STABILITY OF ONE-ELECTRON MOLECULES IN THE BROWN-RAVENHALL MODEL

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ABSTRACT. In appropriate units, the Brown-Ravenhall Hamiltonian for a system of 1 electron relativistic molecules with K fixed nuclei having charge and position $Z_k, R_k,\ k = 1, 2, \dots, K$, is of the form $\mathbf{B}_{1,K} = \Lambda_+(D_0 + \alpha V_c)\Lambda_+$, where Λ_+ is the projection onto the positive spectral subspace of the free Dirac operator D_0 and $V_c = -\sum_{k=1}^{K} \frac{\alpha Z_k}{|\mathbf{x}-R_k|} + \sum_{k<l,\ k,l=1}^{K} \frac{\alpha Z_k Z_l}{|R_k - R_l|}$, with α Sommerfeld's fine structure constant. It is proved that for $\alpha Z_k \le \alpha Z_c = \frac{2}{\pi/2 + 2/\pi}$, $k = 1, 2, \dots, K$, $\mathbf{B}_{1,K} \ge \text{const}\cdot K$.

1. INTRODUCTION

In [4] I. Daubechies and E. Lieb investigated the "stability of matter" problem for a system of one-electron relativistic molecules with static K nuclei modelled by the Hamiltonian

$$\mathbf{H}_{1,K}(\underline{Z},\ \underline{R}) = \left(-\hbar^2 c^2 \Delta + m^2 c^4\right)^{\frac{1}{2}} - \sum_{k=1}^{K} \frac{e^2 Z_k}{|\mathbf{x} - R_k|} + \sum_{k<l,\ k,l=1}^{K} \frac{e^2 Z_k Z_l}{|R_k - R_l|}. \tag{1.1}$$

Here $2\pi\hbar$ is Planck's constant, c the velocity of light, m the electron mass, $-e$ the electron charge, Z_k,R_k the charge and position respectively of the kth nucleus, and we have written $\underline{Z} = (Z_1, \dots, Z_k)$, $\underline{R} = (R_1, \dots, R_k)$. They prove that if $\alpha Z_k \le 2/\pi$, where $\alpha = e^2/(\hbar c)$ is Sommerfeld's fine structure constant which is about $1/137.037$, then the system has stability of the second kind, that is for some constant C, the natural operator defined by (1.1) satisfies

$$\mathbf{H}_{1,K}(\underline{Z},\ \underline{R}) \ge CK. \tag{1.2}$$

The subject of this paper is to investigate the analogous problem for the Brown-Ravenhall Hamiltonian

$$\mathbf{B}_{1,K}(\underline{Z},\ \underline{R}) = \Lambda_+\left(D_0 - \sum_{k=1}^{K} \frac{e^2 Z_k}{|\mathbf{x} - R_k|} + \sum_{k<l,\ k,l=1}^{K} \frac{e^2 Z_k Z_l}{|R_k - R_l|}\right)\Lambda_+. \tag{1.3}$$

In (1.3), the notation is as follows (see [5]):

- D_0 is the free Dirac operator

$$D_0 = c\boldsymbol{\alpha}\cdot \frac{\hbar}{i}\,\nabla + mc^2\beta \equiv \sum_{j=1}^{3} c\frac{\hbar}{i}\alpha_j \frac{\partial}{\partial x_j} + mc^2\beta,$$

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where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are the Dirac matrices given by

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1_2 & 0_2 \\ 0_2 & -1_2 \end{pmatrix}$$

with $\mathbf{0_2}, \mathbf{1_2}$ the zero and unit 2×2 matrices respectively and σ_j the Pauli matrices

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

- Λ_+ denotes the projection of $\mathrm{L}^2(\mathbb{R}^3) \otimes \mathbb{C}^4$ onto the positive spectral subspace of D_0, that is $\chi_{(0,\infty)}(D_0)$, where $\chi_{(0,\infty)}$ is the characteristic function of $(0, \infty)$. If we set

$$\widehat{f}(\mathbf{p}) \equiv \mathcal{F}(f)(\mathbf{p}) = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int_{\mathbb{R}^3} e^{-i\ \mathbf{x}\cdot\mathbf{p}/\hbar} f(\mathbf{x})\, \mathrm{d}\,\mathbf{x}, \tag{1.4}$$

for the Fourier transform of f, then it follows that

$$(\Lambda_+ f)^\wedge(\mathbf{p}) = \Lambda_+(\mathbf{p})\widehat{f}(\mathbf{p}),$$

where

$$\Lambda_+(\mathbf{p}) = \frac{1}{2} + \frac{c\boldsymbol{\alpha}\cdot\mathbf{p} + mc^2\beta}{2\mathbf{e}(p)}, \quad \mathbf{e}(p) = \sqrt{c^2p^2 + m^2c^4} \tag{1.5}$$

with $p = |\mathbf{p}|$.

The underlying Hilbert space in which $\mathbf{B}_{1,K}(\underline{Z},\ \underline{R})$ acts is

$$\mathcal{H}_+ = \Lambda_+(\mathrm{L}^2(\mathbb{R}^3) \otimes \mathbb{C}^4). \tag{1.6}$$

As usual we use the same notations for the formal Hamiltonians (1.1) and (1.3) and the self-adjoint operators defined as Friedrichs extensions when the associated quadratic forms are bounded below. The form domain of $\mathbf{B}_{1,K}(\underline{Z},\ \underline{R})$ is $Q_4(|\mathbf{p}|) = H^{1/2}(\mathbb{R}^3)) \otimes \mathbb{C}^4$.

