and notice that if two operators A and B are such that $A \leqslant B$ then $\max \sigma(\sqrt{W_n} A \sqrt{W_n}) \leqslant \|\sqrt{W_n} B \sqrt{W_n}\|$. Let us call them $A' := \sqrt{W_n} A \sqrt{W_n}$ and $B' := \sqrt{W_n} B \sqrt{W_n}$. It is easy to check that $A' \leqslant B'$. Moreover, by the Weyl's characterization of the spectrum, there exists a normalized sequence $(\varphi_n)_{n\in\mathbb{N}}$ s.t. $(A' - \max \sigma(\sqrt{W_n} A \sqrt{W_n}))\varphi_n$ tends to 0. Then

$$\begin{aligned} 0 &= \lim(\varphi_n, (A' - \max \sigma(\sqrt{W_n} A \sqrt{W_n}))\varphi_n) \\ &\leqslant \lim(\varphi_n, (B' - \max \sigma(\sqrt{W_n} A \sqrt{W_n}))\varphi_n) \\ &= \lim(\varphi_n, B'\varphi_n) - \max \sigma(\sqrt{W_n} A \sqrt{W_n}) \leqslant \|B'\| - \max \sigma(\sqrt{W_n} A \sqrt{W_n}). \end{aligned}$$

Using this fact, Lemma 2.4 and Lemma 2.1, we obtain

$$
\begin{aligned}
&\max \sigma\left(\sqrt{W_n}\frac{1}{D_0+\frac{C-\varepsilon|p|}{2}(\beta+1)}\sqrt{W_n}\right)\\
&\leqslant \left\|\sqrt{W_n}\left(\frac{1}{2}\left(\frac{1}{\alpha\cdot p+\beta+i\sqrt{C}}+\frac{1}{\alpha\cdot p+\beta-i\sqrt{C}}\right)+\frac{8\varepsilon(1+C)}{|p|}\right)\sqrt{W_n}\right\|\\
&\leqslant \left\|\sqrt{V_\mu}\left(\frac{1}{2}\left(\frac{1}{\alpha\cdot p+\beta+i\sqrt{C}}+\frac{1}{\alpha\cdot p+\beta-i\sqrt{C}}\right)+\frac{8\varepsilon(1+C)}{|p|}\right)\sqrt{V_\mu}\right\|\\
&\leqslant 4\pi\varepsilon(1+C)\mu\left(\mathbb{R}^3\right)\\
&\qquad+\frac{1}{2}\left(\left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\beta+i\sqrt{C}}\sqrt{V_\mu}\right\|+\left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\beta-i\sqrt{C}}\sqrt{V_\mu}\right\|\right).
\end{aligned}
$$

We have shown in the proof of Theorem 2.1 that the two operator norms are less than 1 for C large enough. Taking ε small enough we get

$$
\max \sigma\left(\sqrt{W_n}\frac{1}{D_0+\frac{C-\varepsilon|p|}{2}(\beta+1)}\sqrt{W_n}\right)<1. \tag{2.13}
$$

The previous condition implies that

$$
D_0-tW_n+\frac{C-\varepsilon|p|}{2}(\beta+1)
$$

has no eigenvalue in $(-1,0)$ for every $t\in[0,1]$. Indeed, if A is a self-adjoint operator, $\sigma(A)\subset[a,\infty)$ is equivalent to have that $(\varphi,A\varphi)\geqslant a\|\varphi\|^2 \quad \forall\varphi\in\mathcal{D}(A)$, which is true since

$$
\begin{aligned}
\left(\varphi,\sqrt{W_n}\left(-t+\frac{1}{\sqrt{W_n}}\left(D_0+\frac{C-\varepsilon|p|}{2}(\beta+1)\right)\frac{1}{\sqrt{W_n}}\right)\sqrt{W_n}\varphi\right)&\\
\geqslant -t\|\sqrt{W_n}\varphi\|^2+\|\sqrt{W_n}\varphi\|^2\geqslant 0.&
\end{aligned}
$$

Here we used that (2.13) implies that the minimum of the spectrum of the inverse operator is greater then 1. Again from the min-max principle and a continuation argument in t [DES00], this is equivalent to saying that

$$
q_{0,W_n}(\varphi)\geqslant -C\|\varphi\|_{L^2}^2+\varepsilon\left\||p|^{\frac{1}{2}}\varphi\right\|_{L^2}^2
$$

for all $\varphi\in H^1\left(\mathbb{R}^3,\mathbb{C}^2\right)$, where of course q_{0,W_n} denotes the quadratic form with V_μ replaced by W_n. Passing to the limit $n\to\infty$ we obtain also

$$
q_0(\varphi)\geqslant -C\|\varphi\|_{L^2}^2+\varepsilon\||p|^{\frac{1}{2}}\varphi\|_{L^2}^2. \tag{2.14}
$$

Now using Theorem A.2, for $0 < \eta < 1$ we write

$$\begin{aligned} q_0(\varphi) + C\|\varphi\|_{L^2}^2 &= \eta(q_0(\varphi) + C\|\varphi\|_{L^2}^2) + (1-\eta)(q_0(\varphi) + C\|\varphi\|_{L^2}^2) \\ &\geqslant \eta \int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\varphi|^2}{1+\mu * |x|^{-1}} dx - \eta \int_{\mathbb{R}^3} V_\mu |\varphi|^2 + (1-\eta)\varepsilon \left\| |p|^{\frac{1}{2}}\varphi \right\|^2 \\ &\geqslant \eta \int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\varphi|^2}{1+\mu * |x|^{-1}} dx + \left((1-\eta)\varepsilon - \frac{\pi}{2}\eta\mu\left(\mathbb{R}^3\right)\right) \left\| |p|^{\frac{1}{2}}\varphi \right\|^2 . \end{aligned}$$

After taking

$$\eta < \frac{\varepsilon}{\varepsilon + \frac{\pi}{2}\mu\left(\mathbb{R}^3\right)},$$

we see that the quadratic form $q_0 + C\|\cdot\|_{L^2}^2$ is equivalent to the square of the norm of the space $\mathcal{V}_\mu$. This quadratic form is thus closable on $H^1\left(\mathbb{R}^3, \mathbb{C}^2\right)$ and its closure is equivalent to the norm of $\mathcal{V}_\mu$.

Step 2 - Description of the domain via $\mathcal{V}_\mu$

Now, we can apply the results of ([SST20] Theorem 1.1, [EL07] Theorem 4,[EL08] Theorem 1) to the operator $D_0 + C(\beta+1)/2 - V_\mu$, and we obtain a unique self-adjoint extension, distinguished from the property that its domain is included in $\mathcal{V}_\mu \times L^2\left(\mathbb{R}^3, \mathbb{C}^2\right)$ and the domain is given by the functions that are sent by the operator in L^2 functions and whose upper spinor is in $\mathcal{V}_\mu$. Of course, the same holds for $D_0 - V_\mu$ since $C(\beta+1)/2$ is bounded:

$$\mathcal{D}(D_0 - V_\mu) = \left\{ \Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^2) : \varphi \in \mathcal{V}_\mu, (D_0 - V_\mu)\Psi \in L^2(\mathbb{R}^3, \mathbb{C}^2) \right\}.$$

Next, we prove that the domain is included in $\mathcal{V}_\mu \times \mathcal{V}_\mu$. Let $\Psi = (\varphi, \chi) \in \mathcal{V}_\mu \times L^2\left(\mathbb{R}^3, \mathbb{C}^2\right)$ be in the domain. Then we have

$$\begin{cases} \left(1 - V_\mu\right)\varphi + \sigma\cdot p\chi = f \in L^2\left(\mathbb{R}^3, \mathbb{C}^2\right) \\ -\left(1 + V_\mu\right)\chi + \sigma\cdot p\varphi = g \in L^2\left(\mathbb{R}^3, \mathbb{C}^2\right) \end{cases}$$

where the terms on the left side are interpreted as distributions. Since $\varphi \in \mathcal{V}_\mu \subset H^{1/2}\left(\mathbb{R}^3, \mathbb{C}^2\right)$, we have by Theorem A.2 $\|(1+V_\mu)^{1/2}\varphi\|_2^2 = \|\varphi\|_2^2 + \|\sqrt{V_\mu}\varphi\|_2^2 \leqslant \|\varphi\|_2^2 + C\||p|^{1/2}\varphi\|_2^2 \leqslant C\|\varphi\|_{H^{1/2}}^2$. Hence $\left(1+V_\mu\right)^{1/2}\varphi \in L^2\left(\mathbb{R}^3, \mathbb{C}^2\right)$.
But the first equation can then be written in the form

$$\sigma\cdot p\chi = f - 2\varphi + (V_\mu + 1)\varphi = \left(V_\mu + 1\right)^{\frac{1}{2}} \left(\left(V_\mu + 1\right)^{\frac{1}{2}}\varphi + \frac{f - 2\varphi}{\left(V_\mu + 1\right)^{\frac{1}{2}}} \right),$$

where the function in parenthesis belongs to $L^2\left(\mathbb{R}^3, \mathbb{C}^2\right)$. By the characterization (2.10) of $\mathcal{V}_\mu$, this gives immediately that $\chi \in \mathcal{V}_\mu$. Hence $\mathcal{D}\left(D_0 - V_\mu\right) \subset \mathcal{V}_\mu \times \mathcal{V}_\mu \subset$

$H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. By uniqueness in $H^{1/2}$ we conclude that this extension must be the same as the one from Theorem 2.1. The Birman-Schwinger principle was shown in [Kla81], and this ends the proof.

□

2.3 Min-max formulas for the eigenvalues

Related to the above characterization of the domain are the min-max formulas for the eigenvalues. The main result of this chapter is the following.

Theorem 2.4 (Min-max formulas)**.** *Let $\mu \geqslant 0$ be any finite non-trivial Radon measure on $\mathbb{R}^3$ such that*

$$\mu(\{R\}) < 1 \quad \forall R \in \mathbb{R}^3.$$

Define the min-max values

$$\lambda^{(k)} := \inf_{\substack{W \text{ subspace of } F^+ \\ \dim W = k}} \; \sup_{\Psi \in (W \oplus F^-) \setminus \{0\}} \frac{(\Psi, (D_0 - V_\mu)\Psi)}{\|\Psi\|^2}, \quad k \geqslant 1, \tag{2.15}$$

where F is any chosen vector space satisfying $C_c^\infty(\mathbb{R}^3, \mathbb{C}^4) \subseteq F \subseteq H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ and

$$F^+ := \left\{ \Psi = \begin{pmatrix} \varphi \\ 0 \end{pmatrix} \in F \right\}, \quad F^- := \left\{ \Psi = \begin{pmatrix} 0 \\ \chi \end{pmatrix} \in F \right\}.$$

Then, the following holds:

i) $\lambda^{(k)}$ is independent of the chosen space F;

ii) $\lambda^{(k)} \in [-1, 1)$ for all k;

iii) It is a non-decreasing sequence converging to 1: $\lim_{k\to\infty} \lambda^{(k)} = 1$.

Let k_0 be the first integer such that $\lambda^{(k_0)} > -1$, then $\left(\lambda^{(k)}\right)_{k \geqslant k_0}$ are all the eigenvalues of $D_0 - V_\mu$ in non-decreasing order, repeated according to their multiplicity, which are larger than -1 :

$$\sigma\left(D_0 - \mu * \frac{1}{|x|}\right) \cap (-1, 1) = \left\{\lambda^{(k_0)}, \lambda^{(k_0+1)}, \cdots\right\}.$$

By Theorem 1.1 in [DES00], the min-max formula is valid in the case of Coulomb singularities in the domain of the distinguished self-adjoint extension or in any core F on which the operator is essentially self-adjoint. Then it was proved in $H^{1/2}$ in [MM15, Mül16]. Finally in [ELS19] it was extended in any space between $C_c^\infty(\mathbb{R}^3, \mathbb{C}^4)$ and $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. Here we can follow the same approach. The min-max is valid in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ and the density of $C_c^\infty(\mathbb{R}^3, \mathbb{C}^4)$ in $\mathcal{V}_\mu$ allows to conclude that the formula must hold in all spaces in between, following the argument of [ELS19]. In particular, the numbers $\lambda_F^{(k)}$ are independent of the chosen space F. One notable difference is that in those works it is often assumed that $\lambda^{(1)} > -1$, but it was explained in [DES06] how to handle the case where we only have $\lambda^{(k_0)} > -1$ for some $k_0 \geqslant 1$.

Proof. We have to prove that $\lambda^{(k)} \nearrow 1$. Let us first show that for any positive integer k, $\lambda^{(k)} < 1$ if $\mu \neq 0$. For every k we choose a k-dimensional subspace of radial functions in $C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$, denoted by W_k. Let $U_R(f) = R^{-3/2} f(\cdot/R)$ be the unitary operator which dilates the function by a factor R. Let us introduce the space $W_{k,R} := U_R W_k$. Then, for every normalized function $\varphi_R = U_R\varphi \in W_{k,R}$, we have

$$q_\lambda(\varphi_R) = \frac{1}{R^2}\int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\varphi(x)|^2}{1+\lambda+V_\mu(Rx)}dx + \int_{\mathbb{R}^3}(1-\lambda-V_\mu(Rx))\,|\varphi(x)|^2 dx.$$

Decomposing $\mu = \mu\mathbb{1}_{B_\eta} + \mu\mathbb{1}_{B_\eta^c}$ with a large but fixed η, we have

$$\left|\int_{\mathbb{R}^3} V_{\mu\mathbb{1}_{B_\eta^c}}(Rx)|\varphi(x)|^2 dx\right| \leqslant \frac{\mu\left(\mathbb{R}^3\setminus B_\eta\right)\pi}{2R}\|\varphi\|^2_{H^{1/2}}.$$

This is proved exactly like in Theorem A.2 below using that $\mathcal{F}(f(ax))(\xi) = \frac{1}{|a|}\mathcal{F}(f)(\frac{p}{a})$. On the other hand

$$\begin{aligned}
&\left|\int_{\mathbb{R}^3} V_{\mu\mathbb{1}_{B_\eta}}(Rx)|\varphi(x)|^2dx - \frac{\mu(B_\eta)}{R}\int_{\mathbb{R}^3}\frac{|\varphi(x)|^2}{|x|}dx\right| \\
&= \left|\int_{\mathbb{R}^3}\int_{B_\eta}\left(\frac{1}{|Rx-y|}-\frac{1}{R|x|}\right)|\varphi(x)|^2 d\mu(y)dx\right| \\
&\leqslant \int_{\mathbb{R}^3}\int_{B_\eta}\frac{\eta}{R|x||Rx-y|}|\varphi(x)|^2 d\mu(y)dx \\
&\leqslant \frac{\eta}{2R^2}\int_{\mathbb{R}^3}\int_{B_\eta}\frac{|\varphi(x)|^2}{|x|^2}d\mu(y)dx + \frac{\eta}{2R^2}\int_{\mathbb{R}^3}\int_{B_\eta}\frac{|\varphi(x)|^2}{|x-y/R|^2}d\mu(y)dx \\
&\leqslant \frac{\eta\mu(B_\eta)}{R^2}\int|\nabla\varphi|^2 \leqslant \frac{C\eta}{R^2}\|\varphi\|^2_{H^1(\mathbb{R}^3)},
\end{aligned}$$

where in the penultimate inequality we used the Hardy inequality and the fact that it is translation-invariant. We get then

$$\begin{aligned}\int_{\mathbb{R}^3} V_\mu(Rx)|\varphi(x)|^2dx &= \int_{\mathbb{R}^3} V_{\mu\mathbb{1}_{B_\eta}}(Rx)|\varphi(x)|^2dx + \int_{\mathbb{R}^3} V_{\mu\mathbb{1}_{B_\eta^c}}(Rx)|\varphi(x)|^2dx \\ &\geqslant \frac{\mu(B_\eta)}{R}\int_{\mathbb{R}^3}\frac{|\varphi|^2}{|x|}dx - \frac{C\eta}{R^2}\|\varphi\|^2_{H^1} - \frac{\mu(\mathbb{R}^3\setminus B_\eta)\pi}{2R}\|\varphi\|^2_{H^{\frac12}} \\ &\geqslant \frac{\mu(B_\eta)}{RK}\|\varphi\|_2^2 - \frac{C\eta}{R^2}\|\varphi\|^2_{H^1} - \frac{\mu(\mathbb{R}^3\setminus B_\eta)\pi}{2R}\|\varphi\|^2_{H^{\frac12}} \\ &\geqslant \left(c\frac{\mu(B_\eta) - C\mu(\mathbb{R}^3\setminus B_\eta)}{R} - \frac{C\eta}{R^2}\right)\|\varphi\|^2_{L^2(\mathbb{R}^3)},\end{aligned}$$

for some $c > 0$ depending on W_k, since all the functions in $W_{k,R}$ have compact support in a common compact set and, in this finite-dimensional space, all the norms are equivalent. Choosing η large enough and $\lambda = 1 - \varepsilon/R$ with $\varepsilon > 0$ small enough, we deduce that $q_{1-\varepsilon/R}(\varphi_R) < 0$ on $W_{k,R}$ for R large enough. As in [DES00, SST20], the min-max formula (2.15) can be reformulated in terms of the quadratic form q_λ

$$\lambda^{(k)} = \inf\{\lambda : \exists W \subset \mathcal{V}_\mu, \dim(W) = k : q_\lambda(\varphi) \leqslant 0, \forall\varphi \in W\}.$$

Using this characterization, this proves that $\lambda^{(k)} \leqslant 1-\varepsilon/R$, as we wanted. Indeed,

$$\begin{aligned}q_{1-\varepsilon/R}(\varphi_R) &= \frac{1}{R^2}\int_{\mathbb{R}^3}\frac{|\sigma\cdot\nabla\varphi(x)|^2}{2-\varepsilon/R+V_\mu(Rx)}dx + \int_{\mathbb{R}^3}\left(\frac{\varepsilon}{R} - V_\mu(Rx)\right)|\varphi(x)|^2dx \\ &\leqslant \frac{1}{R}\left(\varepsilon - c(\mu(B_\eta) - C\mu(\mathbb{R}^3\setminus B_\eta)\right)\|\varphi\|_2^2 + o\left(\frac{1}{R}\right) < 0\end{aligned}$$

on $W_{k,R}$ for η and R large enough.