To simplify notation, we follow [4] and rescale in the units of the Compton wave-length of the electron, namely $\hbar/(mc)$: replacing $x,\ R_k$ by $(mc/\hbar)x,\ \ (mc/\hbar)R_k$ respectively, and $\mathbf{B}_{1,K}$ by $(mc^2)^{-1}\mathbf{B}_{1,K}$, we obtain

$$\mathbf{B}_{1,K}(\underline{Z},\ \underline{R}) = \Lambda_+\left(D_0 - \sum_{k=1}^{K} \frac{\alpha Z_k}{|\mathbf{x} - R_k|} + \sum_{k<l,\ k,l=1}^{K} \frac{\alpha Z_k Z_l}{|R_k - R_l|}\right)\Lambda_+, \tag{1.7}$$

where now

$$D_0 = \frac{1}{i}\boldsymbol{\alpha}\cdot\nabla + \beta, \quad \Lambda_+(\mathbf{p}) = \frac{1}{2} + \frac{\boldsymbol{\alpha}\cdot\mathbf{p} + \beta}{2\mathbf{e}(p)}, \ \mathbf{e}(p) = \sqrt{p^2 + 1}. \tag{1.8}$$

We shall put $\hbar = 1$ in the Fourier transform $\mathcal{F}$ in (1.4) hereafter.

The case $K = 1$ of this operator (with nucleus at the origin),

$$\mathbf{B}_{1,1}(Z) = \Lambda_+\left(\frac{1}{i}\boldsymbol{\alpha}\cdot\nabla + \beta - \frac{\alpha Z}{|\mathbf{x}|}\right)\Lambda_+, \tag{1.9}$$

was the object of study in [1], [3], [5], [9], [15], [16]. In [5] it was shown that $\mathbf{B}_{1,1}(Z)$ is bounded below in $\mathcal{H}_+$ if and only if

$$Z \le Z_c := \frac{\gamma_c}{\alpha}, \quad \gamma_c = \frac{2}{\frac{\pi}{2} + \frac{2}{\pi}}, \tag{1.10}$$

confirming a prediction of Hardekopf and Sucher in [9] based on numerical considerations. In fact, under (1.10), the operator (1.9) is proved to be positive in [3] and [15], a strict positive lower bound being exhibited in [15] even for $Z = Z_c$. For $\alpha Z \le \gamma_c$, $\sigma_{\mathrm{ess}}(\mathbf{B}_{1,1}(Z)) = [1, \infty)$ and

$\sigma_{sc}(\mathbf{B}_{1,1}(Z)) = \varnothing$ for $\alpha Z < \gamma_c$ (see [5]), where σ_{ess} and σ_{sc} denote the essential and singular continuous spectra respectively, while in [1] a virial theorem is established which implies that for $\alpha Z \leq 3/4$, there are no embedded eigenvalues and hence the spectrum of $\mathbf{B}_{1,1}(Z)$ in $[1,\infty)$ is absolutely continuous. Below 1, when $Z < Z_c$, $\mathbf{B}_{1,1}(Z)$ has an infinite number of eigenvalues accumulating at 1 [16] ; the later result is also a consequence of the result in [8] that the nth eigenvalue of $\mathbf{B}_{1,1}(Z)$ is not greater than that of the Dirac operator $D = D_0 - \alpha Z/|\cdot|$, but they require $Z \leq \frac{\sqrt{3}}{2}\frac{1}{\alpha}$. A significant feature of all these results for (1.9) is that they hold for $Z < Z_c \approx 124.2$, which includes all known elements. Therefore, one has some justification in believing that (1.9) is a better relativistic model than the Herbst operator

$$\mathbf{H}_{1,1}(Z) = (-\Delta + 1)^{1/2} - \frac{\alpha Z}{|\mathbf{x}|}, \tag{1.11}$$

which is the special case $K = 1$ of the rescaled version of (1.1).

The objective in this paper is to establish the result that (1.7) has stability of the second kind for the whole range of nuclear charges allowed by (1.10), namely

$$Z_k \leq Z_c := \frac{2}{\left(\frac{\pi}{2} + \frac{2}{\pi}\right)\alpha}, \quad k = 1, \dots, K. \tag{1.12}$$

As usual for many-particle problems, there is a restriction on the values of α: we require $\alpha \leq \frac{2\pi}{(\pi^2+4)(2+\sqrt{2})} \approx 0.1327$, which covers the physical value $\alpha \approx 1/137 \approx 0.0072$. Note that (1.3) is a restriction to $\mathcal{H}^+$ of $\mathbf{H}_{1,K}\big(\underline{Z},\ \underline{R}\big)\mathbf{1_4}$ in $\mathrm{L}^2(\mathbb{R}^3) \otimes \mathbb{C}^4$. Thus for $Z_k \leq \frac{2}{\pi\alpha}$ the stability of $\mathbf{H}_{1,K}\big(\underline{Z},\ \underline{R}\big)$ in $\mathrm{L}^2(\mathbb{R}^3)$ implies that of $\mathbf{B}_{1,K}\big(\underline{Z},\ \underline{R}\big)$ in the subspace $\mathcal{H}^+$. The problem for the Brown-Ravenhall operator is to extend the range $Z_k \leq 2/(\pi\alpha)$ to $Z_k \leq Z_c$ and hence cover all known elements.

The proof in [4] rests heavily on an inequality in [4, Lemma2.1], which is a refinement of the result (see [11])

$$\|\,|\mathbf{x}|^{-1/2}\ |\mathbf{p}|^{-1/2}\| = \left(\frac{\pi}{2}\right)^{1/2}$$

for compactly supported functions, and makes use of inequalities for symmetric decreasing rearrangements. Our proof depends on an analogous result, but we have to contend with the absence of rearrangement inequalities for the two spinors involved and the fact that the operator $\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|^2}$, unlike $\frac{1}{|\mathbf{p}|}$,does not have a positive kernel.We use the wave decomposition in configuration (x-) space and an interesting sharp inequality

$$\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|^2} \leq \frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|}\frac{1}{|\mathbf{p}|}\frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|} \tag{1.13}$$

(see Lemma 3.2) which we feel might have other useful applications.

Our main result is the following.

Theorem . *Suppose that $\alpha Z_k \leq \gamma_c$, $k = 1, 2, \dots, K$, and $\alpha \leq \gamma_c/(4 + 2\sqrt{2})$, where $\gamma_c = 2/\left(\frac{\pi}{2} + \frac{2}{\pi}\right)$, and $R_k \neq R_l$ for $k \neq l$. Then $\mathbf{B}_{1,K}\big(\underline{Z},\ \underline{R}\big)$ in (1.7) has stability of the second kind, i.e. there exists a constant C such that*

$$\mathbf{B}_{1,K}\big(\underline{Z},\ \underline{R}\big) \geq CK.$$

Remark . Let (1.7) be written as

$$\mathbf{B}_{1,K}\big(\underline{Z},\ \underline{R}\big) = \mathbf{B}^0_{1,K}\big(\underline{Z},\ \underline{R}\big) + \sum_{k<l,\ k,l=1}^{K} \frac{\alpha Z_k Z_l}{|R_k - R_l|}. \tag{1.14}$$

The argument in [5] can be used to give $\sigma_{\text{ess}}\big(\mathbf{B}^0_{1,K}(\underline{Z},\ \underline{R})\big) = [1,\infty)$ for $Z_k \le Z_c$ and hence

$$\sigma_{\text{ess}}\big(\mathbf{B}_{1,K}(\underline{Z},\ \underline{R})\big) = [1 + \sum_{k<l,\ k,l=1}^{K} \frac{\alpha Z_k Z_l}{|R_k - R_l|},\ \infty).$$

2. Preliminaries

The Fourier transform of any spinor ψ in the positive spectral subspace of $D_0 = \frac{1}{i}\boldsymbol{\alpha}\cdot\nabla + \beta$ can be written

$$\widehat{\psi}(\mathbf{p}) = \frac{1}{\mathbf{n}(p)}\begin{pmatrix}[\mathbf{e}(p)+1]\ u(\mathbf{p})\\ (\mathbf{p}\cdot\boldsymbol{\sigma})\ u(\mathbf{p})\end{pmatrix}, \tag{2.1}$$

where $u \in \mathrm{L}^2(\mathbb{R}^3)\otimes\mathbb{C}^2$, a Pauli spinor, $\mathbf{e}(p) = \sqrt{p^2+1}$ and $\mathbf{n}(p) = [2\mathbf{e}(p)(\mathbf{e}(p)+1)]^{1/2}$ (see [5, §2]). Conversely any Dirac spinor of the form (2.1) is in the image of $\mathcal{H}_+$ under the Fourier transform. It is readily shown that , formally, (note that $\mathbf{B}_{1,1}(Z) = \mathbf{B}^0_{1,1}(Z)$)

$$\begin{aligned}\big(\psi, \mathbf{B}^0_{1,1}(Z)\psi\big) &= \big(u, \mathbf{b}^0_{1,1}(Z)u\big)\\ &= \int_{\mathbb{R}^3} \mathbf{e}(p)\,|u(\mathbf{p})|^2\,\mathrm{d}\,\mathbf{p} - \frac{\alpha Z}{2\pi^2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} u(\mathbf{p}')^*\mathbf{k}(\mathbf{p}',\mathbf{p})u(\mathbf{p})\,\mathrm{d}\,\mathbf{p}'\,\mathrm{d}\,\mathbf{p},\end{aligned} \tag{2.2}$$

where $*$ denotes the Hermitian conjugate, $|u(\mathbf{p})|^2 = u(\mathbf{p})^*u(\mathbf{p})$, and the kernel $\mathbf{k}$ is the 2×2 matrix-valued function

$$\mathbf{k}(\mathbf{p}',\mathbf{p}) = \frac{[\mathbf{e}(p')+1][\mathbf{e}(p)+1]\mathbf{1_2} + (\mathbf{p}'\cdot\boldsymbol{\sigma})(\mathbf{p}\cdot\boldsymbol{\sigma})}{\mathbf{n}(p')\,|\mathbf{p}-\mathbf{p}'|^2\,\mathbf{n}(p)}. \tag{2.3}$$

From [1, Lemma 2.4] we have

Lemma 2.1. *The operator $\mathbf{b}^0_{1,1}(Z)$ in (2.2) has the same domain in $\mathrm{L}^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ as the massless operator $\mathfrak{b}^0_{1,1}(Z)$ defined in the form sense by*

$$\mathfrak{b}^0_{1,1}(Z) = |\mathbf{p}| - \frac{1}{2}\gamma\Big(W + PWP\Big), \quad \gamma = \alpha Z, \tag{2.4}$$

where

$$\big(Pu\big)(\mathbf{p}) = \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|}u(\mathbf{p}), \tag{2.5}$$

$$\big(Wu\big)(\mathbf{p}) = \frac{1}{2\pi^2}\int_{\mathbb{R}^3} u(\mathbf{p}')\frac{\mathrm{d}\,\mathbf{p}'}{|\mathbf{p}-\mathbf{p}'|^2}. \tag{2.6}$$

Also , $\mathbf{b}^0_{1,1}(Z) - \mathfrak{b}^0_{1,1}(Z)$ can be extended to a bounded operator on $\mathrm{L}^2(\mathbb{R}^3)\otimes\mathbb{C}^2$.