Let us prove now that $\lambda^{(k)} \to 1$ when $k \to \infty$. Note that $k \mapsto \lambda^{(k)}$ is non-decreasing and < 1 by the previous step. In addition, recall that

$$\sigma_{\text{ess}}(D_0 - V_\mu) = (-\infty, -1] \cup [1 \cup \infty).$$

From this, we conclude that if we have $\lambda^{(k_0)} > -1$ for some k_0, then $\lambda^{(k)}$ is an eigenvalue of $D_0 - V_\mu$ and it can only converge to 1 . By contradiction, Let us assume that $\lambda^{(k)} = -1$ for all $k \geqslant 1$. By the characterization of $\lambda^{(k)}$ there exists a sequence of spaces $W_k \subset \mathcal{V}_\mu$ of dimension $\dim(W_k) = k$ and $\varepsilon_k \to 0^+$ such that $q_{-1+\varepsilon_k}$ is negative on W_k. By monotonicity with respect to λ, we conclude that q_0 is also negative on W_k. This provides a sequence $\varphi_n \in \mathcal{V}_\mu$ such that $\|\varphi_n\|_{L^2} = 1, \varphi_n \to 0$ weakly and $q_0(\varphi_n) < 0$. Indeed

- $k = 1$, $\exists W_1 \subset \mathcal{V}_\mu$ with $\dim(W_1) = 1$ and $q_0 < 0$ on it. So take $\varphi_1 \in W_1$ s.t. $\|\varphi_1\|_2^2 = 1$ and $q_0(\varphi_1) < 0$;

- $k = 2$, $\exists W_2 \subset \mathcal{V}_\mu$ with $\dim(W_2) = 2$ and $q_0 < 0$ on it. So take $\varphi_2 \in W_2$ s.t. $\varphi_2 \perp \varphi_1$, $\|\varphi_2\|_2^2 = 1$ and $q_0(\varphi_1) < 0$;

$\vdots$

- $k = n$, $\exists W_n \subset \mathcal{V}_\mu$ with $\dim(W_n) = n$ and $q_0 < 0$ on it. So take $\varphi_n \in W_2$ s.t. $\varphi_n \perp \varphi_1, \dots, \varphi_{n-1}$, $\|\varphi_n\|_2^2 = 1$ and $q_0(\varphi_1) < 0$;

Since the sequence is orthonormal it converges weakly to 0. By Step 2 in the previous proof we know

$$q_0(\varphi_n) \geqslant \varepsilon \left\| |p|^{\frac{1}{2}} \varphi_n \right\|_2^2 - C_\lambda \|\varphi_n\|_2^2$$

and this proves that the sequence is bounded in $H^{1/2}(\mathbb{R}^3)$. This implies also the boundedness in $\mathcal{V}_\mu$:

$$0 > q_0(\varphi_n) = \|\varphi_n\|_{\mathcal{V}_\mu}^2 - \int V_\mu |\varphi_n|^2 \overset{A.2}{\geqslant} \|\varphi_n\|_{\mathcal{V}_\mu}^2 - \||p|^{1/2}\varphi_n\|_2^2 \geqslant \|\varphi_n\|_{\mathcal{V}_\mu}^2 - C.$$

Next, we pick a localization function $\chi_R(x) = \chi(x/R)$ where $\chi \in C_c^\infty(\mathbb{R}^3, [0,1])$, $\chi \equiv 1$ on B_1 and $\chi \equiv 0$ on $\mathbb{R}^3 \setminus B_2$ and let $\eta_R := \sqrt{1 - \chi_R^2}$. Let $\sum_k J_k^2 = 1$ be any real partition of unity, we use the pointwise IMS formula for the Pauli operator [BDE08] which states that:

$$\begin{aligned}
\sum_k |\sigma \cdot \nabla (J_k \varphi)|^2 =& \sum_k \sum_{i,j=1}^3 \left(\partial_i (J_k \varphi), \sigma_i \sigma_j \partial_j (J_k \varphi)\right)_{\mathbb{C}^2} \\
=& |\sigma \cdot \nabla \varphi|^2 + \sum_k \sum_{i,j=1}^3 (\varphi, \sigma_i \sigma \varphi)_{\mathbb{C}^2} \partial_i J_k \partial_j J_k \\
&+ 2\Re \sum_k \sum_{i,j=1}^3 (\partial_i \varphi, \sigma_i \sigma_j \varphi)_{\mathbb{C}^2} J_k \partial_j J_k \\
=& |\sigma \cdot \nabla \varphi|^2 + |\varphi|^2 \sum_k |\nabla J_k|^2 .
\end{aligned}$$

We have used that $\sigma_i \sigma_j + \sigma_j \sigma_i = 0$ for $i \neq j$ in the second term of the second equality and that $2\sum_k J_k \partial_j J_k = \partial_j \sum_k J_k^2 = 0$ for the last term. Since

$$|\sigma\cdot\nabla\varphi_n|^2 = (\chi_R^2+\eta_R^2)|\sigma\cdot\nabla\varphi_n|^2 = |\sigma\cdot\nabla\chi_R\varphi_n|^2+|\sigma\cdot\nabla\eta_R\varphi_n|^2-(|\nabla\chi_R|^2+|\nabla\eta_R|^2)|\varphi_n|^2,$$

we obtain

$$\begin{aligned}
q_0(\varphi_n) =& \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla (\chi_R \varphi_n)|^2}{1 + V_\mu} - \int_{\mathbb{R}^3} V_\mu \chi_R^2 |\varphi_n|^2 + 1 \\
&+ \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla (\eta_R \varphi_n)|^2}{1 + V_\mu} - \int_{\mathbb{R}^3} V_\mu \eta_R^2 |\varphi_n|^2 - \int_{\mathbb{R}^3} \frac{|\nabla \chi_R|^2 + |\nabla \eta_R|^2}{1 + V_\mu} |\varphi_n|^2 .
\end{aligned}$$

For the first two terms involving χ_R we use that q_0 is bounded from below by (2.14), which yields

$$\int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla (\chi_R \varphi_n)|^2}{1+V_\mu} - \int_{\mathbb{R}^3} V_\mu \chi_R^2 |\varphi_n|^2 \geqslant -C \int_{\mathbb{R}^3} \chi_R^2 |\varphi_n|^2 .$$

Using also that the fourth term is positive, $|\nabla \chi_R|^2 + |\nabla \eta_R|^2 = \frac{1}{R^2}(|\nabla \chi|^2 (\cdot/R) + |\nabla \eta|^2 (\cdot/R)) \leqslant \frac{C}{R^2}$ and φ_n are normalized, we obtain

$$q_0(\varphi_n) \geqslant 1 - C \int_{\mathbb{R}^3} \chi_R^2 |\varphi_n|^2 - \int_{\mathbb{R}^3} V_\mu \eta_R^2 |\varphi_n|^2 - \frac{C}{R^2}.$$

We will prove that the negative terms on the right-hand side are all small in the limit, which gives $q_0(\varphi_n) \geqslant 0$ and leads to a contradiction. Let us start with the second negative term. We decompose $\mu = \mu\chi_{R/4}^2 + \mu\eta_{R/4}^2$ and remark that $V_{\mu\chi_{R/4}^2}\eta_R^2 \leqslant C/R$ since the supports of $\mu\chi_{R/4}^2$ and η_R^2 are at least $R/2$ apart, whereas

$$\int_{\mathbb{R}^3} V_{\mu\eta_{R/4}^2} \eta_R^2 |\varphi_n|^2 \overset{A.2}{\leqslant} \frac{\pi}{2} \mu\left(\mathbb{R}^3 \setminus B_{R/2}\right) \|\eta_R \varphi_n\|_{H^{1/2}}^2 \leqslant C \mu\left(\mathbb{R}^3 \setminus B_{R/2}\right),$$

so that

$$\int_{\mathbb{R}^3} V_\mu \eta_R^2 |\varphi_n|^2 \leqslant C\left(\frac{1}{R} + \mu\left(\mathbb{R}^3 \setminus B_{R/2}\right)\right).$$

We may therefore choose R large enough such that

$$\int_{\mathbb{R}^3} V_\mu \eta_R^2 |\varphi_n|^2 + \frac{C}{R^2} \leqslant \frac{1}{2}.$$

However, due to the weak convergence $\varphi_n \rightharpoonup 0$ in $H^{1/2}$, we have for this fixed R

$$\lim_{n\to\infty} \int_{\mathbb{R}^3} \chi_R^2 |\varphi_n|^2 = 0.$$

This proves, as wanted, that $q_0(\varphi_n) \geqslant 0$ for n large.

□

Chapter 3

The smallest eigenvalue

In this chapter we will focus on the first eigenvalue of the operator $D_0 - V_\mu$. In particular, for $\nu < \nu_1$, where ν_1 is the critical mass that guarantees that $\lambda_1(D_0 - V_\mu)$ does not dive into the lower continuum spectrum for all $\mu(\mathbb{R}^3) < \nu_1$. We will study the minimization problem of the first eigenvalue over all the measures with mass at most ν. The final goal is to check that an optimal measure for that problem has to be concentrated on a compact set of Lebesgue measure zero. All the theorems and their proofs can be found in [ELS21b].

3.1 Two critical coupling constants ν_0 and ν_1

Let us consider any non-negative finite measure $\mu \neq 0$ and denote

$$\nu_{\max}(\mu) := \max_{R \in \mathbb{R}^3} \mu(\{R\}) \in [0, \infty)$$

the charge of its heaviest atom. As proved in the previous chapter, the operator

$$D_0 - t\mu * \frac{1}{|x|}$$

has a distinguished self-adjoint extension for all $0 \leqslant t < \nu_{\max}(\mu)^{-1}$, by Theorem 2.1, and the min-max formula and the Birman-Schwinger principle hold. Next, we consider the ray $(t\mu)_{t>0}$ and ask ourselves for which mass $t\mu(\mathbb{R}^3)$, the first eigenvalue crosses 0 or approaches the bottom -1 of the spectral gap. Therefore, we consider the first min-max level as in (2.15)

$$\lambda_1(D_0 - tV_\mu) := \inf_{\varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2) \setminus \{0\}} \sup_{\chi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)} \frac{\left(\begin{pmatrix} \varphi \\ \chi \end{pmatrix}, (D_0 - tV_\mu) \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \right)}{\|\varphi\|^2 + \|\chi\|^2},$$

for all $0 \leqslant t < \nu_{\max}(\mu)^{-1}$. According to Theorem 2.4, it is the first eigenvalue of $D_0 - tV_\mu$ as soon as it stays above -1, and $t \mapsto \lambda_1(D_0 - tV_\mu)$ is a non-increasing continuous function of t. In the limit $t \to 0$, we have

$$\lim_{t \to 0^+} \lambda_1(D_0 - tV_\mu) = \lambda_1(D_0) = 1;$$

that is, for small t the first eigenvalue emerges from $+1$. We distinguish two cases here: Either the eigenvalue decreases and approaches the bottom of the gap -1 at some critical $t < \nu_{\max}(\mu)^{-1}$, or it stays above it in the whole interval $(0, \nu_{\max}(\mu)^{-1})$. We denote

$$\nu_1(\mu) := \mu(\mathbb{R}^3) \sup\left\{t < \nu_{\max}(\mu)^{-1} : \lambda_1(D_0 - V_{t\mu}) > -1\right\}$$

the corresponding critical mass. Similarly, we may define

$$\nu_0(\mu) := \mu(\mathbb{R}^3) \sup\left\{t < \nu_{\max}(\mu)^{-1} : \lambda_1(D_0 - V_{t\mu}) > 0\right\}.$$

This is the unique value of $t\mu(\mathbb{R}^3)$ for which the first eigenvalue, whenever, it exists is equal to 0, otherwise it is taken equal to $\mu(\mathbb{R}^3)/\nu_{\max}(\mu)$. Clearly, by definition, $\nu_0(\mu) \leqslant \nu_1(\mu)$. By continuity and monotonicity, one also has $\lambda_1(D_0 - tV_\mu) > 0$ for all $0 \leqslant t\mu(\mathbb{R}^3) < \nu_0(\mu)$ and $\lambda_1(D_0 - tV_\mu) > -1$ for all $0 < t\mu(\mathbb{R}^3) < \nu_1(\mu)$. As an example, in the mere Coulomb case where $\mu = \delta_0$, we have

$$\nu_{\max}(\delta_0) = \nu_0(\delta_0) = \nu_1(\delta_0) = 1,$$

since the first eigenvalue reaches 0 but it never approaches -1 .

Note that the definitions are invariant if we multiply the measure μ by any positive number:

$$\nu_{\max}(t\mu) = t\nu_{\max}(\mu), \quad \nu_0(t\mu) = \nu_0(\mu), \quad \nu_1(t\mu) = \nu_1(\mu).$$

When discussing $\nu_0(\mu)$ and $\nu_1(\mu)$, it will often be convenient to take a probability measure for μ. However, while considering the first eigenvalue, the measure μ will be assumed to satisfy just the condition $\mu(\mathbb{R}^3) \leqslant \nu$.

In this section, we are interested in the following minimization problems:

$$\nu_0 := \inf_{\substack{\mu \geqslant 0 \\ \mu \neq 0}} \nu_0(\mu), \quad \nu_1 := \inf_{\substack{\mu \geqslant 0 \\ \mu \neq 0}} \nu_1(\mu) \tag{3.1}$$

which are respectively the smallest charge for which an eigenvalue can approach 0 or -1, for some probability measure μ. For $\nu < \nu_1$ we also study the minimization problem

$$\lambda_1(\nu) = \inf_{\substack{\mu \geqslant 0 \\ \mu(\mathbb{R}^3) \leqslant \nu}} \lambda_1\left(D_0 - \mu * \frac{1}{|x|}\right) \tag{3.2}$$

Since $\nu < \nu_1$, we know that the eigenvalue in the infimum is always greater than -1.

The first main result of this section is a characterization of the two numbers introduced in (3.1) with a help of a formula based on the Birman-Schwinger principle or on Hardy's inequalities. Since we study here ν_0 and ν_1, in the next theorem it is convenient to work with probability measures μ.

Theorem 3.1 (The critical coupling constants ν_0 and ν_1). *We have*

$$\frac{1}{\nu_0} = \sup_{\substack{\mu \geqslant 0 \\ \mu(\mathbb{R}^3)=1}} \left\| \sqrt{V_\mu} \frac{1}{\alpha \cdot p + \beta} \sqrt{V_\mu} \right\|_{L^2(\mathbb{R}^3,\mathbb{C}^4) \to L^2(\mathbb{R}^3,\mathbb{C}^4)}$$

and

$$\begin{aligned} \frac{1}{\nu_1} &= \sup_{\substack{\mu \geqslant 0 \\ \mu(\mathbb{R}^3)=1}} \left\| \sqrt{V_\mu} \frac{1}{\sigma \cdot p} \sqrt{V_\mu} \right\|_{L^2(\mathbb{R}^3,\mathbb{C}^2) \to L^2(\mathbb{R}^3,\mathbb{C}^2)} \\ &= \sup_{\substack{\mu \geqslant 0 \\ \mu(\mathbb{R}^3)=1}} \left\| \sqrt{V_\mu} \frac{1}{\alpha \cdot p} \sqrt{V_\mu} \right\|_{L^2(\mathbb{R}^3,\mathbb{C}^4) \to L^2(\mathbb{R}^3,\mathbb{C}^4)} \\ &= \sup_{\substack{\mu \geqslant 0 \\ \mu(\mathbb{R}^3)=1}} \max \sigma \left(\sqrt{V_\mu} \frac{1}{\alpha \cdot p + \beta + 1} \sqrt{V_\mu} \right). \end{aligned}$$

We first need preliminary lemmas. The first one is about the essential spectrum of K_λ.

Lemma 3.1 (Essential spectrum of K_λ). *Let μ be any probability measure and $\nu_{\max}(\mu) := \max_{R \in \mathbb{R}^3} \mu(\{R\}) \leqslant 1$. Then we have*

$$\sigma_{ess} \left(\sqrt{\mu * \frac{1}{|x|}} \frac{1}{\alpha \cdot p + \varepsilon\beta - \lambda} \sqrt{\mu * \frac{1}{|x|}} \right) = [-\nu_{\max}(\mu), \nu_{\max}(\mu)] \tag{3.3}$$

for all $\varepsilon > 0$ and $|\lambda| < \varepsilon$, as well as

$$\sigma_{ess} \left(\sqrt{\mu * \frac{1}{|x|}} \frac{1}{\alpha \cdot p} \sqrt{\mu * \frac{1}{|x|}} \right) = [-1, 1]. \tag{3.4}$$

Proof. Noticing that

$$\frac{1}{\alpha \cdot p + \varepsilon\beta - \lambda} = \frac{1}{\alpha \cdot p + \varepsilon\beta} + \frac{\lambda}{(\alpha \cdot p + \varepsilon\beta - \lambda)(\alpha \cdot p + \varepsilon\beta)},$$

we see that

$$\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\varepsilon\beta-\lambda}\sqrt{V_\mu}-\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\varepsilon\beta}\sqrt{V_\mu}$$
$$=\underbrace{\sqrt{V_\mu}\frac{1}{|p|^{1/2}}}_{\text{bounded}}\underbrace{\frac{\lambda|p|}{(\alpha\cdot p+\varepsilon\beta-\lambda)(\alpha\cdot p+\varepsilon\beta)}}_{\text{compact}}\underbrace{\frac{1}{|p|^{1/2}}\sqrt{V_\mu}}_{\text{bounded}}$$

is compact. The second operator is compact by the fact that

$$\left\|\frac{\lambda|p|}{(\alpha\cdot p+\varepsilon\beta-\lambda)(\alpha\cdot p+\varepsilon\beta)}\right\|^2 \leqslant \left(\frac{|p|+\varepsilon+\lambda}{|p|^2+\varepsilon^3-\lambda^2}\frac{\lambda|p|}{\sqrt{|p|^2+\varepsilon^2}}\right)^2$$
$$\leqslant \frac{C_{\lambda,\varepsilon}|p|^2}{(1+|p|^2)^2}\in L^2(\mathbb{R}^3)$$

for some constant $C_{\lambda,\varepsilon}$, following an argument similar to the proof of Lemma 2.1. This implies that the essential spectrum is invariant with respect to λ. Indeed if A is self-adjoint and B is compact, then B is A-compact and then, by Weyl's theorem, $\sigma_{\text{ess}}(A)=\sigma_{\text{ess}}(A+B)$. So we can assume $\lambda=0$ for the rest of the proof.

We write now

$$\mu=\sum_{m=1}^{M}\nu_m\delta_{R_m}+\widetilde{\mu},$$

where M can be infinite and $\widetilde{\mu}$ has no atom. Truncating both the sum and $\widetilde{\mu}$ in space, denoting by μ' the truncated measure and using Kato's inequality (A.1), as done in the proof of Theorem 2.1, we see that $\|\sqrt{V_{\mu'}}\frac{1}{\alpha\cdot p+\varepsilon\beta}\sqrt{V_{\mu'}}-\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\varepsilon\beta}\sqrt{V_\mu}\|$ tends to 0. Hence

$$\sigma_{\text{ess}}\left(\sqrt{V_{\mu'}}\frac{1}{\alpha\cdot p+\varepsilon\beta}\sqrt{V_{\mu'}}\right)\to\sigma_{\text{ess}}\left(\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\varepsilon\beta}\sqrt{V_\mu}\right),$$

since the distance of the spectrum of two operators is bounded by the norm of the difference of the operators. Therefore, it suffices to prove the lemma for a finite sum and for $\widetilde{\mu}$ with compact support, all included in a ball of radius N. To simplify the notation, we assume without loss of generality, that $\mu(\mathbb{R}^3)=1$. We have the pointwise estimate

$$\frac{1}{|x|+N}\leqslant V_\mu(x)\leqslant\frac{1}{|x|-N} \tag{3.5}$$

for $|x|>N$ which proves that $|x|V_\mu(x)\to 1$ at infinity.

If μ has no atom, namely $\nu_{\max}(\mu)=0$, and has compact support then by Lemma 2.2 (multiplying and dividing by $|p|^{1/2}$) the operators are compact, and therefore the essential spectrum is just $\{0\}$, proving (3.3) in this case. It is also well-known when μ is a delta measure (see (2.4)). Let us prove now that

$$[-\nu_{\max}(\mu), \nu_{\max}(\mu)] \subset \sigma_{\text{ess}}\left(\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\varepsilon\beta}\sqrt{V_\mu}\right) \tag{3.6}$$

in the case when μ has at least one atom. We assume, without loss of generality, that the delta measure of μ with the largest mass $\nu_{\max}(\mu)$ is located at 0. For $\eta > 0$ one can prove, after some computations (using a change of variable and dominated convergence) that

$$\left\|\left(\underbrace{\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\varepsilon\beta}\sqrt{V_\mu}}_{A_\varepsilon}-k\right)\eta^{3/2}\varphi(\eta\cdot)-\left(\underbrace{\sqrt{\frac{\nu_{\max}(\mu)}{|\cdot|}}\frac{1}{\alpha\cdot p}\sqrt{\frac{\nu_{\max}(\mu)}{|\cdot|}}}_{\nu_{\max}(\mu)A}-k\right)\varphi\right\|_2 \to 0$$

when $\eta \to \infty$, where k is a real number. By (2.4), for fixed $\lambda \in [-1, 1]$, there exists a Weyl's sequence φ_n for A. Then, rescaling it as above by n (with $k = \lambda\nu_{\max}(\mu)$) you find a new Weyl's sequence $n^{3/2}\varphi_n(n\cdot)$ for the operator A_ε related to the eignevalues $\lambda\nu_{\max}(\mu)$. Hence $[-\nu_{\max}(\mu), \nu_{\max}(\mu)]$ is included in the spectrum of A_ε and, being a closed interval, also in the essential spectrum.

Our main task will be to derive the reverse inclusion.