While the Brown-Ravenhall operator is simply expressed in momentum space, it will be necessary for us to work in $x-$space with the operator

$$\begin{aligned}\widetilde{\mathfrak{b}}^0_{1,1}(Z) &= \mathcal{F}^{-1}\mathfrak{b}^0_{1,1}(Z)\mathcal{F}\\ &= |\mathbf{p}| - \frac{1}{2}\gamma\Big(\frac{1}{|\mathbf{x}|} + \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|}\frac{1}{|\mathbf{x}|}\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|}\Big)\end{aligned} \tag{2.7}$$

In (2.7) we have used the fact that $\mathcal{F}\left(\frac{1}{|\cdot|}\right) = \frac{1}{2\pi^2}\frac{1}{|\cdot|^2}$, and hence $\left(\mathcal{F}^{-1}W\mathcal{F}\right)u(\mathbf{x}) = \frac{1}{|\mathbf{x}|}u(\mathbf{x})$, and used the standard notation $|\mathbf{p}|$ for $\mathcal{F}^{-1}\,|\mathbf{p}|\,\mathcal{F}$, and similarly for $\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|}$. We also write $\frac{1}{|\mathbf{x}|}$ for the operator of multiplication by $\frac{1}{|\mathbf{x}|}$ in $x-$space, and omit the tilda in $\widetilde{\mathfrak{b}}^0_{1,1}$

The operator $\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|}$ is a unitary (and self-adjoint) involution; let $P_\pm$ denote the projections onto its eigenspaces corresponding to its eigenvalues at ± 1 . Then, we have $P_\pm = \frac{1}{2}\left(1 \pm \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|}\right)$ and

$$P_\pm\,|\mathbf{p}| = |\mathbf{p}|\,P_\pm, \quad P_\pm\frac{1}{|\mathbf{p}|^{1/2}} = \frac{1}{|\mathbf{p}|^{1/2}}P_\pm, \tag{2.8}$$

$$P_\pm^2 = P_\pm, \quad P_\pm^* = P_\pm. \tag{2.9}$$

Lemma 2.2. *Let* $\mathcal{K} := \gamma_c\frac{1}{|\mathbf{x}|^{1/2}}P_+\frac{1}{|\mathbf{p}|}P_+\frac{1}{|\mathbf{x}|^{1/2}}$. *Then* $\mathcal{K}\geq 0$ *and*

$$\sup_{\|\psi\|=1}\left(\psi, \mathcal{K}\psi\right) = 1.$$

Proof. The operator $\mathfrak{b}^0_{1,1}(Z)$ is homogeneous, and hence non-negative if and only if it is bounded below. We therefore infer from Lemma 2.1 and [5] that $\mathfrak{b}^0_{1,1}(Z)\geq 0$ if and only if $\gamma\leq\gamma_c$. For $\varphi\in H^{1/2}(\mathbb{R}^3)\otimes\mathbb{C}^2 =: Q_2(\,|\mathbf{p}|)$

$$\left(\varphi, P_+\mathfrak{b}^0_{1,1}(Z)P_+\varphi\right) = \left(P_+\varphi,\,|\mathbf{p}|\,P_+\varphi\right) - \gamma\left(\varphi, P_+\frac{1}{|\mathbf{x}|}P_+\varphi\right).$$

Hence, with $\psi = |\mathbf{p}|^{1/2}\varphi$, $\quad\gamma\leq\gamma_c$ is equivalent to

$$\begin{aligned}
\|P_+\psi\|^2 &= \left(P_+\frac{1}{|\mathbf{p}|^{1/2}}\psi,\,|\mathbf{p}|\,P_+\frac{1}{|\mathbf{p}|^{1/2}}\psi\right)\\
&\geq \gamma\left(\frac{1}{|\mathbf{p}|^{1/2}}\psi, P_+\frac{1}{|\mathbf{x}|}P_+\frac{1}{|\mathbf{p}|^{1/2}}\psi\right)\\
&= \gamma\left\|\frac{1}{|\mathbf{x}|^{1/2}}P_+\frac{1}{|\mathbf{p}|^{1/2}}\psi\right\|^2.
\end{aligned}\tag{2.10}$$

Let $A := \frac{1}{|\mathbf{x}|^{1/2}}P_+\frac{1}{|\mathbf{p}|^{1/2}}$. Then $A^* := \frac{1}{|\mathbf{p}|^{1/2}}P_+\frac{1}{|\mathbf{x}|^{1/2}}$ and $\mathcal{K} = \gamma_c AA^*$. It follows from (2.10), and since $A = AP_+$, that

$$\sup_{\|\psi\|=1}\left(\psi, \mathcal{K}\psi\right) = \gamma_c\,\|A^*\|^2 = 1.$$

□

From

$$[(\cdot\ \times\ \mathbf{p})u(\cdot)]^\wedge(\mathbf{p}) = \left(\frac{1}{i}\nabla_\mathbf{p}\ \times\ \mathbf{p}\right)\hat{u}(\mathbf{p})$$

and

$$[(\mathbf{x}\ \times\ \cdot)u(\cdot)]^\vee(\mathbf{x}) = \left(\frac{1}{i}\nabla_\mathbf{x}\ \times\ \mathbf{x}\right)\check{u}(\mathbf{x})$$

it follows that in both $\mathbf{x}$ and $\mathbf{p}$ spaces, the total angular momentum operator $J\equiv\left(J_1,J_2,J_3\right) = \mathbf{x}\,\times\,\mathbf{p}+\frac{1}{2}\boldsymbol{\sigma} = L+\frac{1}{2}\boldsymbol{\sigma}$ depends only on the angular co-ordinates, and commutes with the Brown-Ravenhall operators $\mathbf{b}^0_{1,1}(Z)$ and $\mathfrak{b}^0_{1,1}(Z)$ (see [5, § 2.2]). The eigenvectors $\Omega_{l,m,s}$, $(l,m,s)\in I$

say, of J^2 form an orthonormal basis for $\mathrm{L}^2(\mathbb{S}^3)\otimes\mathbb{C}^2$, and are the spherical spinors

$$\Omega_{l,m,s}(\omega) := \begin{cases} \begin{pmatrix} \sqrt{\frac{l+s+m}{2(l+s)}}Y_{l,m-\frac12}(\omega) \\ \sqrt{\frac{l+s-m}{2(l+s)}}Y_{l,m+\frac12}(\omega) \end{pmatrix} & s=\frac12 \;, \\ \begin{pmatrix} -\sqrt{\frac{l+s-m+1}{2(l+s)+2}}Y_{l,m-\frac12}(\omega) \\ \sqrt{\frac{l+s+m+1}{2(l+s)+2}}Y_{l,m+\frac12}(\omega) \end{pmatrix} & s=-\frac12 \;, \end{cases} \tag{2.11}$$

with $l=0,1,2,...$ and $m=-l-\frac12,...,l+\frac12$, that do not vanish. Here $Y_{l,k}$ are normalized spherical harmonics on the unit sphere $\mathbb{S}^2$ (see, e.g., [13], p. 421) with the convention that $Y_{l,k}=0$, if $|k|>l$. We denote the corresponding index set by I, i.e., $I:=\{(l,m,s)|l\in\mathbb{N}_0, m=-l-\frac12,...,l+\frac12, s=\pm\frac12, \Omega_{l,m,s}\neq 0\}$. The $\Omega_{l,m,s}$ are simultaneous eigenvectors of J^2, J_3, L^2, and $\boldsymbol{\sigma}\cdot L+1$, where $L\equiv\big(L_1,L_2,L_3\big)=\mathbf{x}\;\times\;\mathbf{p}$, with corresponding eigenvalues $(l+s)(l+s+1)$, m, $l(l+1)$ and $-k$ respectively, where

$$k := \begin{cases} -l-1 & \text{if } \; s=\frac12 \;, \\ \;\; l & \text{if } \; s=-\frac12 \;. \end{cases} \tag{2.12}$$

We have the isomorphism

$$\mathcal{H}=\mathrm{L}^2(\mathbb{R}^3)\otimes\mathbb{C}^2 \longrightarrow \mathrm{L}^2(0,\infty,r^2\,\mathrm{d}\,r;\mathrm{L}^2(\mathbb{S}^3)\otimes\mathbb{C}^2):$$

any $f\in\mathcal{H}$ can be written, with $r=|\mathbf{x}|$, $\omega=\mathbf{x}/|\mathbf{x}|$,

$$f(\mathbf{x}) = \sum_{(l,m,s)\in I} c_{l,m,s}(r)\Omega_{l,m,s}(\omega) \tag{2.13}$$

and

$$\|f\|^2 = \sum_{(l,m,s)\in I}\int_0^\infty |c_{l,m,s}(r)|^2 r^2\,\mathrm{d}\,r. \tag{2.14}$$

The Fourier transform takes angular momentum channels into angular momentum channels, and so (2.13) and (2.14) continue to hold when $\mathbf{x}$ is replaced by $\mathbf{p}$. We also need the following identities:

$$\int\limits_{\mathbb{S}^2}\int\limits_{\mathbb{S}^2}\frac{1}{|\mathbf{x}-\mathbf{y}|^2}\Omega^*_{l,m,s}(\omega_x)\;\Omega_{l',m',s'}(\omega_y)\,\mathrm{d}\,\omega_x\,\mathrm{d}\,\omega_y =$$

$$= \frac{2\pi}{|\mathbf{x}|\;|\mathbf{y}|}\mathbf{Q}_l\left(\frac{|\mathbf{x}|^2+\;|\mathbf{y}|^2}{2\,|\mathbf{x}|\;|\mathbf{y}|}\right)\delta_{ll'}\delta_{mm'}\delta_{ss'}, \tag{2.15}$$

$$\left(\frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|}\right)\Omega_{l,m,s}(\omega) = -\Omega_{l+2s,m,-s}(\omega), \quad \omega=\frac{\mathbf{x}}{|\mathbf{x}|}, \tag{2.16}$$

$$\frac{1}{|\mathbf{p}|}\left[\frac{g(r)}{r}\Omega_{l,m,s}(\omega)\right] = \left\{\frac{1}{\pi r}\int_0^\infty g(s)\mathbf{Q}_l\left(\frac{r^2+s^2}{2rs}\right)\mathrm{d}\,s\right\}\Omega_{l,m,s}(\omega), \tag{2.17}$$

$$(\mathbf{p}\cdot\boldsymbol{\sigma})\big[ig(r)\Omega_{l,m,s}(\omega)\big] = -\Omega_{l+2s,m,-s}(\omega)\left[\frac{\mathrm{d}\,g}{\mathrm{d}\,r}+\frac{k+1}{r}g(r)\right], \tag{2.18}$$

see Flügge[6], Greiner[7, p. 171, (12)]. The functions $\mathbf{Q}_l$ are Legendre functions of the second kind, i.e.,

$$\mathbf{Q}_l(z) = \frac12\int_{-1}^1\frac{P_l(t)}{z-t}dt$$

where the P_l are Legendre polynomials. [See Stegun [14] for the notation and some properties of these special functions. The Legendre functions of the second kind appear here for exactly the same reasons as in the treatment of the Schrödinger equation for the hydrogen atom (Flügge [6], Problem 77)].