In the case $\varepsilon = 0$ we can also dilate functions. Let $\lambda \in [-1, 1]$, by (2.4) and a density argument, there exists a (normalized) Weyl sequence $\Psi_n \in C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$ such that $\left(\Psi_n, |x|^{-1/2}(\alpha\cdot p)^{-1}|x|^{-1/2}\Psi_n\right) \to \lambda$. By dilating Ψ_n and by using the scaling invariance of $|x|^{-1/2}(\alpha\cdot p)^{-1}|x|^{-1/2}$, we can assume that Ψ_n is supported outside a ball B_{r_n} with $r_n \to \infty$. Next, we write

$$\left(\Psi_n, \sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\Psi_n\right) = \left(|x|^{\frac12}\sqrt{V_\mu}\Psi_n, \left(\frac{1}{|x|^{\frac12}}\frac{1}{\alpha\cdot p}\frac{1}{|x|^{\frac12}}\right)|x|^{\frac12}\sqrt{V_\mu}\Psi_n\right)$$

and we use the fact that

$$\left\|\left(|x|^{\frac12}\sqrt{V_\mu}-1\right)\Psi_n\right\|_{L^2(\mathbb{R}^3,\mathbb{C}^4)} \leqslant \frac{C}{r_n}\underset{n\to\infty}{\longrightarrow} 0,$$

because $\left||x|^{1/2}\sqrt{V_\mu}-1\right| \leqslant C/\sqrt{r_n}$ on the support of Ψ_n, by (3.19). Since the operator $|x|^{-1/2}(\alpha\cdot p)^{-1}|x|^{-1/2}$ is bounded, we deduce that

$$\lim_{n\to\infty}\left(\Psi_n, \sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\Psi_n\right) = \lim_{n\to\infty}\left(\Psi_n, \frac{1}{|x|^{\frac12}}\frac{1}{\alpha\cdot p}\frac{1}{|x|^{\frac12}}\Psi_n\right) = \lambda.$$

Thus, we have constructed a Weyl sequence for the operator $\sqrt{V_\mu}(\alpha \cdot p)^{-1}\sqrt{V_\mu}$. We may conclude by varying λ that

$$[-1, 1] \subset \sigma_{\text{ess}}\left(\sqrt{V_\mu}\frac{1}{\alpha \cdot p}\sqrt{V_\mu}\right). \tag{3.7}$$

We now discuss the reverse inclusions. Similarly as in the proof of Theorem 2.1, we consider the following partition of unity

$$1 = \sum_{m=1}^{M} \mathbb{1}_{B_\eta(R_m)} + \mathbb{1}_{B_R \setminus \cup_{m=1}^M B_\eta(R_m)} + \mathbb{1}_{\mathbb{R}^3 \setminus B_R},$$

where R is chosen large enough and η is chosen small enough, so that the balls $B_\eta(R_m)$ do not intersect and are all included in $B_{R/2}$. We insert our partition of unity on both sides of our operator and expand. We claim that all the cross terms are compact, so that

$$\begin{aligned} A_\varepsilon &:= \sqrt{V_\mu}\frac{1}{\alpha \cdot p + \varepsilon\beta}\sqrt{V_\mu} \\ &= \sum_{m=1}^{M} \mathbb{1}_{B_\eta(R_m)} A_\varepsilon \mathbb{1}_{B_\eta(R_m)} + \mathbb{1}_{\mathbb{R}^3 \setminus B_R} A_\varepsilon \mathbb{1}_{\mathbb{R}^3 \setminus B_R} + \mathcal{K}, \end{aligned}$$

where $\mathcal{K}$ is compact. For instance, the compactness of

$$\mathbb{1}_{B_\eta(R_m)} A_\varepsilon \mathbb{1}_{B_\eta(R_\ell)}$$

with $\ell \neq m$ follows from the same proof as in Lemma 2.1. The functions $\mathbb{1}_{B_\eta(R_\ell)}\sqrt{V_\mu}$ are in L^2, and the kernel of the operator $(\alpha \cdot p + \varepsilon\beta)^{-1}$ is

$$(\alpha \cdot p + \varepsilon\beta)^{-1}(x, y) = (-i\alpha \cdot \nabla_x + \varepsilon\beta)\,\frac{e^{-\sqrt{\varepsilon}|x-y|}}{4\pi|x-y|}.$$

It is exponentially decaying at infinity for $\varepsilon > 0$ and equal to

$$(\alpha \cdot p)^{-1}(x, y) = i\frac{\alpha \cdot (x-y)}{4\pi|x-y|^3}$$

when $\varepsilon = 0$. Similarly,

$$\mathbb{1}_{\mathbb{R}^3 \setminus B_R} A_\varepsilon \mathbb{1}_{B_\eta(R_m)}, \quad \mathbb{1}_{B_\eta(R_m)} A_\varepsilon \mathbb{1}_{\mathbb{R}^3 \setminus B_R}$$

are compact because V_μ behaves like $1/|x|$ at infinity and

$$\int_{\mathbb{R}^3 \setminus B_R} \frac{\left|(\alpha \cdot p + \varepsilon\beta)^{-1}(x, 0)\right|^2}{|x|}dx < \infty.$$

Indeed, when $\varepsilon > 0$ the integrand is exponentially decaying whereas when $\varepsilon = 0$ it behaves like $|x|^{-5}$. Finally, all the terms involving $\mathbb{1}_{B_R \setminus \cup_{m=1}^M B_\eta(R_m)}$ are easier to treat since we can write:

$$V_\mu = \left(\frac{1}{|B_{\eta/2}|} \sum_{m=1}^M \nu_m \mathbb{1}_{B_{\eta/2}(R_m)} + \widetilde{\mu} \right) * \frac{1}{|x|} \qquad \text{on } \mathbb{R}^3 \setminus \cup_{m=1}^M B_\eta(R_m).$$

Then

$$\frac{1}{|p|^{\frac{1}{2}}} \sqrt{V_\mu} \mathbb{1}_{B_R \setminus \cup_{m=1}^M B_\eta(R_m)}$$

is compact by Lemma 2.2. By the same argument we can actually infer that

$$\mathbb{1}_{B_\eta(R_m)} A_\varepsilon \mathbb{1}_{B_\eta(R_m)} = \nu_m \frac{\mathbb{1}_{B_\eta(R_m)}}{|x - R_m|^{1/2}} \frac{1}{\alpha \cdot p + \varepsilon\beta} \frac{\mathbb{1}_{B_\eta(R_m)}}{|x - R_m|^{1/2}} + \mathcal{K},$$

where $\mathcal{K}$ is compact. Therefore, we have shown that

$$\begin{aligned} A_\varepsilon &= \sqrt{V_\mu} \frac{1}{\alpha \cdot p + \varepsilon\beta} \sqrt{V_\mu} \\ &= \sum_{m=1}^M \nu_m \frac{\mathbb{1}_{B_\eta(R_m)}}{|x - R_m|^{1/2}} \frac{1}{\alpha \cdot p + \varepsilon\beta} \frac{\mathbb{1}_{B_\eta(R_m)}}{|x - R_m|^{1/2}} \\ &+ \mathbb{1}_{\mathbb{R}^3 \setminus B_R} \sqrt{V_\mu} \frac{1}{\alpha \cdot p + \varepsilon\beta} \sqrt{V_\mu} \mathbb{1}_{\mathbb{R}^3 \setminus B_R} + \mathcal{K}_{R,\eta,\varepsilon}, \end{aligned}$$

where $\mathcal{K}_{R,\eta,\varepsilon}$ is compact. By (2.5), as already done in the proof of Theorem 2.1, we have the operator bound

$$\frac{\mathbb{1}_{B_\eta(R_m)}}{|x - R_m|^{\frac{1}{2}}} \frac{1}{\alpha \cdot p + \varepsilon\beta} \frac{\mathbb{1}_{B_\eta(R_m)}}{|x - R_m|^{\frac{1}{2}}} \leqslant \mathbb{1}_{B_\eta(R_m)}$$

and, therefore, we infer

$$\begin{aligned} A_\varepsilon &\leqslant \nu_{\max}(\mu) \mathbb{1}_{\cup_{m=1}^M B_\eta}(R_m) \\ &+ \mathbb{1}_{\mathbb{R}^3 \setminus B_R} \sqrt{V_\mu} \frac{1}{\alpha \cdot p + \varepsilon\beta} \sqrt{V_\mu} \mathbb{1}_{\mathbb{R}^3 \setminus B_R} + \mathcal{K}_{R,\eta,\varepsilon}. \end{aligned}$$

When $\varepsilon > 0$ the operator

$$\mathbb{1}_{\mathbb{R}^3 \setminus B_R} \sqrt{V_\mu} \frac{1}{\alpha \cdot p + \varepsilon\beta} \sqrt{V_\mu} \mathbb{1}_{\mathbb{R}^3 \setminus B_R}$$

is also compact, using (2.7) with $z = 0$, and the fact that $\mathbb{1}_{\mathbb{R}^3 \setminus B_R} \sqrt{V_\mu} \leqslant \sqrt{\frac{\mu(\mathbb{R}^3)}{R - N}}$ is bounded. Let $\Psi_n \rightharpoonup 0$ be a Weyl sequence such that $(A_\varepsilon - \lambda)\Psi_n \to 0$ with

$\lambda := \max \sigma_{\text{ess}}\,(A_\varepsilon)$. Then, we have

$$(\Psi_n, (A_\varepsilon - \lambda)\Psi_n) \leqslant \nu_{\max}(\mu) + (\Psi_n, \mathbb{1}_{\mathbb{R}^3\setminus B_R}\sqrt{V_\mu}\frac{1}{\alpha\cdot p + \varepsilon\beta}\sqrt{V_\mu}\mathbb{1}_{\mathbb{R}^3\setminus B_R}\Psi_n) \\ + (\Psi_n, \mathcal{K}_{R,\eta,\varepsilon}\Psi_n) - \lambda.$$

Using that the compact terms and the left-hand side tend to 0, we obtain $\lambda \leqslant \nu_{\max}(\mu)$. By charge-conjugation invariance (see Section 1.3), the spectrum and essential spectrum of A_ε are symmetric with respect to the origin. This obeservation, together with (3.6), proves (3.3).

When $\varepsilon = 0$ we instead use the behavior at infinity of V_μ to infer that

$$\begin{aligned}\mathbb{1}_{\mathbb{R}^3\setminus B_R}\sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\mathbb{1}_{\mathbb{R}^3\setminus B_R} &\leqslant \mathbb{1}_{\mathbb{R}^3\setminus B_R}\sqrt{\frac{1}{R-N}}\frac{1}{\alpha\cdot p}\sqrt{\frac{1}{R-N}}\mathbb{1}_{\mathbb{R}^3\setminus B_R} \\ &\leqslant \frac{1}{1-\frac{N}{R}}\mathbb{1}_{\mathbb{R}^3\setminus B_R}\sqrt{|x|^{-1}}\frac{1}{\alpha\cdot p}\sqrt{|x|^{-1}}\mathbb{1}_{\mathbb{R}^3\setminus B_R} \\ &\overset{2.5}{\leqslant} \frac{\mathbb{1}_{\mathbb{R}^3\setminus B_R}}{1-\frac{N}{R}},\end{aligned}$$

where $\mathrm{supp}(\mu) \subset B_N$, and we obtain

$$A_\varepsilon \leqslant \nu_{\max}(\mu)\mathbb{1}_{\cup_{m=1}^M B_\eta}(R_m) + \frac{\mathbb{1}_{\mathbb{R}^3\setminus B_R}}{1-\frac{N}{R}} + \mathcal{K}_{R,\eta,\varepsilon} \leqslant \frac{1}{1-\frac{N}{R}} + \mathcal{K}_{R,\eta,\varepsilon},$$

since $\nu_m \leqslant 1$ for all m. After taking $R \to \infty$, as done for the case $\varepsilon \neq 0$, this proves the reverse inclusion to (3.7) and concludes the proof of (3.4). □

In the previous proof, we have introduced the compact operator $\mathcal{K}_{R,\eta,\varepsilon}$. The following lemma provides its limit as $\varepsilon \to 0$.

Lemma 3.2 (Behavior of $\mathcal{K}_{R,\eta,\varepsilon}$)**.** *The sequence of operators $\mathcal{K}_{R,\eta,\varepsilon}$ converges in norm to the corresponding compact operator $\mathcal{K}_{R,\eta,0}$ when $\varepsilon \to 0^+$.*

Proof. The operator $\mathcal{K}_{R,\eta,\varepsilon}$ can be written in the form

$$\mathcal{K}_{R,\eta,\varepsilon} = \sum \sqrt{V_j}(\alpha\cdot p + \varepsilon\beta)^{-1}\sqrt{V_j'},$$

where for each j, either V_j or V_j' has compact support, thus belongs to L^r for any $1 \leqslant r < 3$. In addition, the supports of V_j and V_j' do not intersect, except for only one term involving $W = \mathbb{1}_{B_R\setminus\cup_{m=1}^M B_\eta(R_m)}\sqrt{V_\mu}$ twice. The terms involving W are rather easy to deal with, since they can be written in the form

$$\sqrt{V_j}\frac{1}{\alpha\cdot p + \varepsilon\beta}\sqrt{W} = \sqrt{V_j}\frac{1}{|p|^{\frac{1}{2}}}\frac{|p|}{\alpha\cdot p + \varepsilon\beta}\frac{1}{|p|^{\frac{1}{2}}}\sqrt{W}.$$

Since $|p|^{-1/2}\sqrt{W}$ is compact by Lemma 2.2, the convergence holds in norm by Theorem A.5. Therefore, we only have to treat the case where V_j and V_j' correspond to either two disjoint balls around some nuclei, or one such ball and the potential $V_\mu \mathbb{1}_{\mathbb{R}^3\setminus B_R}$.

In order to deal with these more complicated terms, it is convenient to use pointwise kernel bounds like in Lemma 2.1. Recall also that if $|A(x,y)| \leqslant B(x,y)$, then $\|A\| \leqslant \|B\|$. First we compute the kernel of the difference

$$\left(\frac{1}{\alpha\cdot p+\varepsilon\beta}-\frac{1}{\alpha\cdot p}\right)(x,y) = -i\frac{\alpha\cdot(x-y)}{4\pi|x-y|^3}\left(1-e^{-\sqrt{\varepsilon}|x-y|}\right) - i\sqrt{\varepsilon}\frac{\alpha\cdot(x-y)}{4\pi|x-y|^2}e^{-\sqrt{\varepsilon}|x-y|}+\varepsilon\beta\frac{e^{-\sqrt{\varepsilon}|x-y|}}{4\pi|x-y|}.$$

Using for instance that

$$\frac{1-e^{-r}}{r^2}\leqslant\frac{1}{r^{\frac32}},\qquad \frac{e^{-r}}{r}\leqslant\frac{1}{r^{\frac32}},$$

we obtain the bound for ε small enough

$$\left|\left(\frac{1}{\alpha\cdot p+\varepsilon\beta}-\frac{1}{\alpha\cdot p}\right)(x,y)\right|\leqslant\frac{3\varepsilon^{\frac14}}{4\pi|x-y|^{\frac32}}.$$

In the case of two non-overlapping balls around two different singularities, $|x-y|$ stays bounded and never vanishes. Hence, we find by Lemma 2.1 (with $s=3/2$)

$$\left\|\mathbb{1}_{B_\eta(R_m)}\sqrt{V_\mu}\left(\frac{1}{\alpha\cdot p+\varepsilon\beta}-\frac{1}{\alpha\cdot p}\right)\mathbb{1}_{B_\eta(R_\ell)}\sqrt{V_\mu}\right\| \leqslant C\varepsilon^{\frac14}\left\|\mathbb{1}_{B_\eta(R_m)}\sqrt{V_\mu}\frac{1}{|p|^{3/2}}\mathbb{1}_{B_\eta(R_\ell)}\sqrt{V_\mu}\right\|\leqslant C\varepsilon^{\frac14}$$

with $m\neq\ell$. For the cross term involving one singularity and $V_\mu\mathbb{1}_{\mathbb{R}^3\setminus B_R}$ we obtain, again by Lemma 2.1,

$$\begin{aligned}\left\|\mathbb{1}_{\mathbb{R}^3\setminus B_R}\sqrt{V_\mu}\left(\frac{1}{\alpha\cdot p+\varepsilon\beta}-\frac{1}{\alpha\cdot p}\right)\mathbb{1}_{B_\eta(R_\ell)}\sqrt{V_\mu}\right\| &\leqslant C\varepsilon^{\frac14}\left\|\mathbb{1}_{\mathbb{R}^3\setminus B_R}\sqrt{V_\mu}\frac{1}{|p|^{3/2}}\mathbb{1}_{B_\eta(R_\ell)}\sqrt{V_\mu}\right\| \\ &\leqslant C\varepsilon^{\frac14}\left(\int_{\mathbb{R}^3\setminus B_R}\frac{V_\mu}{(1+|x|)^3}\right)^{\frac12}\leqslant C\varepsilon^{\frac14}\left(\int_{\mathbb{R}^3\setminus B_R}\frac{dx}{|x|^4}\right)^{\frac12}.\end{aligned}$$

which concludes the proof that $\mathcal{K}_{R,\eta,\varepsilon}\to\mathcal{K}_{R,\eta,0}$ in norm. □

After these preparatory lemmas, we are able to prove the following result, which will be the main ingredient for the proof of Theorem 3.1 in the case of the critical number ν_1.

Lemma 3.3. *For every probability measure μ, we have*

$$\lim_{\varepsilon\to 0^+} \max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0+1-\varepsilon}\sqrt{V_\mu}\right) \leqslant \left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\right\|.$$

This limit exists because the function in the left-hand side is increasing with respect to ε.