It follows from (2.17) and (2.18) that $1/|\mathbf{p}|$ preserves the angular momentum channels, but $(\mathbf{p}\cdot\boldsymbol{\sigma})/|\mathbf{p}|$ does not.However $(\mathbf{p}\cdot\boldsymbol{\sigma})/|\mathbf{p}|$ and P_+ have the following invariant subspaces. We can write the decomposition represented by (2.13) as

$$\mathcal{H} \equiv \mathrm{L}^2(\mathbb{R}^3)\otimes\mathbb{C}^2 = \bigoplus_{l\geq 0,\ m=-l-1/2,\dots,l+1/2} \mathcal{H}_{l,m},$$

where $\mathcal{H}_{l,m}$ is the space of functions of the form

$$c_{l,m,\frac12}(r)\Omega_{l,m,\frac12}(\omega) + c_{l+1,m,-\frac12}(r)\Omega_{l+1,m,-\frac12}(\omega). \tag{2.19}$$

Then, by (2.17) and (2.18)

$$P_+ : \mathcal{H}_{l,m} \to \mathcal{H}_{l,m}. \tag{2.20}$$

Finally in this section, we give a brief survey of the properties of the Mellin transform that we shall need subsequently. The Mellin transform $\mathcal{M}$ is defined on $\mathrm{L}^2(\mathbb{R}^+) \equiv \mathrm{L}^2((0,\infty);\frac{\mathrm{d}r}{r})$ by

$$\psi^\sharp(s) := \big(\mathcal{M}\psi\big)(s) := \frac{1}{\sqrt{2\pi}}\int_0^\infty p^{-\frac12 - is}\psi(p)\,\mathrm{d}\,p\ , \quad s\in\mathbb{R}, \tag{2.21}$$

and has inverse

$$\big(\mathcal{M}^{-1}\psi^\sharp\big)(p) = \frac{1}{\sqrt{2\pi}}\int_0^\infty s^{-\frac12+ip}\psi^\sharp(s)\,\mathrm{d}\,s\ , \quad p\in\mathbb{R}^+. \tag{2.22}$$

It is a unitary map from $\mathrm{L}^2(\mathbb{R}^+)$ onto $\mathrm{L}^2(\mathbb{R})$. Convolution on $\mathrm{L}^2(\mathbb{R}^+)$ is defined by

$$(\psi * \varphi)(s) = \int_0^\infty \psi(p)\varphi\big(\frac{s}{p}\big)\frac{\mathrm{d}\,p}{p} \tag{2.23}$$

and we have that

$$\mathcal{M}(\psi * \varphi) = \psi^\sharp * \varphi^\sharp. \tag{2.24}$$

The Mellin transform of the Legendre functions of the second kind satisfies

$$\mathcal{M}\big[\mathbf{Q}_l\big(\frac{\cdot}{2}+\frac{2}{\cdot}\big)\big](z) = \frac{\pi}{2}\frac{\Gamma([l+1-iz]/2)\Gamma([l+1+iz]/2)}{\Gamma([l+2-iz]/2)\Gamma([l+2+iz]/2)} \tag{2.25}$$

(see [12]).

3. Fundamental inequalities

The following result is the analogue of Lemma 2.1 in [4], and has a crucial role in the proof of our main theorem. It is a refinement of Lemma 2.2 to compactly supported functions. Let $B(\mathbf{a},R)$ denotes the ball $\{\mathbf{x} : |\mathbf{x}-\mathbf{a}| < R\}$.

Theorem 3.1. *Let $\mathcal{K} = \gamma_c\frac{1}{|\mathbf{x}|^{1/2}}P_+\frac{1}{|\mathbf{p}|}P_+\frac{1}{|\mathbf{x}|^{1/2}}$. Then for all $\psi\in\mathrm{L}^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ with $\operatorname{supp}\psi\subset B(\mathbf{0},R)$ we have*

$$(\psi,\mathcal{K}\psi) \leq \|\psi\|^2 - \frac{C}{R^2}\bigg(\int_{\mathbb{R}^3}|\psi(\mathbf{x})|\frac{\mathrm{d}\,\mathbf{x}}{\sqrt{|\mathbf{x}|}}\bigg)^2 \tag{3.1}$$

where $C = 1/(\pi^3+4\pi)$.

To prove the theorem we need some preliminary lemmas.

Lemma 3.2.
$$\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|^2} \le \frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|}\frac{1}{|\mathbf{p}|}\frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|}. \tag{3.2}$$

Proof. Let
$$\tilde{\mathcal{K}} = \frac{\gamma_c}{2}\frac{1}{|\mathbf{x}|^{1/2}}\left(\frac{1}{|\mathbf{p}|} + \frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|}\frac{1}{|\mathbf{p}|}\frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|}\right)\frac{1}{|\mathbf{x}|^{1/2}}. \tag{3.3}$$
We shall prove that for all $\psi \in \mathrm{L}^2(\mathbb{R}^3)\otimes\mathbb{C}^2$
$$\big(\psi,\mathcal{K}\psi\big) \le \Big(\psi,\tilde{\mathcal{K}}\psi\Big)$$
whence the lemma.

Let $\psi \in \mathcal{H}_{l,m}$ be of the form
$$\frac{1}{r}f(r)\Omega_{l,m,\frac{1}{2}}(\omega) + \frac{1}{r}g(r)\Omega_{l+1,m,-\frac{1}{2}}(\omega) \tag{3.4}$$
with $f,g \in C_0^1(0,\infty)$; such spinors are dense in $\mathcal{H}_{l,m}$. In
$$\big(\psi,\mathcal{K}\psi\big) = \frac{\gamma_c}{2}\left(\frac{1}{|\mathbf{x}|^{1/2}}\psi, \frac{1}{|\mathbf{p}|}\frac{1}{|\mathbf{x}|^{1/2}}\psi\right) + \frac{\gamma_c}{2}\left(\frac{1}{|\mathbf{x}|^{1/2}}\psi, \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|^2}\frac{1}{|\mathbf{x}|^{1/2}}\psi\right)$$
it follows from (2.17) and (2.18) that the first term is diagonal and the second off-diagonal in f and g . The diagonal term is