Proof. For $0<\varepsilon\leqslant 1$, we write

$$\begin{aligned}
\frac{1}{D_0+1-\varepsilon} &= \frac{\alpha\cdot p+\beta-1+\varepsilon}{|p|^2+\varepsilon(2-\varepsilon)}\\
&= \frac{1}{\alpha\cdot p+\beta\sqrt{\varepsilon(2-\varepsilon)}} + \frac{(1-\sqrt{\varepsilon(2-\varepsilon)})\beta-1+\varepsilon}{|p|^2+\varepsilon(2-\varepsilon)}\\
&\leqslant \frac{1}{\alpha\cdot p+\beta\sqrt{\varepsilon(2-\varepsilon)}},
\end{aligned}$$

where we have used that

$$(1-\sqrt{\varepsilon(2-\varepsilon)})\beta-1+\varepsilon \leqslant \varepsilon-\sqrt{\varepsilon(2-\varepsilon)}\leqslant 0.$$

We obtain the operator inequality

$$\sqrt{V_\mu}\frac{1}{D_0+1-\varepsilon}\sqrt{V_\mu} \leqslant \sqrt{V_\mu}\frac{1}{\alpha\cdot p+\sqrt{\varepsilon(2-\varepsilon)}\beta}\sqrt{V_\mu},$$

which implies, as seen in the proof of Theorem 2.3, that

$$\max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0+1-\varepsilon}\sqrt{V_\mu}\right) \leqslant \left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\sqrt{\varepsilon(2-\varepsilon)}\beta}\sqrt{V_\mu}\right\|.$$

We now show that

$$\lim_{\varepsilon\to 0^+}\left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\varepsilon\beta}\sqrt{V_\mu}\right\| = \left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\right\|. \tag{3.8}$$

We will use the fact that

$$A_\varepsilon := \sqrt{V_\mu}\frac{1}{\alpha\cdot p+\varepsilon\beta}\sqrt{V_\mu} \underset{\varepsilon\to 0^+}{\longrightarrow} \sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu} =: A_0$$

strongly in the operator sense; that is, $A_\varepsilon \Psi \to A_0 \Psi$ for any $\Psi \in L^2(\mathbb{R}^3, \mathbb{C}^4)$. Actually, we have $\|A_\varepsilon\| \leqslant \pi/2$ for every $\varepsilon \geqslant 0$ by Kato's inequality, and the limit holds when $\Psi \in C_c^\infty(\mathbb{R}^3, \mathbb{C}^4)$ by the dominated convergence, theorem. Therefore, the convergence holds true everywhere by a density argument. Note that the operator norm is lower semi-continuous for the strong convergence. Indeed, let $\Psi \in L^2(\mathbb{R}^3, \mathbb{C}^4)$ with norm equal to 1, then

$$\liminf_{\varepsilon\to 0} \|A_\varepsilon\| = \liminf_{\varepsilon\to 0} \|A_\varepsilon\|\|\Psi\| \geqslant \liminf_{\varepsilon\to 0} \|A_\varepsilon \Psi\| = \|A_0\Psi\|.$$

Passing to the infimum over the normalized functions in last term in the right-hand side, we get $\|A_0\| \leqslant \liminf \|A_\varepsilon\|$. It remains to prove the reverse inequality. Let us assume by contradiction, that, after extracting a subsequence, $\|A_{\varepsilon_n}\| \to \lambda > \|A_0\|$. Since $\|A_0\| \geqslant 1$ by Lemma 3.1, this implies $\|A_{\varepsilon_n}\| > 1$ for n large enough. By charge conjugation, the spectrum is symmetric. Hence, the maximum is equal to the spectral radius, which is also equal to the norm for bounded self-adjoint operators (see Section 1.3). Therefore, $\|A_{\varepsilon_n}\| = \max \sigma(A_{\varepsilon_n}) \in \sigma(A_{\varepsilon_n}) \setminus \sigma_{\text{ess}}(A_{\varepsilon_n})$ by (3.1. Thus, $\|A_{\varepsilon_n}\| =: \lambda_n$ is an eigenvalue of A_{ε_n} whenever n is large enough. Let u_n be a corresponding normalized eigenfunction, then $A_{\varepsilon_n} u_n = \lambda_n u_n$. Since the sequence of eigenfucntion is bounded in L^2, we can assume that $u_n \rightharpoonup u$ weakly, to a function $u \in L^2$, up to a subsequence. This implies that $A_0 u = \lambda u$. Indeed, for every $f \in L^2$, one has

$$\begin{aligned}(A_0 u, f) &= ((A_0 - A_{\varepsilon_n})u, f) + (A_{\varepsilon_n}(u-u_n), f) + (A_{\varepsilon_n} u_n, f)\\ &= \underset{\substack{\downarrow\ A_{\varepsilon_n}u\to A_0 u\\ 0}}{((A_0 - A_{\varepsilon_n})u, f)} + \underset{\substack{u_n\rightharpoonup u\ \downarrow\ A_{\varepsilon_n}f\to A_0 f\\ 0}}{(u-u_n, A_{\varepsilon_n} f)} + \underset{\substack{\lambda_n\to\lambda\ \downarrow\ u_n\rightharpoonup u\\ (\lambda u, f).}}{(A_{\varepsilon_n} u_n, f)}\end{aligned}$$

Since $\lambda > \|A_0\|$, it means that $u = 0$. Otherwise, we would have $\|A_0\|\|u\|_2 < \lambda\|u\|_2 = \|A_0 u\|_2 \leqslant \|A_0\|u\|_2$. Now

$$\lim_{n\to\infty} (u_n, \mathcal{K}_{R,\eta,\varepsilon_n} u_n) = \lim_{n\to\infty} (u_n, \mathcal{K}_{R,\eta,0} u_n) = 0,$$

due to the norm convergence $\mathcal{K}_{R,\eta,R,\varepsilon} \to \mathcal{K}_{R,\eta,0}$ from (3.2) and to the compactness of the operator $\mathcal{K}_{R,\eta,0}$, which implies $\mathcal{K}_{R,\eta,0} u_n \to 0$. Hence, we find

$$\lambda = \lim_{n\to\infty} (u_n, A_{\varepsilon_n} u_n) \overset{3.2}{\leqslant} \lim_{n\to\infty} \left(u_n, \left(\frac{1}{1-\frac{N}{R}} + \mathcal{K}_{R,\eta,R,\varepsilon} \right) u_n \right) = \frac{1}{1-\frac{N}{R}}.$$

Taking $R \to \infty$ we conclude that $\lambda \leqslant 1$, and we reach a contradiction. Therefore, we have proved (3.8). This concludes the proof of Lemma 3.3. □

We finally turn to the proof of Theorem 3.1.

Proof of Theorem 3.1. **Step 1 - Proof of the characterization of ν_0**

According to Theorem 2.3, the Birman-Schwinger principle tells us that λ is an eigenvalue of $D_0 - tV_\mu$ if and only if $1/t$ is an eigenvalue of the bounded operator $K_\lambda = \sqrt{V_\mu}\,(D_0-\lambda)^{-1}\sqrt{V_\mu}$. The ordered eigenvalues of this latter operator (outside of the essential spectrum) are increasing with respect to λ and are Lipschitz continuous : Since $z \mapsto K_z$ is an analytic family of bounded operators, they are indeed real analytic curves that may cross (see [Kat13, Chapter 7]). We conclude that λ is the first eigenvalue of $D_0 - tV_\mu$ if and only if $1/t$ is the largest eigenvalue of K_λ.

Due to the definition of $\nu_0(\mu)$ there are two cases:

- If the eigenvalue crosses 0 before t reaches $1/\nu_{\max}(\mu)$, then $\lambda_1(D_0 - \nu_0(\mu)V_\mu) = 0$ and the Birman-Schwinger principle ensures that 0 is the first eigenvalue iff $\nu_0(\mu)^{-1}$ is the largest eigenvalue of K_0 :
$$\frac{1}{\nu_0(\mu)} = \max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0}\sqrt{V_\mu}\right) = \left\|\sqrt{V_\mu}\frac{1}{D_0}\sqrt{V_\mu}\right\|. \tag{3.9}$$
The last equality holds true because the spectrum is symmetric, by charge conjugation;

- If t reaches $1/\nu_{\max}(\mu)$ before the eigenvalue crosses the origin, from the Birman-Schwinger principle this means that necessarily
$$\max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0}\sqrt{V_\mu}\right) \leqslant \nu_{\max}(\mu) = \frac{1}{\nu_0(\mu)}.$$
Otherwise the eigenvalue would have crossed the origin earlier. However, by Lemma 3.1 we know that $\sigma_{\mathrm{ess}}(\sqrt{V_\mu}\frac{1}{D_0}\sqrt{V_\mu}) = [-\nu_{\max}(\mu), \nu_{\max}(\mu)]$, so that the maximum of the spectrum is always larger than or equal to $\nu_{\max}(\mu)$. Thus, there must be equality, and we conclude that (3.9) holds in all cases.

Taking the supremum over μ yields to
$$\sup_\mu\left\|\sqrt{V_\mu}\frac{1}{D_0}\sqrt{V_\mu}\right\| = \sup_\mu\frac{1}{\nu_0(\mu)} = \frac{1}{\inf_\mu \nu_0(\mu)} = \frac{1}{\nu_0}.$$

Step 2 - Proof of the characterization of ν_1

The argument for $\nu_1(\mu)$ is similar but a little more subtle since we are approaching the negative part of the essential spectrum. We have by Lemma 3.1
$$\sigma_{\mathrm{ess}}\left(\sqrt{V_\mu}\frac{1}{D_0+1-\varepsilon}\sqrt{V_\mu}\right) = [-\nu_{\max}(\mu), \nu_{\max}(\mu)]$$

and therefore

$$\max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0+1-\varepsilon}\sqrt{V_\mu}\right)\geqslant\nu_{\max}(\mu) \tag{3.10}$$

for all $0<\varepsilon<2$. Again we have two cases:

- If $\lambda_1\left(D_0-tV_\mu\right)$ approaches -1 before t reaches $1/\nu_{\max}(\mu)$, then the Birman-Schwinger principle provides as above

$$\begin{aligned}\frac{1}{\nu_1(\mu)}&=\lim_{\varepsilon\to0^+}\sup\left\{t<\frac{1}{\nu_{\max}(\mu)}:\lambda_1(D_0-tV_\mu)>-1+\varepsilon\right\}\\&=\lim_{\varepsilon\to0^+}\max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0+1-\varepsilon}\sqrt{V_\mu}\right).\end{aligned}$$

- If t reaches $1/\nu_{\max}(\mu)$ before the eigenvalue touches -1 , then necessarily

$$\lim_{\varepsilon\to0^+}\max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0+1-\varepsilon}\sqrt{V_\mu}\right)\leqslant\nu_{\max}(\mu).$$

  But, since the other inequality holds by (3.10), we see that there must be equality. We thus conclude that $\nu_1(\mu)^{-1}=\lim_{\varepsilon\to0^+}\max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0+1-\varepsilon}\sqrt{V_\mu}\right)$ holds for every probability measure μ.

Using Lemma 3.3, we obtain the upper bound

$$\frac{1}{\nu_1(\mu)}\leqslant\left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\right\|_{L^2(\mathbb{R}^3,\mathbb{C}^4)\to L^2(\mathbb{R}^3,\mathbb{C}^4)}.$$

On the other hand, using the dominated convergence theorem, we have

$$\left\langle\sqrt{V_\mu}\Psi,\frac{1}{D_0+1-\varepsilon}\sqrt{V_\mu}\Psi\right\rangle\underset{\varepsilon\to0^+}{\longrightarrow}\left\langle\sqrt{V_\mu}\Psi,\frac{1}{D_0+1}\sqrt{V_\mu}\Psi\right\rangle$$

for any Ψ in the form domain of $\sqrt{V_\mu}\left(D_0+1\right)^{-1}\sqrt{V_\mu}$. For a bounded self-adjoint operator A the maximum of the spectrum is

$$\max\sigma(A)=\sup_{\|\Psi\|=1}(\Psi,A\Psi).$$

Indeed, by the spectral theorem there exists a measured space (X,m), a unitary isomorphism $U:L^2(\mathbb{R}^3,\mathbb{C}^4)\to L^2(X,m)$ and a function $f:X\to\mathbb{R}\cup\{\pm\infty\}$ s.t. for every φ in the domain of A one has $UA\varphi=fU\varphi\quad m-a.e.$ in X. Moreover

$$\sigma(A)=\mathrm{essrange}(f)=\{y\in\mathbb{R}:\forall\varepsilon>0\quad m(f^{-1}([y-\varepsilon,y+\varepsilon]))>0\}.$$

Since A is bounded, we may assume that $\max\sigma(A) = \max \operatorname{essrange}(f) = \|f\|_\infty > 0$, up to a translation of the operator. In addition

$$(\varphi, A\varphi) = (U\varphi, fU\varphi) = \int_X f|U\varphi|^2 dm \leqslant \|f\|_\infty \|U\varphi\|^2_{L^2(X,dm)} = \|f\|_\infty \|\varphi\|_2^2.$$

Hence we obtain that $\max\sigma(A) \geqslant \sup_{\|\Psi\|=1}(\Psi, A\Psi)$. But, taking for $\varepsilon > 0$ $U\varphi = \mathbb{1}_{f^{-1}([\|f\|_\infty-\varepsilon,\|f\|_\infty])}/\|\mathbb{1}_{f^{-1}([\|f\|_\infty-\varepsilon,\|f\|_\infty])}\|_2$ – the norm at the denominator being positive by the definition of L^∞-norm) – we have $(\varphi, A\varphi) = (U\varphi, fU\varphi) \geqslant (\|f\|_\infty - \varepsilon)\|\varphi\|_2^2$ and letting $\varepsilon \to 0$ we get the reverse inequality. This implies that the max of the spectrum is lower semi-continuous, as done in the proof of the previous lemma. Hence

$$\lim_{\varepsilon\to 0^+} \max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0+1-\varepsilon}\sqrt{V_\mu}\right) \geqslant \max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0+1}\sqrt{V_\mu}\right).$$

Therefore we have shown that

$$\max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0+1}\sqrt{V_\mu}\right) \leqslant \frac{1}{\nu_1(\mu)} \leqslant \left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\right\|_{L^2(\mathbb{R}^3,\mathbb{C}^4)\to L^2(\mathbb{R}^3,\mathbb{C}^4)}$$

for every probability measure μ. After maximizing over μ we obtain

$$\begin{aligned}\sup_{\substack{\mu\geqslant 0\\ \mu(\mathbb{R}^3)=1}} \ &\max\sigma\left(\sqrt{V_\mu}\frac{1}{D_0+1}\sqrt{V_\mu}\right)\\ &\leqslant \frac{1}{\nu_1} \leqslant \sup_{\substack{\mu\geqslant 0\\ \mu(\mathbb{R}^3)=1}} \left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\right\|_{L^2(\mathbb{R}^3,\mathbb{C}^4)\to L^2(\mathbb{R}^3,\mathbb{C}^4)}.\end{aligned} \tag{3.11}$$

We want to show that these inequalities are in fact equalities. Let us write

$$\sqrt{V_\mu}\frac{1}{\alpha\cdot p+\varepsilon(\beta+1)}\sqrt{V_\mu} = \sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu} + \varepsilon(\beta-1)\sqrt{V_\mu}\frac{1}{|p|^2}\sqrt{V_\mu}.$$

Next, we use the fact that if A and B are two self-adjoint operators with B being bounded and A being non-negative (but possibly unbounded), then

$$\lim_{\varepsilon\to 0^+}\max\sigma(B-\varepsilon A) = \max\sigma(B).$$

$\leqslant$) Let Ψ_n a Weyl's sequence for $\max\sigma(B-\varepsilon A)$, then

$$\begin{aligned}\max\sigma(B-\varepsilon A) &= \lim_{n\to\infty}(\Psi_n,(B-\varepsilon A)\Psi_n) \leqslant (\Psi_n, B\Psi_n)\\ &\leqslant \sup_{\|\Psi\|=1}(\Psi_n, B\Psi_n) = \max\sigma(B);\end{aligned}$$

$\geqslant$) By density of $\mathcal{D}(A)$ for any $\eta > 0$ we can find a normalized vector $v \in \mathcal{D}(A)$ such that $(v, Bv) \geqslant \max\sigma(B) - \eta$. Let Ψ_n be again a Weyl's sequence for $\max\sigma(B - \varepsilon A) =: \lambda$, then

$$(v, (B - \varepsilon A)v) \leqslant \|B - \varepsilon A\| = \inf_{\|\Psi\|=1} \|(B - \varepsilon A)\Psi\|$$
$$\leqslant \|(B - \varepsilon A - \lambda)\Psi_n\| + \lambda\|\Psi_n\|^2 \to \max\sigma(B - \varepsilon A).$$

Therefore, we get

$$\liminf_{\varepsilon\to 0^+} \max\sigma(B - \varepsilon A) \geqslant \lim_{\varepsilon\to 0^+} (\langle v, Bv\rangle - \varepsilon\langle v, Av\rangle) \geqslant \max\sigma(B) - \eta.$$

The claim follows after taking $\eta \to 0$.

We therefore obtain that

$$\lim_{\varepsilon\to 0^+} \max\sigma\left(\sqrt{V_\mu}\,\frac{1}{\alpha\cdot p + \varepsilon(\beta+1)}\sqrt{V_\mu}\right)$$
$$= \max\sigma\left(\sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\right) = \left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\right\|,$$

where the last equality follows from the symmetry of the spectrum. But, the left-hand side is unitarily equivalent to $\sqrt{V_{\mu_\varepsilon}}\,(D_0+1)^{-1}\sqrt{V_{\mu_\varepsilon}}$ with $\mu_\varepsilon = \frac{1}{\varepsilon^3}\mu\left(\varepsilon^{-1}\cdot\right)$ via the unitary operator $U_\varepsilon f = \frac{1}{\varepsilon^{3/2}} f(\cdot/\varepsilon)$ (hence the spectrum is the same), and therefore

$$\left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\right\| = \lim_{\varepsilon\to 0^+} \max\sigma\left(\sqrt{V_{\mu_\varepsilon}}\frac{1}{D_0+1}\sqrt{V_{\mu_\varepsilon}}\right)$$
$$\leqslant \sup_{\substack{\mu'\geqslant 0\\ \mu'(\mathbb{R}^3)=1}} \max\sigma\left(\sqrt{V_{\mu'}}\frac{1}{D_0+1}\sqrt{V_{\mu'}}\right).$$

Taking the supremum over the probability measures μ, this shows that there are only equalities in (3.11) and proves the second and third equalities in the characterization of ν_1.

To conclude, it remains to notice that

$$\frac{1}{\alpha\cdot p} = \begin{pmatrix} 0 & \frac{1}{\sigma\cdot p} \\ \frac{1}{\sigma\cdot p} & 0 \end{pmatrix}.$$

Hence the norm of the operator in $L^2(\mathbb{R}^3, \mathbb{C}^4)$ is the same as the one of the off-diagonal term in $L^2(\mathbb{R}^3, \mathbb{C}^2)$:

$$\left\|\sqrt{V_\mu}\frac{1}{\alpha\cdot p}\sqrt{V_\mu}\right\|_{L^2(\mathbb{R}^3,\mathbb{C}^4)\to L^2(\mathbb{R}^3,\mathbb{C}^4)} = \left\|\sqrt{V_\mu}\frac{1}{\sigma\cdot p}\sqrt{V_\mu}\right\|_{L^2(\mathbb{R}^3,\mathbb{C}^2)\to L^2(\mathbb{R}^3,\mathbb{C}^2)}.$$

This concludes the proof of Theorem 3.1 □

Remark: The characterization of ν_1 can be interepreted in terms of Hardy-type inequalities. Indeed, for all $u \in L^2(\mathbb{R}^3, \mathbb{C}^2)$ and for all positive measures μ

$$\left\| \sqrt{V_\mu} \frac{1}{\sigma \cdot p} \sqrt{V_\mu} u \right\|^2_{L^2(\mathbb{R}^3,\mathbb{C}^2)} \leqslant \frac{\|u\|^2_{L^2(\mathbb{R}^3,\mathbb{C}^2)}}{\nu_1^2} \mu(\mathbb{R}^3)^2.$$

Taking $u = V_\mu^{-1/2} \sigma \cdot p\varphi$ with $\varphi \in H^1(\mathbb{R}^3, \mathbb{C}^2)$, we obtain that ν_1 is also the best constant in the Hardy-type inequality

$$\int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla\varphi|^2}{\mu * |x|^{-1}} dx \geqslant \frac{\nu_1^2}{\mu(\mathbb{R}^3)^2} \int_{\mathbb{R}^3} \left(\mu * \frac{1}{|x|}\right) |\varphi|^2 dx \tag{3.12}$$

for every $\varphi \in H^1(\mathbb{R}^3, \mathbb{C}^2)$ and every positive measure μ on $\mathbb{R}^3$.

3.2 Continuity of the first eigenvalue for the vague topology

Before proving the main result of the thesis regarding the existence of an optimal measure for the variational problem $\lambda_1(\nu)$ defined in (3.2), we will prove in this section the continuity of the map $\mu \mapsto \lambda_1(D_0 - \mu * |x|^{-1})$, using Lions' concentration-compactness method [Lio84a, Lio84b, Lio85a, Lio85b, Lew10]. Before we provide the detailed statement, we prove some preliminary results which are going to be useful in the argument. The first one will be used to deal with the case of *vanishing sequences* (μ_n), which contain no compact bubble at all and have all of their mass disappearing locally.

Lemma 3.4 (Estimate in terms of the largest local mass)**.** *Let μ be a nonnegative finite measure over $\mathbb{R}^3$. Then there exists a universal constant C such that for all $R \geqslant 4$*

$$\left\| V_\mu \frac{1}{D_0} \right\| \leqslant C \sup_{x \in \mathbb{R}^3} \mu(B_R(x)) + \frac{C\mu(\mathbb{R}^3)}{R}.$$

Proof. Let us consider a partition of unity $\sum_{j\in\mathbb{Z}^3} \chi_j = 1$ of $\mathbb{R}^3$ with each $\chi_j \in C_c^\infty(\mathbb{R}^3)$ supported over the cube $j + (-1,1)^3$. Let $R \geqslant 1$ and $\chi_{R,j}(x) := \chi_j(x/R)$ be the dilated partition of unity. Arguing as in the proof of Lemma 2.2, we write

$$\begin{aligned} \chi_{R,j} V_\mu &= \chi_{R,j} V_{\mu \mathbb{1}_{B_{4R}(j)}} + \chi_{R,j} V_{\mu \mathbb{1}_{\mathbb{R}^3 \setminus B_{4R}(j)}} \\ &\leqslant \chi_{R,j} V_{\mu \mathbb{1}_{B_{4R}(j)}} + \frac{C\mu(\mathbb{R}^3)}{R} \chi_{R,j}, \end{aligned}$$

where C is the distance between the sphere and the cube. This gives

$$0 \leqslant V_\mu \leqslant \sum_{j\in\mathbb{Z}^3} \chi_{R,j} V_{\mu \mathbb{1}_{B_{4R}(j)}} + \frac{C\mu\left(\mathbb{R}^3\right)}{R}.$$

Hence

$$\left\| V_\mu \frac{1}{D_0} \right\| \overset{A.4}{=} \left\| V_\mu \frac{1}{\sqrt{1-\Delta}} \right\| \leqslant \left\| \sum_{j\in\mathbb{Z}^3} \chi_{R,j} V_{\mu \mathbb{1}_{B_{4R}(Rj)}} \frac{1}{\sqrt{1-\Delta}} \right\| + \frac{C\mu\left(\mathbb{R}^3\right)}{R}.$$

To estimate the first term in the right-hand side, we write

$$\begin{aligned}\sum_{j\in\mathbb{Z}^3} & \chi_{R,j} V_{\mu \mathbb{1}_{B_{4R}(j)}} \frac{1}{\sqrt{1-\Delta}} \\ &= \sum_{j\in\mathbb{Z}^3} \chi_{R,j} V_{\mu \mathbb{1}_{B_{4R}(j)}} \frac{1}{\sqrt{1-\Delta}} \left(\mathbb{1}_{B_{4R}(j)} + \mathbb{1}_{\mathbb{R}^3 \setminus B_{4R}(j)}\right)\end{aligned}$$

and we estimate the corresponding positive kernels pointwise. Using that

$$\frac{1}{\sqrt{1-\Delta}}(x-y) \leqslant C \frac{e^{-|x-y|}}{|x-y|^2} \leqslant C \frac{1}{|x-y|^2},$$

we obtain

$$\begin{aligned}\sum_{j\in\mathbb{Z}^3} \chi_{R,j} V_{\mu \mathbb{1}_{B_{4R}(j)}} \frac{1}{\sqrt{1-\Delta}}(x,y) &\leqslant C \sum_{j\in\mathbb{Z}^3} \mathbb{1}_{B_{4R}(j)}(x) \frac{V_{\mu \mathbb{1}_{B_{4R}(j)}}(x)}{|x-y|^2} \\ &\leqslant C \left(\sum_{j\in\mathbb{Z}^3} \mathbb{1}_{B_{4R}(j)}(x) \right) \sup_{j\in\mathbb{Z}^3} V_{\mu \mathbb{1}_{B_{4R}(j)}}(x) \frac{1}{|x-y|^2}.\end{aligned}$$

Note that the right-hand side is the kernel of the operator

$$C \left(\sum_{j\in\mathbb{Z}^3} \mathbb{1}_{B_{4R}(j)} \right) \sup_{j\in\mathbb{Z}^3} V_{\mu \mathbb{1}_{B_{4R}(j)}} \frac{1}{|p|}.$$

Therefore we have, by Hardy's inequality and the fact that $\sum_{j\in\mathbb{Z}^3} \mathbb{1}_{B_{4R}(j)} \leqslant C$, the following norm estimate

$$\begin{aligned}\left\| \sum_{j\in\mathbb{Z}^3} \chi_{R,j} V_{\mu \mathbb{1}_{B_{4R}(Rj)}} \frac{1}{\sqrt{1-\Delta}} \right\| &\leqslant C \left\| \left(\sum_{j\in\mathbb{Z}^3} \mathbb{1}_{B_{4R}(j)} \right) \sup_{j\in\mathbb{Z}^3} V_{\mu \mathbb{1}_{B_{4R}(j)}} \frac{1}{|p|} \right\| \\ &\leqslant C \left\| \sup_{j\in\mathbb{Z}^3} V_{\mu \mathbb{1}_{B_{4R}(j)}} \frac{1}{|p|} \right\| \leqslant C \sup_{j\in\mathbb{Z}^3} \mu\left(B_{4R}(j)\right).\end{aligned}$$

Thus we conclude that

$$\left\|V_\mu \frac{1}{D_0}\right\| \leqslant C \sup_{x\in\mathbb{R}^3} \mu\left(B_{R'}(x)\right) + \frac{C\mu\left(\mathbb{R}^3\right)}{R'} \quad \forall R' \geqslant 4.$$

$\square$

The second lemma is about the convergence of the Coulomb potential V_{μ_n} in the case where μ_n converges tightly or vaguely to a limit (see Appendix A.1 for an introduction to finite measures).

Lemma 3.5 (Convergence of the potential)**.** *Let $\mu_n \rightharpoonup \mu$ be a sequence of measures which converges tightly. Then the associated potential $V_{\mu_n} = \mu_n * |x|^{-1}$ converges to $V_\mu = \mu * |x|^{-1}$ strongly in $\left(L^2 + L^\infty\right)\left(\mathbb{R}^3\right)$, hence also almost everywhere after extraction of a subsequence. In particular, we have the norm convergence*

$$\sqrt{V_{\mu_n}}\frac{1}{D_0-\lambda} \longrightarrow \sqrt{V_\mu}\frac{1}{D_0-\lambda}$$

for every $\lambda \in (-1,1)$, uniformly on compact subsets of $(-1,1)$. If $\mu_n \rightharpoonup^* \mu$ converges vaguely (but not tightly), then we still have $V_{\mu_n}(x) \to V_\mu(x)$ strongly in $L^2_{\text{loc}}\left(\mathbb{R}^3\right)$, hence also almost-everywhere after extraction of a subsequence.

Proof. The tight convergence $\mu_n \rightharpoonup \mu$ implies that the Fourier transforms $\widehat{\mu_n}(k) \to \widehat{\mu}(k)$ converge for all $k \in \mathbb{R}^3$, since the function $x \mapsto e^{-2\pi i(x,k)}$ is continuous and bounded. Then

$$\begin{aligned}\widehat{V_{\mu_n}}(k) - \widehat{V_\mu}(k) &= \mathcal{F}\left((\mu_n-\mu) * \frac{1}{|\cdot|}\right) = \widehat{\mu_n-\mu}\cdot\widehat{\frac{1}{|x|}} = 4\pi\frac{\widehat{\mu_n}(k)-\widehat{\mu}(k)}{|k|^2} \\ &= 4\pi\frac{\widehat{\mu_n}(k)-\widehat{\mu}(k)}{|k|^2}\mathbb{1}_{B_1}(k) + 4\pi\frac{\widehat{\mu_n}(k)-\widehat{\mu}(k)}{|k|^2}\mathbb{1}_{\mathbb{R}^3\setminus B_1}(k),\end{aligned}$$

where the first term in the last equation is in $L^1\left(B_1\right)$ and the second one in $L^2\left(\mathbb{R}^3\setminus B_1\right)$. From the dominated convergence theorem – using that $\widehat{\mu_n}$ is uniformly bounded –, we infer that both terms converge to 0, the first one in L^1 and the second one in L^2. Applying the inverse of the Fourier transform, the convergence in L^2 remains the same, while the convergence in L^1 becomes convergence in L^∞. Thus $V_{\mu_n} \to V_\mu$ strongly in $\left(L^2+L^\infty\right)\left(\mathbb{R}^3\right)$, hence in $L^2_{\text{loc}}\left(\mathbb{R}^3\right)$.

The norm convergence follows from the inequality

$$\begin{aligned}&\left\|f(x)\frac{1}{D_0-\lambda}\right\| \\ &\quad\leqslant \min\left(\frac{\|f\|_{L^\infty}}{\min(|\lambda-1|,|\lambda+1|)}, \frac{\|f\|_{L^4}}{(2\pi)^3}\left(\int_{\mathbb{R}^3}\left\|\frac{1}{\alpha\cdot p+\beta-\lambda}\right\|^4 dp\right)^{\frac14}\right).\end{aligned} \tag{3.13}$$

Indeed

$$\left\|(\sqrt{V_{\mu_n}}-\sqrt{V_\mu})\frac{1}{D_0-\lambda}\right\| \leqslant \left\|(\sqrt{V_{\mu_n}}-\sqrt{V_\mu})\mathbb{1}_{B_1}\frac{1}{D_0-\lambda}\right\| + \left\|(\sqrt{V_{\mu_n}}-\sqrt{V_\mu})\mathbb{1}_{B_1^c}\frac{1}{D_0-\lambda}\right\|$$

and, using (3.13) on both terms and the fact that the L^∞-norm of $(\sqrt{V_{\mu_n}}-\sqrt{V_\mu})\mathbb{1}_{B_1}$ and the L^4-norm of $(\sqrt{V_{\mu_n}}-\sqrt{V_\mu})\mathbb{1}_{B_1^c}$ go to zero, we get the norm convergence. Let us prove (3.13). We have

$$\left\|f\frac{1}{D_0-\lambda}\right\| \leqslant \|f\|\|\frac{1}{D_0-\lambda}\| \leqslant \frac{\|f\|_{L^\infty}}{\mathrm{dist}(\lambda,\sigma(D_0))} \leqslant \frac{\|f\|_{L^\infty}}{\min(|\lambda-1|,|\lambda+1|)};$$

and

$$\begin{aligned}\left\|f\frac{1}{D_0-\lambda}\varphi\right\|_2 &\overset{C-S}{\leqslant} \|f\|_4\left\|\mathcal{F}^{-1}\left(\frac{1}{\alpha\cdot p+\beta-\lambda}\widehat{\varphi}\right)\right\|_4\\ &\leqslant \frac{\|f\|_4}{(2\pi)^3}\left\|\frac{1}{\alpha\cdot p+\beta-\lambda}\widehat{\varphi}\right\|_{4/3}\\ &\leqslant \frac{\|f\|_4}{(2\pi)^3}\left(\int_{\mathbb{R}^3}\left\|\frac{1}{\alpha\cdot p+\beta-\lambda}\right\|^{4/3}|\widehat{\varphi}|^{4/3}dp\right)^{\frac{3}{4}}\\ &\overset{C-S}{\leqslant} \frac{\|f\|_{L^4}}{(2\pi)^3}\left(\int_{\mathbb{R}^3}\left\|\frac{1}{\alpha\cdot p+\beta-\lambda}\right\|^{4}dp\right)^{\frac{1}{4}}\|\widehat{\varphi}\|_2.\end{aligned}$$

Finally, if $\mu_n \rightharpoonup^* \mu$ vaguely (but not tightly), then we may always choose a radius r_n diverging to infinity sufficiently slowly such that $\mu_n(B_{r_n}) \to \mu(\mathbb{R}^3)$. It is equivalent to show that, for fixed r_k diverging you can find a subsequence n_k which goes to infinity rapidly s.t. $\mu_{n_k}(B_{r_k}) \to \mu(\mathbb{R}^3)$. Thnaks to the vague convergence, we have $\mu_n(B_{r_k}) \to \mu(B_{r_k})$ as $n\to\infty$. Extracting a subsequence we may assume $|\mu_{n_k}(B_{r_k})-\mu(B_{r_k})| \leqslant \frac{1}{k}$. We then deduce that

$$\left|\mu_{n_k}(B_{r_k})-\mu(\mathbb{R}^3)\right| \leqslant \frac{1}{k}+\mu(\mathbb{R}^3\setminus B_{r_k}) \underset{k\to\infty}{\longrightarrow} 0. \tag{3.14}$$

Then, $\mu_n\mathbb{1}_{B_{r_n}}$ converges tightly and, on any fixed ball B_R, we have

$$\mathbb{1}_{B_R}\left|V_{\mu_n}-V_{\mu_n\mathbb{1}_{B_{r_n}}}\right| = \mathbb{1}_{B_R}\left|V_{\mu_n\mathbb{1}_{\mathbb{R}^3\setminus B_{r_n}}}\right| \leqslant \frac{\mu_n(\mathbb{R}^3)}{|r_n-R|} \to 0.$$

By the tight case, $V_{\mu_n\mathbb{1}_{B_{r_n}}} \to V_\mu$ in L^2_{loc} and for any compact set K there exists $R>0$ s.t. $K\subset B_R$. Hence,

$$\begin{aligned}\|V_{\mu_n}-V_\mu\|_{L^2(K)} &\leqslant \|V_{\mu_n}-V_{\mu_n\mathbb{1}_{B_{r_n}}}\|_{L^2(B_R)}+\|V_{\mu_n\mathbb{1}_{B_{r_n}}}-V_\mu\|_{L^2(B_R)}\\ &\leqslant \left(\frac{\mu_n(B_{r_n}^c)}{|r_n-R|}\right)^2|B_R|+\|V_{\mu_n\mathbb{1}_{B_{r_n}}}-V_\mu\|_{L^2(B_R)} \underset{n\to\infty}{\longrightarrow} 0,\end{aligned}$$

which concludes the proof $\square$

With these results in hand, we are now able to provide the proof of the main theorem of this section.

Theorem 3.2 (Weak continuity)**.** *Let* $0 \leqslant \nu < \nu_1$ *and let* (μ_n) *be an arbitrary sequence of non-negative measures such that* $\mu_n(\mathbb{R}^3) \leqslant \nu$. *Then, there exists a subsequence* (μ_{n_k}), *a sequence of space translations* $(x_k) \subset \mathbb{R}^3$ *and a measure* μ *such that* $\mu_{n_k}(\cdot + x_k) \rightharpoonup^* \mu$ *vaguely and*

$$\lim_{k\to\infty} \lambda_1\left(D_0 - \mu_{n_k} * \frac{1}{|x|}\right) = \lambda_1\left(D_0 - \mu * \frac{1}{|x|}\right).$$

Proof. Firstly, we notice that

$$\lim_{n\to\infty} \lambda_1\left(D_0 - V_{\mu*\zeta_n}\right) = \lambda_1\left(D_0 - V_\mu\right)$$

for any $0 \leqslant \mu(\mathbb{R}^3) < 1$ and $\zeta_n \in C_c^\infty(\mathbb{R}^3) \rightharpoonup^* \delta_0$ a regularizing sequence (we can also assume that $\int_{\mathbb{R}^3} \zeta_n = 1$ and ζ_n symmetric w.r.t the origin). This follows from the resolvent convergence in Theorem 2.1. Moreover, $\mu * \zeta_n \rightharpoonup^* \mu$ tightly: for every $f \in C_b$ one has $(\mu * \zeta_n, f) = (\mu, \zeta_n * f) \to (\mu, f)$ by the dominated convergence theorem. Hence, in the whole proof we can assume for simplicity that $\mu_n \in C^\infty(\mathbb{R}^3, \mathbb{R}_+)$. By Theorem 2.1, this property ensures that the domain of the corresponding Dirac operator is $H^1(\mathbb{R}^3)$. Indeed $\mu_n(\{R\}) = 0$ for every $R \in \mathbb{R}^3$, and this allows us to perform some computations more easily. Let

$$\ell := \lim_{n\to\infty} \lambda_1\left(D_0 - V_{\mu_n}\right)$$

be the limit of the eigenvalues, which always exists after extraction of an appropriate subsequence, since the sequence is bounded in $(-1, 1)$.

We split the proof of the proposition into several steps. In the first step we deal with the easy case where $\ell = 1$, which contains in particular the case of *vanishing sequences* in the sense of the concentration-compactness method, as we will explain. The central argument is in Step 2 where we prove that $\ell > -1$; that is, the eigenvalue cannot approach the lower essential spectrum. In Step 3, we will find the bubble μ which has the lowest possible eigenvalue and show that this is the limit of $\lambda_1(D_0 - \mu_n * |x|^{-1})$.

Step 1 – The case $\ell = 1$

If $\ell = 1$, we can always find a sequence (x_n) diverging fast enough to infinity such that $\mu_n(\cdot + x_n) \rightharpoonup^* 0 =: \mu$. Indeed, for $f \in C_0$, one has $(f, \mu_n(\cdot + x_n)) =$

$(f(\cdot - x_n), \mu_n) \to 0$ by the dominated convergence theorem, by using the fact that f goes to 0 at ∞. Since $\lambda_1(D_0 - V_0) = \lambda_1(D_0) = 1$, the proposition is proved, and $\mu = 0$ in this case. In the rest of the proof, we therefore assume that

$$\ell < 1.$$

Step 2 – The proof that $\ell > -1$

Under this assumption, $\mu_n(\mathbb{R}^3)$ cannot have a subsequence tending to 0. Otherwise, by Hardy's inequality, we would have

$$\left\| V_{\mu_{n_k}} \frac{1}{D_0} \right\| \leqslant 2\mu_{n_k}\left(\mathbb{R}^3\right) \to 0,$$

and this would imply that $\lambda_1(D_0 - V_{n_k})$ converges to ± 1 by [Lew22, Theorem 5.4]. Since $\ell < 1$, the only remaining possibility is -1. In particular, for k large enough $\lambda_1(D_0 - V_{n_k})$ stays away below 0. For every such k, by the continuity of the function $t \mapsto f(t) = \lambda_1(D_0 - tV_{n_k})$ and since $f(0) = 1$ and $f(1) < 0$, there exists $t_k \in (0,1)$ such that $f(t_k) = \lambda_1(D_0 - t_k V_{n_k}) = 0$. And we reach a contradiction again since by the same argument as above $\lambda_1(D_0 - t_k V_{n_k}) \to \pm 1$. Thus, we have

$$\liminf_{n\to\infty} \mu_n\left(\mathbb{R}^3\right) > 0.$$

Moreover

$$\lim_{n\to\infty} \sup_{x\in\mathbb{R}^3} \mu_n(B_R(x)) > 0$$

for all $R > 0$. Therefore, the sequence μ_n cannot vanish in the sense of the concentration-compactness terminology [Lio84a, Lio84b, Lio85a, Lio85b, Lew10]). Otherwise by Lemma 3.4 we would again deduce that $\left\|V_{\mu_n} D_0^{-1}\right\| \to 0$, and thus $\lambda_1(D_0 - V_{\mu_n}) \to 1$, which is in contradiction with $\ell < 1$.