$$\begin{aligned}
&\frac{\gamma_c}{4\pi^2}\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3}\frac{\bar{f}(r)}{r^{3/2}}\frac{f(r')}{r'^{3/2}}\frac{1}{|\mathbf{x}-\mathbf{x}'|^2}\Omega^*_{l,m,\frac{1}{2}}(\omega)\Omega_{l,m,\frac{1}{2}}(\omega')\,\mathrm{d}\,\mathbf{x}\,\mathrm{d}\,\mathbf{x}' + \\
&\qquad + \frac{\gamma_c}{4\pi^2}\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3}\frac{\bar{g}(r)}{r^{3/2}}\frac{g(r')}{r'^{3/2}}\frac{1}{|\mathbf{x}-\mathbf{x}'|^2}\Omega^*_{l+1,m,-\frac{1}{2}}(\omega)\Omega_{l+1,m,-\frac{1}{2}}(\omega')\,\mathrm{d}\,\mathbf{x}\,\mathrm{d}\,\mathbf{x}' \\
&= \frac{\gamma_c}{2\pi}\int\limits_0^\infty\int\limits_0^\infty\frac{\bar{f}(r)}{\sqrt{r}}\frac{f(r')}{\sqrt{r'}}\mathbf{Q}_l\left(\frac{r^2+r'^2}{2rr'}\right)\mathrm{d}\,r\,\mathrm{d}\,r' + \frac{\gamma_c}{2\pi}\int\limits_0^\infty\int\limits_0^\infty\frac{\bar{g}(r)}{\sqrt{r}}\frac{g(r')}{\sqrt{r'}}\mathbf{Q}_{l+1}\left(\frac{r^2+r'^2}{2rr'}\right)\mathrm{d}\,r\,\mathrm{d}\,r'
\end{aligned} \tag{3.5}$$

from (2.15). The off diagonal term in $\Big(\psi,\mathcal{K}\psi\Big)$ is
$$\begin{aligned}
&\frac{\gamma_c}{8\pi}\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3}\frac{\bar{f}(r')}{r'^{3/2}}\Omega^*_{l,m,\frac{1}{2}}(\omega')\frac{1}{|\mathbf{x}-\mathbf{x}'|}\mathbf{p}\cdot\boldsymbol{\sigma}\left\{\frac{g(r)}{r^{3/2}}\Omega_{l+1,m,-\frac{1}{2}}(\omega)\right\}\mathrm{d}\,\mathbf{x}\,\mathrm{d}\,\mathbf{x}' + \\
&\qquad + \frac{\gamma_c}{8\pi}\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3}\frac{\bar{g}(r')}{r'^{3/2}}\Omega^*_{l+1,m,-\frac{1}{2}}(\omega')\frac{1}{|\mathbf{x}-\mathbf{x}'|}\mathbf{p}\cdot\boldsymbol{\sigma}\left\{\frac{f(r)}{r^{3/2}}\Omega_{l,m,\frac{1}{2}}(\omega)\right\}\mathrm{d}\,\mathbf{x}\,\mathrm{d}\,\mathbf{x}' \\
&\qquad\qquad =: \gamma_c\big(I_1+I_2\big)
\end{aligned} \tag{3.6}$$
say; in (3.6) we have used the fact that $\frac{1}{|\mathbf{p}|^2}$ has kernel $\frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|}$. We shall also need
$$\int\limits_{\mathbb{S}^2}\int\limits_{\mathbb{S}^2}\frac{1}{|\mathbf{x}-\mathbf{x}'|}\Omega^*_{l,m,s}(\omega_x),\Omega_{l,m,s}(\omega_{x'})\,\mathrm{d}\,\omega_x\,\mathrm{d}\,\omega_{x'} == \frac{4\pi}{2l+1}\frac{r_<^l}{r_>^{l+1}}, \tag{3.7}$$

where $r_< = \min(|\mathbf{x}|\,,\,|\mathbf{x}'|)$ and $r_> = \max(|\mathbf{x}|\,,\,|\mathbf{x}'|)$. In I_1, we set $G(r) = g(r)/r^{3/2}$. From (2.18) we have

$$(\mathbf{p}\cdot\boldsymbol{\sigma})\{G(r)\Omega_{l+1,m,-\frac{1}{2}}(\omega)\} = i\Omega_{l,m,\frac{1}{2}}(\omega)\left(\frac{\mathrm{d}\,G}{\mathrm{d}\,r} + \frac{l+2}{r}G(r)\right),$$

and on using(3.6), we get

$$\begin{aligned} I_1 &= \frac{1}{2(2l+1)}\int_0^\infty\int_0^\infty \frac{\bar{f}(r')}{r'^{3/2}} i\frac{r_<^l}{r_>^{l+1}}\left(\frac{\mathrm{d}\,G}{\mathrm{d}\,r} + \frac{l+2}{r}G(r)\right) r^2 r'^2\,\mathrm{d}\,r\,\mathrm{d}\,r' = \\ &= \frac{i}{2(2l+1)}\int_0^\infty\int_0^\infty \bar{f}(r')\left(\frac{r_<}{r_>}\right)^{l+\frac{1}{2}}\left\{\frac{\mathrm{d}\,g}{\mathrm{d}\,r} + \frac{l+\frac{1}{2}}{r}g(r)\right\}\mathrm{d}\,r\,\mathrm{d}\,r' = \\ &= \frac{i}{2}\int_0^\infty\int_0^r \bar{f}(r')g(r)\left(\frac{r'}{r}\right)^{l+\frac{1}{2}}\frac{\mathrm{d}\,r\,\mathrm{d}\,r'}{r}. \end{aligned} \tag{3.8}$$

Similarly

$$I_2 = \frac{-i}{2}\int_0^\infty\int_0^r \bar{g}(r)f(r')\left(\frac{r'}{r}\right)^{l+\frac{1}{2}}\frac{\mathrm{d}\,r\,\mathrm{d}\,r'}{r}. \tag{3.9}$$