We argue by contradiction and assume that $\ell = -1$. Let us denote

$$M := \sup\left\{\mu\left(\mathbb{R}^3\right) : \exists\,(x_k) \subset \mathbb{R}^3, \mu_{n_k}(\cdot - x_k) \rightharpoonup^* \mu \text{ vaguely}\right\}$$

the largest mass of all the possible vague limits of μ_n, up to translations and extraction of subsequences. If $M = 0$, then $\mu_n(\cdot - x_n) \rightharpoonup^* 0$ for any $(x_n) \subset \mathbb{R}^3$ and this implies that $\mu_n(B_R(x_n)) \to 0$ for every $R > 0$. This cannot happen because $\lim_{n\to\infty} \sup_{x\in\mathbb{R}^3} \mu_n(B_R(x)) > 0$. Therefore, $M > 0$, and there exists a sequence of translations (x_k) and a subsequence such that $\mu_{n_k}(\cdot - x_k) \rightharpoonup^* \mu \neq 0$ vaguely with, for instance, $\mu(\mathbb{R}^3) \geqslant M/2$. The problem being translation-invariant, we may assume for simplicity of notation that $x_k \equiv 0$ and that $\mu_n \rightharpoonup^* \mu$ vaguely, after extraction of a subsequence. To simplify the notation, we introduce the shorthands

$$\lambda_n := \lambda_1(D_0 - V_n) = -1 + \varepsilon_n, \quad V_n := \mu_n * \frac{1}{|x|}$$

with $\varepsilon_n \to 0^+$. Let $\Psi_n \in H^1(\mathbb{R}^3, \mathbb{C}^4)$ be an eigenvector solving

$$(D_0 - V_n)\,\Psi_n = \lambda_n \Psi_n, \quad \Psi_n = \begin{pmatrix} \varphi_n \\ \chi_n \end{pmatrix}.$$

Considering the min-max formula (2.15) for $k = 1$ and solving the maximization over χ_n, one finds that λ_n is the lowest $\lambda \in [-1, 1]$ such that

$$0 \in \sigma\left(-\sigma \cdot \nabla \frac{1}{\varepsilon_n + V_n} \sigma \cdot \nabla + 2 - \varepsilon_n - V_n\right). \tag{3.15}$$

Since $\lambda_n > -1$, it is the first eigenvalue of $D_0 - V_n$ and φ_n is the first eigenfunction of the operator in (3.15); that is

$$\left(-\sigma \cdot \nabla \frac{1}{\varepsilon_n + V_n} \sigma \cdot \nabla + 2 - \varepsilon_n - V_n\right) \varphi_n = 0 \tag{3.16}$$

and

$$\chi_n = \frac{-i\sigma \cdot \nabla \varphi_n}{\varepsilon_n + V_n}.$$

The quadratic form associated with the operator in (3.15) is

$$q_{\lambda_n}(\varphi) := \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \varphi(x)|^2}{\varepsilon_n + V_n(x)} dx + \int_{\mathbb{R}^3} (2 - \varepsilon_n - V_n(x))\, |\varphi(x)|^2 dx \geqslant 0.$$

It is non-negative because φ_n is the first eigenfunction related to the eigenvalue 0, which is therefore the lowest eigenvalue. In the whole argument we normalize our solution in order that the upper spinor itself is normalized in L^2 :

$$\int_{\mathbb{R}^3} |\varphi_n(x)|^2\, dx = 1.$$

Let $0 \leqslant \zeta \leqslant 1$ be a smooth function with support in the ball B_4, which equals one in B_2, and set $\zeta_R(x) := \zeta(x/R)$ and $\eta_R = \sqrt{1 - \zeta_R^2}$. As done in the proof of Theorem 2.3, we will use the pointwise IMS formula for the Pauli operator which states that

$$\sum_k |\sigma \cdot \nabla (J_k \varphi)|^2 = |\sigma \cdot \nabla \varphi|^2 + |\varphi|^2 \sum_k |\nabla J_k|^2$$

for a partition of unity $\sum_k J_k^2 = 1$. Here again we obtain

$$\begin{aligned} 0 &= q_{\lambda_n}(\varphi_n) \\ &= q_{\lambda_n}(\zeta_R \varphi_n) + q_{\lambda_n}(\eta_R \varphi_n) \\ &\quad - \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \zeta_R(x)|^2 + |\sigma \cdot \nabla \eta_R(x)|^2}{\varepsilon_n + V_n(x)} |\varphi_n(x)|^2\, dx \\ &\geqslant q_{\lambda_n}(\zeta_R \varphi_n) + q_{\lambda_n}(\eta_R \varphi_n) - \frac{C}{R^2} \int_{2R \leqslant |x| \leqslant 4R} \frac{|\varphi_n(x)|^2}{\varepsilon_n + V_n(x)} dx. \end{aligned}$$

On $B_{4R} \setminus B_{2R}$ we have

$$V_n(x) \geqslant (\mu_n \mathbb{1}_{B_R}) * \frac{1}{|x|} \geqslant \frac{\mu_n (B_R)}{5R},$$

where $5R$ is the largest possible distance between the points in the annulus and the points in the ball B_R. Since $\mu_n (B_R) \to \mu (B_R)$ with $\mu (\mathbb{R}^3) \geqslant M/2 > 0$ due to the vague convergence, we deduce that for R large enough we have

$$q_{\lambda_n} (\zeta_R \varphi_n) + q_{\lambda_n} (\eta_R \varphi_n) \leqslant \frac{C}{R} \int_{B_{4R} \setminus B_{2R}} |\varphi_n|^2 \leqslant \frac{C}{R}.$$

Recall that $q_{\lambda_n} \geqslant 0$, hence this gives a bound on $q_{\lambda_n} (\zeta_R \varphi_n)$ and $q_{\lambda_n} (\eta_R \varphi_n)$ separately.

We first look at the local part $q_{\lambda_n} (\zeta_R \varphi_n)$ which gives, after discarding the L^2 term,

$$\int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \zeta_R \varphi_n|^2}{\varepsilon_n + V_n} dx - \int_{\mathbb{R}^3} V_n |\zeta_R \varphi_n|^2 dx \leqslant q_{\lambda_n}(\zeta_r \varphi_n) \leqslant \frac{C}{R}.$$

For the second term in the left-hand side, by the characterization of ν_1 in terms of the Hardy-type inequality (3.12) on $\zeta_R \varphi_n$, we have

$$\int_{\mathbb{R}^3} V_n |\zeta_R \varphi_n|^2 dx \leqslant \frac{\mu_n (\mathbb{R}^3)^2}{\nu_1^2} \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \zeta_R \varphi_n|^2}{V_n} dx. \tag{3.17}$$

For the first term, we use instead the lower bound

$$\frac{1}{\varepsilon_n + V_n} = \frac{1}{V_n} \left(1 - \frac{\varepsilon_n}{V_n + \varepsilon_n}\right) \geqslant \frac{1}{V_n} \left(1 - \frac{\varepsilon_n}{\frac{1}{CR} + \varepsilon_n}\right) = \frac{1}{V_n} \left(1 - \frac{C\varepsilon_n R}{1 + C\varepsilon_n R}\right),$$

where in above inequality we have used that

$$V_n \geqslant \frac{\mu_n (B_{4R})}{8R} \geqslant \frac{1}{CR} \quad \text{on } B_{4R} \text{ for } n \text{ and } R \text{ large enough.}$$

We arrive at

$$\int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \zeta_R \varphi_n|^2}{\varepsilon_n + V_n} dx \geqslant \frac{1}{1 + C\varepsilon_n R} \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \zeta_R \varphi_n|^2}{V_n} dx.$$

We have therefore proved the following bound

$$\left(\frac{1}{1 + C\varepsilon_n R} - \frac{\mu_n (\mathbb{R}^3)^2}{\nu_1^2}\right) \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \zeta_R \varphi_n|^2}{V_n} dx \leqslant \frac{C}{R}. \tag{3.18}$$

Since $\mu_n(\mathbb{R}^3) \leqslant \nu < \nu_1$ and $\varepsilon_n \to 0$ by assumption, this shows that the integral in the left-hand side is uniformly bounded for fixed R. In particular, $\zeta_R\varphi_n$ is also uniformly bounded in $\mathcal{V}_{\mu_n}$:

$$\|\zeta_R\varphi_n\|^2_{\mathcal{V}_{\mu_n}} = \int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\zeta_R\varphi_n|^2}{1+V_n}dx + \|\zeta_R\varphi_n\|_2^2 \leqslant \int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\zeta_R\varphi_n|^2}{V_n}dx + 1.$$

Next, we prove an $H^{1/2}$ bound. In Theorem 2.2 we have shown the inequality

$$\frac{\|\varphi\|^2_{H^{1/2}(\mathbb{R}^3,\mathbb{C}^2)}}{\max(2, 16m(\mathbb{R}^3))} \leqslant \|\varphi\|^2_{\mathcal{V}_m} \leqslant \|\varphi\|^2_{H^1(\mathbb{R}^3,\mathbb{C}^2)}. \tag{3.19}$$

Scaling φ and m in this way $\varphi' = \frac{1}{\lambda^{3/2}}\varphi(\cdot/\lambda)$, $m' = \frac{1}{\lambda^{7/2}}m(\cdot/\lambda)$, one gets, after some computations, $\|\varphi'\|_2 = \|\varphi\|_2$, $(\varphi', |p|\varphi') = \frac{1}{\lambda^6}(\varphi, |p|\varphi)$, $m'(\mathbb{R}^3) = \frac{1}{\lambda^{1/2}}m(\mathbb{R}^3)$ and $V_{m'} = \frac{1}{\lambda^{3/2}}V_m(\cdot/\lambda)$. Inserting φ' and m' in (3.19) we obtain the inequality

$$\int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\varphi(x)|^2}{\lambda^{3/2}+V_m(x)}dx \geqslant \frac{(\varphi,|p|\varphi)}{2\lambda^{11/2}\max\left(1, \frac{8}{\lambda^{1/2}}m(\mathbb{R}^3)\right)} - \lambda^{1/2}\|\varphi\|^2_{L^2(\mathbb{R}^3)},$$

for all $\varphi \in H^1(\mathbb{R}^3, \mathbb{C}^2)$, all positive measure m and all $\lambda > 0$. For λ small

$$\frac{(\varphi,|p|\varphi)}{2\lambda^{11/2}\max\left(1, \frac{8}{\lambda^{1/2}}m(\mathbb{R}^3)\right)} = \frac{(\varphi,|p|\varphi)}{16\lambda^5 m(\mathbb{R}^3)} \geqslant \frac{(\varphi,|p|\varphi)}{16m(\mathbb{R}^3)}.$$

Hence, taking $\lambda \to 0$ yields to

$$(\varphi,|p|\varphi) \leqslant 16m(\mathbb{R}^3)\int_{\mathbb{R}^3}\frac{|\sigma\cdot\nabla\varphi(x)|^2}{V_m(x)}dx.$$

So by (3.18) we get

$$\left(\frac{1}{1+C\varepsilon_n R} - \frac{\mu_n(\mathbb{R}^3)^2}{\nu_1^2}\right)(\zeta_R\varphi_n, |p|\zeta_R\varphi_n) \leqslant \frac{C}{R}. \tag{3.20}$$

This shows that $\zeta_R\varphi_n$ is bounded in $H^{1/2}$ for every R large enough. In other words, φ_n is bounded in $H^{1/2}_{\text{loc}}$.

After extraction of a subsequence, we may assume that $\varphi_n \rightharpoonup \varphi$ weakly in L^2 and strongly in L^2_{loc}, hence also almost everywhere. From Lemma 3.5, since μ_n converges vaguely to μ, we also have that $V_n(x) \to V_\mu(x)$ almost everywhere. Then passing to the limit in (3.17) and (3.18), we obtain from Fatou's lemma

$$\begin{aligned}\int_{\mathbb{R}^3} V_\mu|\zeta_R\varphi|^2 &\leqslant \liminf \int_{\mathbb{R}^3} V_\mu|\zeta_R\varphi_n|^2 \leqslant \liminf \frac{\mu_n(\mathbb{R}^3)^2}{\nu_1^2}\int_{\mathbb{R}^3}\frac{|\sigma\cdot\nabla\zeta_R\varphi_n|^2}{V_n}\\ &\leqslant \liminf \frac{\mu_n(\mathbb{R}^3)^2}{\nu_1^2}\left(\frac{1}{1+C\varepsilon_n R} - \frac{\mu_n(\mathbb{R}^3)^2}{\nu_1^2}\right)^{-1}\frac{C}{R} \leqslant \frac{C}{R}.\end{aligned}$$

Finally, taking $R \to \infty$ gives $\varphi \equiv 0$ ($V_\mu > 0$). Using the strong local compactness, we can choose $R = R_n \to \infty$ sufficiently slowly, (see (3.14) and [Lew10] for a similar argument) to ensure that

$$\begin{gathered}\varepsilon_n R_n \to 0, \quad \mu_n\left(B_{R_n}\right) \to \mu\left(\mathbb{R}^3\right), \quad \mu_n\left(B_{8R_n} \setminus B_{R_n}\right) \to 0, \\ \int_{B_{8R_n}} \left|\varphi_n\right|^2 \to 0.\end{gathered} \tag{3.21}$$

From (3.20) we also have $\|\zeta_{R_n}\varphi_n\|_{H^{1/2}} \to 0$. All this shows that nothing is happening in the region under investigation. The mass of φ_n must excape at infinity.

At this stage, we have shown that φ_n has no L^2 mass in the region where μ_n converges to μ. The next step is to apply the whole argument again to $\eta_{R_n}\varphi_n$. Namely, following the concentration compactness method [Lio84a, Lio84b, Lio85a, Lio85b, Lew10], we extract the next profile in the sequence μ_n and use the same argument to show that φ_n has no mass in the corresponding region. After finitely many steps, the remainder $\mu_n^{'}$ will be composed of a piece which can vanish and another piece with an arbitrarily small mass (for instance a mass $\leqslant 1/4$). For simplicity of exposition, we provide the end of the argument in the simplest situation, namely we assume that

$$\mu_n \mathbb{1}_{\mathbb{R}^3 \setminus B_{R_n}} = \mu_n^{(1)} + \mu_n^{(2)},$$

where $\mu_n^{(1)}$ vanishes in the sense of concentration-compactness, i.e.

$$\lim_{n\to\infty} \sup_{x\in\mathbb{R}^3} \mu_n\left(B_R(x)\right) = 0 \tag{3.22}$$

for every $R > 0$, and $\mu_n^{(2)}\left(\mathbb{R}^3 \setminus B_{R_n}\right) \leqslant 1/4$. Then $\|V_{\mu_n \mathbb{1}_{\mathbb{R}^3\setminus B_{R_n}}} \frac{1}{D_0}\| \leqslant \|V_{\mu_n^{(1)}} \frac{1}{D_0}\| + \|V_{\mu_n^{(2)}} \frac{1}{D_0}\| \leqslant \frac{2}{3}$, for n large, since by Lemma 3.4 the first one tends to 0 due to (3.22) and the second one is below $1/2$ by Hardy's inequality. This, using [Lew22, Theorem 5.4] and the same argument presented at the beginning of this step, implies that

$$\lambda_1\left(D_0 - V_{\mu_n \mathbb{1}_{\mathbb{R}^3\setminus B_{R_n}}}\right) \geqslant 1/3 \geqslant 0$$

for n large enough. Hence, by the min-max principle and the characterization in terms of the quadratic form q_λ [DES00], this tells us that

$$q_{0,\mu_n \mathbb{1}_{\mathbb{R}^3\setminus B_{R_n}}}(\varphi) = \int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\varphi|^2}{1 + V_{\mu_n \mathbb{1}_{\mathbb{R}^3\setminus B_{R_n}}}} dx + \int_{\mathbb{R}^3} \left(1 - V_{\mu_n \mathbb{1}_{\mathbb{R}^3\setminus B_R}}\right)|\varphi|^2 dx \geqslant 0, \tag{3.23}$$

for every $\varphi \in H^1\left(\mathbb{R}^3, \mathbb{C}^2\right)$. On the support of η_{R_n}, which is contained in $B^c_{2R_n}$, we have

$$V_n = V_{\mu_n \mathbb{1}_{\mathbb{R}^3\setminus B_R}} + V_{\mu_n \mathbb{1}_{B_{R_n}}} \leqslant V_{\mu_n \mathbb{1}_{\mathbb{R}^3\setminus B_{R_n}}} + \frac{C}{R_n}.$$

Hence, using that $\varepsilon_n + CR_n^{-1} \to 0$, we obtain

$$\begin{aligned}
q_{\lambda_n}(\eta_{R_n}\varphi_n) &= \int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla(\eta_{R_n}\varphi_n)|^2}{\varepsilon_n + V_{\mu_n}}dx + \int_{\mathbb{R}^3}(2-\varepsilon_n - V_{\mu_n})|\eta_{R_n}\varphi_n|^2\,dx \\
&\geqslant \int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla(\eta_{R_n}\varphi_n)|^2}{\varepsilon_n + CR_n^{-1} + V_{\mu_n\mathbb{1}_{\mathbb{R}^3\setminus B_{Rn}}}}dx \\
&\qquad + \int_{\mathbb{R}^3}\left(2-\varepsilon_n - \frac{C}{R_n} - V_{\mu_n\mathbb{1}_{\mathbb{R}^3\setminus B_{R_n}}}\right)|\eta_{R_n}\varphi_n|^2\,dx \\
&\geqslant \int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla(\eta_{R_n}\varphi_n)|^2}{1 + V_{\mu_n\mathbb{1}_{\mathbb{R}^3\setminus B_{Rn}}}}dx \\
&\qquad + \int_{\mathbb{R}^3}\left(2-\varepsilon_n - \frac{C}{R_n} - V_{\mu_n\mathbb{1}_{\mathbb{R}^3\setminus B_{R_n}}}\right)|\eta_{R_n}\varphi_n|^2\,dx \\
&\overset{3.23}{\geqslant} \int_{\mathbb{R}^3}\left(1-\varepsilon_n - \frac{C}{R_n}\right)|\eta_{R_n}\varphi_n|^2\,dx \geqslant \frac{1}{2}\int_{\mathbb{R}^3}|\eta_{R_n}\varphi_n|^2\,dx.
\end{aligned} \tag{3.24}$$

Since the left-hand side is bounded from above by C/R_n that goes to 0, this shows that

$$\|\varphi_n\|_2^2 = \|\eta_{R_n}\varphi_n\|_2^2 + \|\zeta_{R_n}\varphi_n\|_2^2 \leqslant \|\eta_{R_n}\varphi_n\|_2^2 + \int_{B_{8R_n}} |\varphi_n|^2 \overset{3.21}{\longrightarrow} 0,$$

and we reach a contradiction with its normalization. We conclude that $\ell = -1$ cannot happen.

Our next goal is to extract from μ_n one piece of mass $\widetilde{\mu}_n = \mu_n \mathbb{1}_{B_{R_n}(x_n)} \rightharpoonup \mu \neq 0$ tightly for a proper space translation $(x_n) \subset \mathbb{R}^3$, such that the corresponding eigenvalue $\lambda_1(D_0 - V_{\widetilde{\mu}_n})$ has the same limit ℓ as the original sequence μ_n. Then we will also obtain that $\lambda_1(D_0 - V_{\widetilde{\mu}_n}) \to \lambda_1(D_0 - V_\mu)$, using the following lemma.

Lemma 3.6 (Convergence in the tight case)**.** *Let $0 \leqslant \nu < \nu_1$. Let (μ_n) be a sequence of non-negative measures such that $\mu_n(\mathbb{R}^3) \leqslant \nu$ and which converges tightly to a measure μ. Then we have*

$$\lim_{n\to\infty} \lambda_1\left(D_0 - \mu_n * \frac{1}{|x|}\right) = \lambda_1\left(D_0 - \mu * \frac{1}{|x|}\right).$$

Proof. Since $\nu < \nu_1$, there exists $\eta > 0$ such that $\nu(1+\eta) < \nu_1$. We consider $V_n' := (1+\eta)\mu_n * |x|^{-1} = (1+\eta)V_n$ where $(1+\eta)\mu_n(\mathbb{R}^3) \leqslant (1+\eta)\nu < \nu_1$. The previous step implies that there exists $\varepsilon_0 > 0$ such that

$$\lambda_1(D_0 - (1+\eta)V_n) > -1 + \varepsilon_0$$

for n large enough. As seen in the beginning of the proof of Theorem 3.1, from the Birman-Schwinger principle in Theorem 2.3 it follows that λ is the first eigenvalue of $D_0 - V\mu$ iff 1 is the largest eigenvalue of K_λ. Then, since the eigenvalues are increasing with λ, we obtain

$$\begin{aligned}
&\max\sigma\left((1+\eta)\sqrt{V_n}\frac{1}{D_0+1-\varepsilon_0}\sqrt{V_n}\right)\\
&<\max\sigma\left((1+\eta)\sqrt{V_n}\frac{1}{D_0+\lambda_1\left(D_0-(1+\eta)V_n\right)}\sqrt{V_n}\right)=1\\
&\implies \max\sigma\left(\sqrt{V_n}\frac{1}{D_0+1-\varepsilon_0}\sqrt{V_n}\right)<\frac{1}{1+\eta}<1.
\end{aligned}$$

Therefore, we have the operator bound

$$K_n=\sqrt{V_n}\frac{1}{D_0+1-\varepsilon_0}\sqrt{V_n}<\frac{1}{1+\eta}. \tag{3.25}$$

Indeed, if there exists Ψ s.t. $\|\Psi\|_2=1$ and $(\Psi,K_n\Psi)>\max\sigma(K_n)$, then $\max\sigma(K_n)=\sup_{\|\Psi\|=1}(\Psi,K_n\Psi)>\max\sigma(K_n)$, which is absurd. By Lemma 3.5 we get the strong convergence $K_n\to K=\sqrt{V}\frac{1}{D_0+1-\varepsilon_0}\sqrt{V}$:

$$\begin{aligned}
&\left\|\left(\sqrt{V_n}\frac{1}{D_0+1-\varepsilon_0}\sqrt{V_n}-\sqrt{V}\frac{1}{D_0+1-\varepsilon_0}\sqrt{V}\right)\Psi\right\|_2^2\\
&\leqslant\left\|\left(\sqrt{V_n}\frac{1}{D_0+1-\varepsilon_0}-\sqrt{V}\frac{1}{D_0+1-\varepsilon_0}\right)\sqrt{V_n}\Psi\right\|^2\ (\xrightarrow{3.5}0)\\
&+\left\|\sqrt{V}\frac{1}{D_0+1-\varepsilon_0}(\sqrt{V_n}-\sqrt{V})\Psi\right\|_2^2\ (\longrightarrow 0\quad\text{by dominated convergence}).
\end{aligned}$$

The uniform upper bound implies from the functional calculus that

$$(1-K_n)^{-1}\to(1-K)^{-1}$$

strongly as well. In addition, Lemma 3.5 also provides the norm convergence of $\sqrt{V_n}\,(D_0+1-\varepsilon_0)^{-1}$. From the resolvent formula (2.6)

$$\begin{aligned}
\frac{1}{D_0-V-E}&=\frac{1}{D_0-E}\\
&\quad-\underbrace{\frac{1}{D_0-E}\sqrt{V_n}}_{A_n}\underbrace{\frac{1}{1-\sqrt{V_n}\frac{1}{D_0-E}\sqrt{V_n}}}_{B_n}\underbrace{\sqrt{V_n}\frac{1}{D_0-E}}_{C_n}
\end{aligned} \tag{3.26}$$

with $E=-1+\varepsilon_0$, we conclude that, if $A_nB_nC_n$ converges in norm to ABC (where A,B,C are the corresponding limits with V_μ in place of V_n), one has

$$(D_0-V_n+1-\varepsilon_0)^{-1}\to(D_0-V+1-\varepsilon_0)^{-1}$$

in norm as $n \to \infty$. Since A_n converges in norm to A, it is enough to prove that B_nC_n does the same to BC. C_n is compact by (2.7). Therefore for every $\varepsilon > 0$ there exists a finite rank operator T_ε s.t. $\|T_\varepsilon - C_n\| \leqslant \varepsilon$. We can also assume $\|T_\varepsilon - C\| \leqslant 2\varepsilon$ because C_n converges in norm to C. T_ε being a finite rank operator, we have $\|(B_n - B)T_\varepsilon\| \to 0$ as $n \to \infty$ since strong and norm convergences are equivalent in finite dimensional spaces. Finally, we get

$$\begin{aligned}\|B_nC_n - BC\| &\leqslant \|B_n(C_n - T_\varepsilon)\| + \|(B_n - B)T_\varepsilon\| + \|B(T_\varepsilon - C)\| \\ &\leqslant k\varepsilon + \|(B_n - B)T_\varepsilon\| + 2k\varepsilon \underset{n\to\infty}{\longrightarrow} 3k\varepsilon.\end{aligned}$$

Letting $\varepsilon \to 0$ we obtain the norm convergence of the resolvent, which implies the convergence of the spectrum (see [Ree12, Chapter 8]). In particular, the first eigenvalue $\lambda_1(D_0 - V_n)$ (which is known to be larger than $-1 + \varepsilon_0$ by the above arguments) converges to $\lambda_1(D_0 - \mu * |x|^{-1})$, as wanted. □

Step 3 - Extraction of a tight minimizing sequence

We go back to our initial minimizing sequence μ_n, for which we know that $-1 < \ell < 1$. We apply the same strategy as in Step 2 and extract finitely many weak limits of μ_n up to translations, so that the remainder can be written in the form $\mu_n' = \mu_n^{(1)} + \mu_n^{(2)}$, where $\mu_n^{(1)}$ vanishes in the sense of concentration-compactness and $\mu_n^{(2)}$ has an arbitrarily small mass. By an argument similar to the one in (3.24), we can prove that φ_n converges to 0 in L^2 on the support of μ_n'. Hence, it must have a non zero mass in one of the regions where μ_n converges tightly to a non-zero measure. We then show that the eigenvalue of this particular tight piece converges to ℓ.

For the sake of clarity, we write again the whole argument in the simplest situation where we only have one tight piece. Thus, we have like above that $\mu_n \mathbb{1}_{B_{R_n}} \rightharpoonup \mu$ tightly, whereas $\mu_n' := \mu_n \mathbb{1}_{\mathbb{R}^3 \setminus B_{R_n}} = \mu_n^{(1)} + \mu_n^{(2)}$ where $\mu_n^{(1)}$ vanishes and $\mu_n^{(2)}(\mathbb{R}^3 \setminus B_{R_n})$ is as small as we want. Then from (3.24) we know that $\eta_{R_n}\varphi_n \to 0$, which implies, since the sequence is normalized, that

$$\lim_{n\to\infty} \int_{\mathbb{R}^3} |\zeta_{R_n}\varphi_n|^2 = 1.$$

We have in addition

$$q_{\lambda_n}(\zeta_{R_n}\varphi_n) \leqslant \frac{C}{R_n} \leqslant \frac{C'}{R_n}\int_{\mathbb{R}^3} |\zeta_{R_n}\varphi_n|^2,$$

since the last integral converges to 1. On the support of ζ_{R_n} we have as before

$$V_n \leqslant V_{\mu_n \mathbb{1}_{B_{8R_n}}} + \frac{C}{R_n}.$$

Hence, we obtain

$$0 \geqslant \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla (\zeta_{R_n} \varphi_n)|^2}{1 + \lambda_n + (C + C')/R_n + V_{\mu_n \mathbb{1}_{B_{8R_n}}}} dx + \int_{\mathbb{R}^3} \left(1 - \lambda_n - \frac{C + C'}{R_n} - V_{\mu_n \mathbb{1}_{B_{8R_n}}}\right) |\zeta_{R_n} \varphi_n|^2 \, dx.$$

From the characterization of the first eigenvalue via the quadratic form, this proves that

$$\lambda_1 \left(D_0 - V_{\mu_n \mathbb{1}_{B_{8R_n}}}\right) \leqslant \lambda_n + \frac{C + C'}{R_n} = \lambda_1(D_0 - V_n) + \frac{C + C'}{R_n} \to \ell.$$

From Lemma 3.5, the tight convergence implies that the left-hand side converges to $\lambda_1 (D_0 - V_\mu)$. Therefore, we obtain after passing to the limit

$$\lambda_1 (D_0 - V_\mu) \leqslant \ell.$$

On the other hand, for every fixed $\varphi \in C_c^\infty (\mathbb{R}^3, \mathbb{C}^2)$ we have, as already seen, $q_{\lambda_n, \mu_n}(\varphi) \geqslant 0$ and using the strong local convergence of V_n from Lemma 3.5, we obtain $q_{\lambda_n, \mu_n}(\varphi) \to q_{\ell, \mu}(\varphi)$. So passing to the limit $q_{\ell, \mu}(\varphi) \geqslant 0$ and this precisely means that

$$\ell \leqslant \lambda_1 (D_0 - V_\mu).$$

Thus we have proved, as desired, that $\lim \lambda_1(D_0 - V_{\mu_n}) = \ell = \lambda_1 (D_0 - V_\mu)$ and this concludes the proof of Theorem 3.2. □

3.3 Existence of an optimal measure

The main result under study in this thesis is the following theorem concerning the existence of an optimal measure for the variational problem $\lambda_1(\nu)$ defined in (3.2) and all sub-critical coupling constant $0 \leqslant \nu < \nu_1$, with ν_1 as in (3.1).

Theorem 3.3 (Optimal measure)**.** *We have the following results:*

1. *The function $\nu \mapsto \lambda_1(\nu)$ is locally Lipschitz-continuous on $[0, \nu_1)$, decreasing and takes its values in $(-1, 1]$ with $\lambda_1(0) = 1$.*

2. *For any $\nu \in [0, \nu_1)$, there exists a positive measure μ_ν with $\mu_\nu (\mathbb{R}^3) = \nu$ such that*
$$\lambda_1 \left(D_0 - \mu_\nu * \frac{1}{|x|}\right) = \lambda_1(\nu).$$
More precisely, any minimizing sequence (μ_n) for $\lambda_1(\nu)$ is tight up to space translations and converges tightly to an optimal measure for $\lambda_1(\nu)$.

3. *Any such minimizer μ_ν concentrates on the compact set*

$$K := \left\{ x \in \mathbb{R}^3 : |\Psi_\nu|^2 * \frac{1}{|\cdot|}(x) = \max_{\mathbb{R}^3} \left(|\Psi_\nu|^2 * \frac{1}{|\cdot|} \right) \right\},$$

where Ψ_ν is any eigenfunction of $D_0 - V_{\mu_\nu}$ asscoiated to the eigenvalue $\lambda_1(\nu)$. The compact set K has a zero Lebesgue measure. In particular, μ_ν is singular with respect to the Lebesgue measure.

Proof. **Step 1 - Existence of an optimizer**

Let $(\mu_n)_{n\in\mathbb{N}}$ be any minimizing sequence of $\lambda_1(\nu)$, with $0 < \nu < \nu_1$ and $\mu_n(\mathbb{R}^3) = \nu$. From Theorem 3.2, we know that there exists a subsequence and space translations $(x_k) \subset \mathbb{R}^3$ such that $\mu_{n_k}(\cdot + x_k) \rightharpoonup^* \mu$ vaguely (hence $\mu(\mathbb{R}^3) \leqslant \nu$) and

$$\lambda_1(\nu) = \lim_{n\to\infty} \lambda_1(D_0 - V_{\mu_n}) = \lambda_1(D_0 - V_\mu).$$

The measure μ is the desired optimizer. To prove that the convergence is in fact tight, we have to show that $\mu(\mathbb{R}^3) = \nu$. The argument here relies on the strict monotonicity of the eigenvalue. First, for $\nu > 0$ we have

$$\lambda_1(\nu) \leqslant \lambda_1(D_0 - \nu/|x|) = \sqrt{1-\nu^2} < 1$$

from which we deduce that $\mu \neq 0$ (that is, the sequence μ_n cannot vanish). On the other hand, if $\mu(\mathbb{R}^3) < \nu$, we have

$$\lambda_1(\nu) = \lambda_1(D_0 - V_\mu) > \lambda_1\left(D_0 - \frac{\nu}{\mu(\mathbb{R}^3)} V_\mu\right) \geqslant \lambda_1(\nu),$$

and we reach a contradiction. Hence $\mu(\mathbb{R}^3) = \nu$ and the original sequence must be tight. In the previous inequality we have used that $t \mapsto \lambda_1(D_0 - tV_\mu)$ is decreasing for a fixed μ. This follows from the min-max principle and the characterization in terms of quadratic forms [DES00]. Indeed, if $\varphi_\nu \neq 0$ is an eigenfunction associated with $\lambda_1(D_0 - V_\mu)$, we have

$$\int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\varphi_\nu|^2}{1+\lambda_1(D_0 - V_\mu) + tV_\mu} dx + \int_{\mathbb{R}^3} (1 - \lambda_1(D_0 - V_\mu) - tV_\mu)\, |\varphi_\nu|^2\, dx$$
$$< q_{\lambda_1(D_0 - V_\mu)}(\varphi_\nu) = 0$$

for $t > 1$, since $V_\mu > 0$ everywhere. This implies that $\lambda_1(D_0 - tV_\mu) < \lambda_1(D_0 - V_\mu)$ for $t > 1$.

Step 2 - Properties of $\nu \mapsto \lambda_1(\nu)$

The function $\nu \mapsto \lambda_1(\nu)$ is obviously non-increasing for $\nu \in [0, \nu_1)$. Since there exists a minimizer μ for every ν it is actually decreasing: if $\lambda_1(\nu_1) = \lambda_1(\nu_2)$ for $\nu_1 < \nu_2$, let μ_1, μ_2 be optimal measures respectively for $\lambda_1(\nu_1), \lambda_1(\nu_2)$, then again we have the following contradiction

$$\lambda_1(\nu_1) = \lambda_1(D_0 - V_{\mu_2}) > \lambda_1 \left(D_0 - \frac{\nu_1}{\mu_2 (\mathbb{R}^3)} V_{\mu_2} \right) \geqslant \lambda_1(\nu_1).$$

Hence it is continuous except possibly on a countable set.

To prove the continuity, consider a sequence $\nu_n \to \nu \in (0, \nu_1)$ together with an associated sequence of optimizers μ_n such that $\lambda_1 (D_0 - V_{\mu_n}) = \lambda_1 (\nu_n)$. From Theorem 3.1 we know that we can assume $\mu_n \rightharpoonup^* \mu \neq 0$ vaguely after an appropriate translation and extraction of a subsequence, so that

$$\liminf_{n\to\infty} \lambda_1 (D_0 - V_{\mu_n}) = \lim_{n\to\infty} \lambda_1 (D_0 - V_{\mu_n}) = \lambda_1 (D_0 - V_\mu) \geqslant \lambda_1(\nu),$$

because $\mu(\mathbb{R}^3) \leqslant \liminf \mu_n(\mathbb{R}^3) = \lim \nu_n = \nu$. Let now μ be an optimizer for $\lambda_1(\nu)$, then

$$\limsup_{n\to\infty} \lambda_1 (\nu_n) \leqslant \lim_{n\to\infty} \lambda_1 \left(D_0 - \frac{\nu_n}{\nu} V_\mu \right) = \lambda_1 (D_0 - V_\mu) = \lambda_1(\nu),$$

since the map $t \mapsto \lambda_1 (D_0 - tV_\mu)$ is continuous for a fixed μ. This concludes the proof of the continuity of $\nu \mapsto \lambda_1(\nu)$.

Finally, we discuss the regularity of $\nu \mapsto \lambda_1(\nu)$. It is well known that for every fixed μ, the function $t \mapsto \lambda_1 (D_0 - tV_\mu)$ is locally Lipschitz in $[0, \nu_1/\mu (\mathbb{R}^3))$ [Kat13]. This follows from the resolvent formula

$$\begin{aligned} &\frac{1}{D_0 - tV_\mu + 1 - \varepsilon_0} - \frac{1}{D_0 - t'V_\mu + 1 - \varepsilon_0} \\ &\qquad = (t - t') \frac{1}{D_0 - tV_\mu + 1 - \varepsilon_0} V_\mu \frac{1}{D_0 - t'V_\mu + 1 - \varepsilon_0}, \end{aligned}$$

which implies by Kato's inequality

$$\begin{aligned} &\left\| \frac{1}{D_0 - tV_\mu + 1 - \varepsilon_0} - \frac{1}{D_0 - t'V_\mu + 1 - \varepsilon_0} \right\| \\ &\leqslant C \left|t - t'\right| \left\| \frac{1}{D_0 - tV_\mu + 1 - \varepsilon_0} \left|D_0\right|^{\frac{1}{2}} \right\| \left\| \left|D_0\right|^{\frac{1}{2}} \frac{1}{D_0 - t'V_\mu + 1 - \varepsilon_0} \right\|. \end{aligned}$$

Here $\varepsilon_0 := \lambda_1 (\nu_1 - \eta) + 1 > 0$ where $\eta > 0$ is chosen so that $t, t' < (\nu_1 - 2\eta) / \mu (\mathbb{R}^3)$. The two norms can be estimated uniformly in μ using the resolvent formula (3.26) and the fact that (as in (3.25))

$$\sqrt{V_\mu} \frac{1}{D_0 + 1 - \varepsilon_0} \sqrt{V_\mu} \leqslant \frac{\mu(\mathbb{R}^3)}{\nu_1 - \eta}.$$

To see that the Lipschitz property at fixed μ implies a similar property for $\lambda_1(\nu)$, we remark that for $0 \leqslant \nu < \nu^{'} \leqslant \nu_1 - \varepsilon$

$$\lambda_1(\nu) \leqslant \lambda_1 \left(D_0 - \frac{\nu}{\nu_1 - \varepsilon} V_{\frac{\nu_1-\varepsilon}{\nu'}\mu'} \right) \leqslant \lambda_1 \left(D_0 - \frac{\nu'}{\nu_1 - \varepsilon} V_{\frac{\nu_1-\varepsilon}{\nu'}\mu'} \right) + C(\nu^{'} - \nu)$$
$$= \lambda_1(\nu') + C(\nu^{'} - \nu),$$

where $\mu^{'}$ is a minimizer for $\lambda_1(\nu^{'})$ with $\mu'(\mathbb{R}^3) = \nu'$. This is because $t \mapsto \lambda_1 (D_0 - tV_\mu)$ is locally Lipschitz in $[0, \nu_1/\mu(\mathbb{R}^3))$ and $\frac{\nu}{\nu_1-\varepsilon}, \frac{\nu'}{\nu_1-\varepsilon} \in [0,1]$, which is a compact set of $[0, \frac{\nu_1}{\frac{\nu_1-\varepsilon}{\nu'}\mu'(\mathbb{R}^3)}) = [0, \frac{\nu_1}{\nu_1-\varepsilon})$.

Step 3 - Euler-Lagrange equation

Let μ be a minimizer for $\lambda_1(\nu)$ and let $\Psi = (\varphi, \chi)$ be any corresponding eigenfunction. Recall that φ solves (3.16) and that

$$\chi = \frac{-i\sigma \cdot \nabla\varphi}{1 + \lambda_1(\nu) + V_\mu}.$$

Let μ' be any other probability measure and $\mu_t := (1-t)\mu + t\mu'$, for $t \in [0,1]$. Then we have $\lambda_1 (D_0 - V_{\mu_t}) \geqslant \lambda_1 (D_0 - V_\mu) = \lambda_1(\nu)$ and this implies that $q_{\lambda_1,\mu_t}(\varphi) \geqslant 0$ for all $t \in [0,1]$, and in $t = 0$ it equals 0. Then we have

$$\begin{aligned} 0 \leqslant \frac{d}{dt} q_{\lambda_1,\mu_t}(\varphi)\Big|_{t=0} &= \int_{\mathbb{R}^3} \frac{|\sigma\cdot\nabla\varphi|^2 (V_\mu - V_{\mu'})}{(1+\lambda_1(\nu) + (1-t)V_\mu + tV_{\mu'})^2} + (V_\mu - V_{\mu'})|\varphi|^2 \Big|_{t=0} \\ &= \int_{\mathbb{R}^3} \left(\frac{|\sigma\cdot\nabla\varphi|^2}{(1+\lambda_1(\nu)+V_\mu)^2} + |\varphi|^2 \right) (V_\mu - V_{\mu'}) \\ &= \int_{\mathbb{R}^3} |\Psi|^2 (V_\mu - V_{\mu'}) = \int_{\mathbb{R}^3} \left(|\Psi|^2 * \frac{1}{|\cdot|} \right) d(\mu - \mu')(x), \end{aligned}$$

where $|\Psi|^2 = |\varphi|^2 + |\chi|^2$. In other words, μ solves the maximization problem

$$\sup_{\substack{\mu' \geq 0 \\ \mu'(\mathbb{R}^3)=1}} \int_{\mathbb{R}^3} \left(|\Psi|^2 * \frac{1}{|\cdot|} \right)(x) d\mu'(x).$$

Since $\Psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ by Theorem 2.1, and $H^{1/2} \subset L^{3,2}$, where $L^{3,2}$ is the usual Lorentz space [Tar98, Appendix IV], we have $|\Psi|^2 \in L^{3/2,1} = (L^{3,\infty})^*$. But $|x|^{-1} \in L^{3,\infty}$ and therefore the potential $|\Psi|^2 * |x|^{-1}$, being the convolution of two functions in dual spaces, is actually a continuous function tending to zero at infinity. The solutions to the maximization problem are exactly the measures supported on the compact set where this function attains its maximum. In particular, μ concentrates on the compact set

$$K := \operatorname{argmax}\left(|\Psi|^2 * \frac{1}{|x|}\right).$$

Step 4 - K has zero measure

The final step is to prove that K has zero Lebesgue measure. Assume by contraddiction that $|K| > 0$ and denote by

$$\Omega := \mathbb{R}^3 \setminus \{R_1, \ldots, R_K\}$$

the set obtained after removing the largest singularities of μ, for instance all the points such that $\mu(\{R_j\}) \geqslant \min(1/4, \varepsilon_0/4)$ where ε_0 is the universal constant from ([ELS21b], Theorem 14). Then $|K \cap \Omega| > 0$ as well. Let us denote by

$$U := \max_{\mathbb{R}^3}\left(|\Psi|^2 * \frac{1}{|x|}\right) - |\Psi|^2 * \frac{1}{|x|} \geqslant 0$$

the shifted potential which satisfies $U \equiv 0$ on K as well as the equation $\Delta U = 4\pi|\Psi|^2 \geqslant 0$ on $\mathbb{R}^3$. Consider a point of full measure $x_0 \in \Omega \cap K$, that is, such that

$$\lim_{r \to 0} \frac{|B_r(x_0) \setminus K|}{|B_r(x_0)|} = 0.$$

Without loss of generality we may assume that $x_0 = 0$. Let $\chi \in C_c^\infty(B_2)$ be such that $\chi_{|B_1} \equiv 1$ and set $\chi_r(x) := \chi(x/r)$. Then we have

$$\begin{aligned} -\chi_r U \Delta(\chi_r U) &= -\chi_r U(\chi_r \Delta U + 2\nabla\chi_r \cdot \nabla\chi U + U\Delta\chi_r) \\ &= -4\pi\chi_r^2 U|\Psi|^2 - \chi_r U^2 \Delta\chi_r - \frac{1}{2}\nabla\chi_r^2 \cdot \nabla U^2. \end{aligned}$$

The first term in the right-hand side is non-positive since $U \geqslant 0$. Integrating and using that $\frac{1}{2}\Delta\chi_r^2 = \chi_r\Delta\chi_r + |\nabla\chi_r|^2$ we obtain

$$\int_{\mathbb{R}^3} |\nabla(\chi_r U)|^2 \leqslant -\int_{\mathbb{R}^3} \chi_r U^2 \Delta\chi_r + \frac{1}{2}\int_{\mathbb{R}^3} U^2 \Delta\chi_r^2 = \int_{\mathbb{R}^3} U^2 |\nabla\chi_r|^2 \leqslant \frac{C}{r^2}\int_{\mathbb{R}^3} U^2$$

and therefore

$$\begin{aligned} \int_{B_r}\left(\frac{U^2}{r^2} + |\nabla U|^2\right) &\leqslant \int_{\mathbb{R}^3}\left(\frac{\chi_r^2 U^2}{r^2} + |\nabla(\chi_r U)|^2\right) \\ &\leqslant \frac{C}{r^2}\int_{B_{2r}} U^2 = \frac{C}{r^2}\int_{B_{2r}\setminus K} U^2, \end{aligned}$$

since $U \equiv 0$ on K by definition. Next, we use the Sobolev inequality ([AF03], Theorem 4.12) in the ball B_{2r}: $\|U\|^2_{L^6(B_{2r})} \leqslant C\|U\|^2_{W^{1,2}(B_{2r})}$. Applying it to the scaled $U(r\cdot)$ we get also

$$\|U\|^2_{L^6(B_{2r})} \leqslant C \int_{B_{2r}} \left(\frac{U^2}{r^2} + |\nabla U|^2\right).$$

Therefore, by Hölder's inequality we obtain

$$\frac{C}{r^2}\int_{B_{2r}\setminus K} U^2 \leqslant \frac{C\,|B_{2r}\setminus K|^{\frac{2}{3}}}{r^2}\|U\|^2_{L^6(B_{2r})} \leqslant \frac{C\,|B_{2r}\setminus K|^{\frac{2}{3}}}{r^2}\int_{B_{2r}} \left(\frac{U^2}{r^2} + |\nabla U|^2\right).$$

Hence, in summary, we have proved that

$$\int_{B_r} \left(\frac{U^2}{r^2} + |\nabla U|^2\right) \leqslant C\left(\frac{|B_{2r}\setminus K|}{|B_r|}\right)^{\frac{2}{3}} \int_{B_{2r}} \left(\frac{U^2}{r^2} + |\nabla U|^2\right)$$

for a universal constant C. By arguing like in ([DFG92], Section 3) this proves that the integrand has a zero of infinite order, i.e.

$$\lim_{r\to 0^+} r^{-\alpha}\int_{B_r} \left(\frac{U^2}{r^2} + |\nabla U|^2\right) = 0 \quad \forall \alpha > 0, \tag{3.27}$$

that is, U and ∇U vanish to all orders at $x_0 = 0$.

Next, we prove that Ψ also vanishes to all orders at the same point. We use Green's formula in the form

$$4\pi\int_{B_r} |\Psi|^2 = \int_{B_r} \Delta U = -\int_{S_r} \nabla U \cdot n,$$

where n is the outward normal to the sphere S_r of radius r. After passing to spherical coordinates we see that

$$-4\pi\int_{B_s} |\Psi|^2 = \int_{S_s} \nabla U \cdot n = s^2\frac{d}{dr}\left(\frac{1}{r^2}\int_{S_r} U\right)\bigg|_{r=s}.$$

Therefore, after integrating over s between r and $2r$, we obtain

$$\frac{1}{r^2}\int_{S_r} U - \frac{1}{4r^2}\int_{S_{2r}} U = 4\pi\int_r^{2r}\int_{B_s} |\Psi|^2\frac{ds}{s^2} \geqslant \frac{\pi}{r}\int_{B_r} |\Psi|^2,$$

because $1/s^2 \geqslant 1/4r^2$ and $\int_{B_s} |\Psi|^2 \geqslant \int_{B_r} |\Psi|^2$ for $r \leqslant s \leqslant 2r$. Since $U \geqslant 0$ we have shown the inequality

$$\pi\int_{B_r} |\Psi|^2 \leqslant \frac{1}{r}\int_{S_r} U.$$

From the continuity of boundary traces ($\|U\|_{L^2(\partial B_r)} \leqslant C\|U\|_{W^{1,2}(B_r)}$) and a scaling like above we have

$$\int_{S_r} U \leqslant |S_r|^{1/2} \left(\int_{S_r} U^2 \right)^{1/2} \leqslant Cr \int_{B_r} \left(\frac{U^2}{r^2} + |\nabla U|^2 \right).$$

We finally get

$$\int_{B_r} |\Psi|^2 \leqslant C \int_{B_r} \left(\frac{U^2}{r^2} + |\nabla U|^2 \right),$$

which vanishes to all orders, as we have shown in (3.27), that is Ψ also vanishes to all orders at the same point. This is impossible by ([ELS21b], Corollary 15). Hence we must have $|K| = 0$ and this concludes the proof of Theorem. $\square$

Appendix A

In this appendix I include some of the theorems I did not prove during the thesis in order not to disrupt the thread of speech, to allow for a more smooth reading.

Theorem A.1 (Kato's inequality)**.** *For all $f \in \{u : |\cdot|^{1/2}\widehat{u} \in L^2(\mathbb{R}^3)\}$,*

$$\int_{\mathbb{R}^3} |x|^{-1}|f(x)|^2 dx \leqslant \frac{\pi}{2}\int_{\mathbb{R}^3} |p||\widehat{f}(p)|^2 dp, \quad i.e \quad \frac{1}{|x|} \leqslant \frac{\pi}{2}|p|.$$

The constant $\pi/2$ is sharp.

Proof. We will prove the statement for a generic constant C in place of $\pi/2$, for the sharp case see ([BE11], Theorem 2.2.4). By Paserval's formula one has

$$\begin{aligned}
\int_{\mathbb{R}^3} \frac{|f(x)|^2}{|x|} dx &= \int_{\mathbb{R}^3} \mathcal{F}\left(\frac{f(x)}{|x|}\right)(p) \cdot \overline{\mathcal{F}(f(x))}(p) dp \\
&= \int_{\mathbb{R}^3} \left(\mathcal{F}\left(f(x)\right) * \mathcal{F}(|x|^{-1})\right)(p) \cdot \overline{\mathcal{F}(f(x))}(p) dp \\
&= C\int_{\mathbb{R}^3} \left(\mathcal{F}\left(f(x)\right) * |\cdot|^{-2})\right)(p) \cdot \overline{\mathcal{F}(f(x))}(p) dp \\
&= C\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\mathcal{F}(f)(q) \cdot \overline{\mathcal{F}(f)}(p)}{|p-q|^2} dq dp \\
&= C\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\mathcal{F}(f)(q)\frac{|q|}{|p|} \cdot \overline{\mathcal{F}(f)}(p)\frac{|p|}{|q|}}{|p-q|^2} dq dp \\
&\overset{C-S}{\leqslant} C\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|\mathcal{F}(f)(p)|^2\frac{|p|^2}{|q|^2}}{|p-q|^2} dq dp \\
&= C\int_{\mathbb{R}^3} |\mathcal{F}(f)(p)|^2|p|^2 \left(\int_{\mathbb{R}^3} \frac{dq}{|q|^2|p-q|^2}\right) dp.
\end{aligned}$$

The function $p \mapsto \int_{\mathbb{R}^3} \frac{dq}{|q|^2|p-q|^2}$ has been computed in ([LL01], Section 5.10) and it is equal to $C|p|^{-1}$ so we finally get, as desired,

$$\int_{\mathbb{R}^3} \frac{|f(x)|^2}{|x|} dx \leqslant C \int_{\mathbb{R}^3} |p| |\mathcal{F}(f)(p)|^2 dp.$$

$\square$

Theorem A.2. *From Kato's inequality,*

$$\frac{1}{|x|} \leqslant \frac{\pi}{2}|p|,$$

it follows that, for every $\mu \geqslant 0$ positive finite Radon measure, one has

$$\mu * \frac{1}{|\cdot|} \leqslant \frac{\pi}{2}\mu(\mathbb{R}^3)|p|, \quad \textit{or equivalently that } \frac{1}{|p|} \leqslant \frac{\pi}{2}\mu(\mathbb{R}^3)\frac{1}{V_\mu}.$$

Proof. Kato's inequality implies that

$$\int \frac{|\varphi|^2}{|x|} \leqslant \frac{\pi}{2} \int \overline{\varphi} \cdot |p| \varphi = \frac{\pi}{2} \int \left| |p|^{\frac{1}{2}} \varphi \right|^2 \qquad \text{for every } \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^4).$$

Hence for every $x \in \mathbb{R}^3$ we have

$$\begin{aligned}\int \frac{|\varphi(y)|^2}{|x-y|} dy &= \int \frac{|\varphi(z+x)|^2}{|z|} dz \leqslant \frac{\pi}{2} \int \left| |p|^{\frac{1}{2}} \varphi(z+x) \right|^2 dz \\ &= \frac{\pi}{2} \int \left| |p|^{\frac{1}{2}} \mathcal{F}(\varphi(\cdot + x))(p) \right|^2 dp = \frac{\pi}{2} \int \left| |p|^{\frac{1}{2}} e^{-ip\cdot x} \mathcal{F}(\varphi)(p) \right|^2 dp \\ &= \frac{\pi}{2} \int \left| |p|^{\frac{1}{2}} \mathcal{F}(\varphi)(p) \right|^2 dp = \frac{\pi}{2} \int \left| |p|^{\frac{1}{2}} \varphi \right|^2.\end{aligned}$$

Then, integrating on x and using that μ is a positive measure we get

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\varphi(y)|^2}{|x-y|} dy d\mu(x) \leqslant \left\| |\varphi|^2 * \frac{1}{|\cdot|} \right\|_\infty \mu(\mathbb{R}^3) \leqslant \frac{\pi}{2}\mu(\mathbb{R}^3) \int \left| |p|^{\frac{1}{2}} \varphi \right|^2$$

$\forall \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^4)$, which means that

$$\mu * \frac{1}{|\cdot|} \leqslant \frac{\pi}{2}\mu(\mathbb{R}^3)|p|, \text{ or equivalently that } \frac{1}{|p|} \leqslant \frac{\pi}{2}\mu(\mathbb{R}^3)\frac{1}{V_\mu}. \tag{A.1}$$

$\square$

Theorem A.3. *Let $\mu \geqslant 0$ be a finite positive Borel measure, then, using $|x|^{-2} \leqslant 4(D_0)^2$, one has*

$$\|V_\mu \varphi\|_2 \leqslant 2\mu(\mathbb{R}^3)\|D_0\varphi\|_2.$$

Proof. Using the very same argument as in Theorem A.2, by $|x|^{-2} \leqslant 4(D_0)^2$ one gets

$$\int\int \frac{|\varphi(y)|^2}{|x-y|^2} dy d\mu(x) \leqslant 4\mu(\mathbb{R}^3) \int |D_0\varphi|^2.$$

But, using that $\|\cdot\|_{L^1(\mathbb{R}^3,d\mu)} \leqslant \sqrt{\mu(\mathbb{R}^3)}\|\cdot\|_{L^2(\mathbb{R}^3,d\mu)}$, we have

$$\int V_\mu^2(y)|\varphi(y)|^2 dy = \int \left(\int \frac{d\mu(x)}{|x-y|} \right)^2 |\varphi(y)|^2 dy$$
$$\leqslant \mu(\mathbb{R}^3) \int \left(\int \frac{d\mu(x)}{|x-y|^2} \right) |\varphi(y)|^2 dy \leqslant 4\mu(\mathbb{R}^3)^2 \int |D_0\varphi|^2.$$

□

Theorem A.4. *Let A, B be bounded operators. Then we have the following*

- *if A is positive then $\|A^{1/2}\| = \|A\|^{1/2}$;*
- $\|A\| = \||A|\|$;
- *If A, B are positive and commute, then $(AB)^{1/2} = A^{1/2}B^{1/2}$;*
- *if A, B are self-adjoint and commute, then $|AB| = |A||B|$;*
- *if $A^*A = AA^*$ (in particular if A is self-adjoint), then we have $|A|^{-1} = |A^{-1}|$.*

Proof.
- Recall that $\|A^*A\| = \|AA^*\| = \|A\|^2$. Since the positive square root $A^{1/2}$ is self-adjoint, it follows that

$$\|A\| = \|A^{1/2}A^{1/2}\| = \|A^{1/2}(A^{1/2})^*\| = \|A^{1/2}\|^2.$$

- $\||A|\| = \|(A^*A)^{1/2}\| = \|A^*A\|^{1/2} = \|A\|$.
- By uniqueness of square roots for positive operators, it is enough to prove that $(A^{1/2}B^{1/2})^2 = AB$. Since A, B commute, also their square roots and $(A^{1/2}B^{1/2})^2 = A^{1/2}B^{1/2}A^{1/2}B^{1/2} = A^{1/2}A^{1/2}B^{1/2}B^{1/2} = AB$.
- If A, B commute, then also the squares, and hence we have

$$|AB| = (BAAB)^{1/2} = (A^2B^2)^{1/2} = (A^2)^{1/2}(B^2)^{1/2} = |A||B|.$$

- Finally, if $A^*A = AA^*$ one has

$$|A^{-1}||A| = \sqrt{(A^{-1})^*A^{-1}}\sqrt{A^*A}$$
$$\underset{(A^{-1})^*=(A^*)^{-1}}{=} \sqrt{(AA^*)^{-1}(A^*A)} = \sqrt{(A^*A)^{-1}(A^*A)} = \mathbb{1},$$

where in the second equality we have used also the third point.

□

Theorem A.5. *Let B be a bounded operator, A_s a sequence of operators such that $A_s \to 0$ strongly with $\|A_s\| \leqslant C$ uniformly in s and K a compact operator. Then one has $\|BA_sK\| \underset{s\to\infty}{\to} 0$.*

Proof. Since K is compact, there exists a sequence of finite rank operators $(K_n)_{n\in\mathbb{N}}$ s.t. $\|K - K_n\| \underset{n\to\infty}{\longrightarrow} 0$ and the K_n's are given by

$$K_n\varphi = \sum_{j=1}^{n} \lambda_n \varphi_n(\varphi, \varphi_n),$$

where $(\varphi_n)_{n\in\mathbb{N}}$ is a complete eigenbasis of L^2 given by K and $(\lambda_n)_{n\in\mathbb{N}}$ the associated eigenvalues. Then, one has

$$\begin{aligned}
\|BA_sK_n\varphi\|_2 \leqslant \|B\|\|A_sK_n\varphi\|_2 &= \|B\| \left\| \sum_{j=1}^{n} \lambda_n A_s\varphi_n(\varphi, \varphi_n) \right\|_2 \\
&\leqslant \|B\| \left(\sum_{j=1}^{n} |\lambda_n|\|\varphi_n\|_2\|A_s\varphi_n\|_2 \right) \|\varphi\|_2 \\
\Rightarrow \|BA_sK_n\| \leqslant \|B\| &\left(\sum_{j=1}^{n} |\lambda_n|\|\varphi_n\|_2\|A_s\varphi_n\|_2 \right) \underset{s\to\infty}{\longrightarrow} 0,
\end{aligned}$$

because the sum is finite and $A_s \to 0$ implies $\Rightarrow \|A_s\varphi_n\|_2 \to 0$ for every n. Finally, for every $n \in \mathbb{N}$

$$\|BA_sK\| \leqslant \|BA_s(K - K_n)\| + \|BA_sK_n\| \leqslant C\|B\|\|K - K_n\| + \|BA_sK_n\|,$$

so, letting first $s \to \infty$ and then $n \to \infty$, we get the claim. □

A.1 Finite measure Theory

Now, I recall some definitions and results about finite (positive) measure since they are extensively used during the thesis. One can find all the results in [Wil95, Cas].

Definition (Finite measure space)**.** Let $\Omega \subset \mathbb{R}^n$ be an open set. (We will use $\Omega = \mathbb{R}^3$). The space of finite measure on Ω, denoted $\mathcal{M}(\Omega)$, is the space of continuous linear maps on $C_0(\Omega) = \{f : \Omega \to \mathbb{C} : f$ continuous and tending to 0 at $\infty\}$. $\mathcal{M}(\Omega)$ is equipped with the norm

$$\|\mu\| := \sup_{u\in C_0(\Omega)\setminus\{0\}} \frac{|(\mu, u)|}{\|u\|_\infty} = \sup_{u\in C_0(\Omega)\setminus\{0\}} \frac{|\int_\Omega u d\mu|}{\|u\|_\infty}.$$

The set of positive finite measure is denoted $\mathcal{M}^+(\Omega)$.

Note that if $\mu \in \mathcal{M}^+(\Omega)$, then $\|\mu\| = (\mu, 1) = \mu(\Omega)$.

Definition (Vague convergence)**.** Let $(\mu_n)_{n\in\mathbb{N}}$ and μ be measures in $\mathcal{M}^+(\Omega)$, we say that μ_n converges vaguely or weakly*, $\mu_n \rightharpoonup^* \mu$ if

$$\lim_{n\to\infty} \int_\Omega u d\mu_n = \int_\Omega u d\mu \quad \forall u \in C_0(\Omega).$$

Note that if $\mu_n \rightharpoonup^* \mu$ vaguely, then it is not true that $\mu_n(A) \to \mu(A)$ for every $A \subset \Omega$. It holds for A bounded, but in general we have only $\mu(A) \leqslant \liminf_n \mu_n(A)$. Moreover, by uniform boundedness principle, if a sequence μ_n converges vaguely then there is a uniform bound on $\mu_n(\Omega)$.

Definition (Tight convergence)**.** Let $(\mu_n)_{n\in\mathbb{N}}$ and μ be measures in $\mathcal{M}^+(\Omega)$, we say that μ_n converges tightly, $\mu_n \rightharpoonup \mu$ if

$$\lim_{n\to\infty} \int_\Omega u d\mu_n = \int_\Omega u d\mu \quad \forall u \in C_b(\Omega),$$

where $C_b(\Omega)$ is the set of continuous bounded functions on Ω.

The name *tight* is not classical, it comes from a translation from French. Often in literature it is called Narrow convergence or (by abuse of notation) weakly convergence.

Clearly tight convercence is stronger than vague convergence and they coincide only if Ω is bounded. Unlike the vague case, for tight convergence we have $\mu_n(A) \to \mu(A)$ for every $A \subset \Omega$. We have the following characterization.

Theorem A.6. *Let $(\mu_n)_{n\in\mathbb{N}}$ and μ be measures in $\mathcal{M}^+(\Omega)$, then the followings are equivalent:*

1. *$\mu_n \rightharpoonup \mu$ tightly;*
2. *$\mu_n \rightharpoonup^* \mu$ vaguely and $\|\mu_n\| = \mu_n(\Omega) \to \|\mu\| = \mu(\Omega)$.*

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