Hence, for $\psi \in \mathcal{H}_{l,m}$ given by (3.4), we have

$$\begin{aligned} (\psi, \mathcal{K}\psi) &= \frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty \frac{\bar{f}(r)}{\sqrt{r}}\frac{f(r')}{\sqrt{r'}}\mathbf{Q}_l\left(\frac{r^2+r'^2}{2rr'}\right)\mathrm{d}\,r\,\mathrm{d}\,r' + \\ &+ \frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty \frac{\bar{g}(r)}{\sqrt{r}}\frac{g(r')}{\sqrt{r'}}\mathbf{Q}_{l+1}\left(\frac{r^2+r'^2}{2rr'}\right)\mathrm{d}\,r\,\mathrm{d}\,r' - \gamma_c\,\mathrm{Im}\left[\int_0^\infty\int_0^r \bar{f}(r')g(r)\left(\frac{r'}{r}\right)^{l+\frac{1}{2}}\frac{\mathrm{d}\,r\,\mathrm{d}\,r'}{r}\right]. \end{aligned} \tag{3.10}$$

In

$$(\psi, \tilde{\mathcal{K}}\psi) = \frac{\gamma_c}{2}\left(\frac{1}{|\mathbf{x}|^{1/2}}\psi, \frac{1}{|\mathbf{p}|}\frac{1}{|\mathbf{x}|^{1/2}}\psi\right) + \frac{\gamma_c}{2}\left(\frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|}\frac{1}{|\mathbf{x}|^{1/2}}\psi, \frac{1}{|\mathbf{p}|}\frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|}\frac{1}{|\mathbf{x}|^{1/2}}\psi\right) \tag{3.11}$$

the first term is the same as that in $(\psi, \mathcal{K}\psi)$, whilst in the second we have from (2.16)

$$\left(\boldsymbol{\sigma}\cdot\frac{\mathbf{x}}{|\mathbf{x}|}\right)\psi(x) = -\frac{1}{r}f(r)\Omega_{l+1,m,-\frac{1}{2}}(\omega) - \frac{1}{r}g(r)\Omega_{l,m,\frac{1}{2}}(\omega).$$

Hence both term in (3.11) are diagonal and

$$\begin{aligned} &(\psi, \tilde{\mathcal{K}}\psi) = \\ &= \frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty \frac{\bar{f}(r)}{\sqrt{r}}\frac{f(r')}{\sqrt{r'}}\mathbf{Q}_l\left(\frac{r^2+r'^2}{2rr'}\right)\mathrm{d}\,r\,\mathrm{d}\,r' + \frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty \frac{\bar{g}(r)}{\sqrt{r}}\frac{g(r')}{\sqrt{r'}}\mathbf{Q}_{l+1}\left(\frac{r^2+r'^2}{2rr'}\right)\mathrm{d}\,r\,\mathrm{d}\,r' + \\ &\quad + \frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty \frac{\bar{g}(r)}{\sqrt{r}}\frac{g(r')}{\sqrt{r'}}\mathbf{Q}_l\left(\frac{r^2+r'^2}{2rr'}\right)\mathrm{d}\,r\,\mathrm{d}\,r' + \frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty \frac{\bar{f}(r)}{\sqrt{r}}\frac{f(r')}{\sqrt{r'}}\mathbf{Q}_{l+1}\left(\frac{r^2+r'^2}{2rr'}\right)\mathrm{d}\,r\,\mathrm{d}\,r'. \end{aligned} \tag{3.12}$$

Hence, from (3.10) and (3.12),

$$\big(\psi,\tilde{\mathcal{K}}\psi\big)-\big(\psi,\mathcal{K}\psi\big)=\frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty\frac{\bar{g}(r)}{\sqrt{r}}\frac{g(r')}{\sqrt{r'}}\mathbf{Q}_l\Big(\frac{r^2+r'^2}{2rr'}\Big)\,\mathrm{d}\,r\,\mathrm{d}\,r'+$$

$$+\frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty\frac{\bar{f}(r)}{\sqrt{r}}\frac{f(r')}{\sqrt{r'}}\mathbf{Q}_{l+1}\Big(\frac{r^2+r'^2}{2rr'}\Big)\,\mathrm{d}\,r\,\mathrm{d}\,r'+\gamma_c\,\mathrm{Im}\Big[\int_0^\infty\int_0^r\bar{f}(r')g(r)\Big(\frac{r'}{r}\Big)^{l+\frac{1}{2}}\frac{\mathrm{d}\,r\,\mathrm{d}\,r'}{r}\Big]. \quad (3.13)$$

We need to prove that the right-hand side of (3.13) is non-negative. For this we use the Mellin transform.

Let $2\pi\mathbf{Q}_l^\sharp(z)$ denote the function on the right-hand side of (2.25). We then have in the first term of (3.10), with $F(r)=\sqrt{r}f(r)$,

$$\frac{1}{2\pi}\int_0^\infty\int_0^\infty\frac{\bar{f}(r)}{\sqrt{r}}\frac{f(r')}{\sqrt{r'}}\mathbf{Q}_l\Big(\frac{r^2+r'^2}{2rr'}\Big)\,\mathrm{d}\,r\,\mathrm{d}\,r'=$$

$$\frac{1}{2\pi}\int_0^\infty\int_0^\infty\bar{F}(r)F(r')\mathbf{Q}_l\Big(\frac{r^2+r'^2}{2rr'}\Big)\frac{\mathrm{d}\,r\,\mathrm{d}\,r'}{rr'}=\int_{-\infty}^\infty\big|F^\sharp(s)\big|^2\mathbf{Q}_l^\sharp(s)\,\mathrm{d}\,s.$$

Similarly for the second term of (3.10). In (3.8) and (3.9) we set $\Theta(x)=x^{l+1}\chi(x)$, where χ is the characteristic function of $[0,1]$. Then, with $G(r)=\sqrt{r}g(r)$

$$I_1=\frac{i}{2}\int_0^\infty\int_0^\infty\bar{F}(r')G(r)\Theta\Big(\frac{r'}{r}\Big)\frac{\mathrm{d}\,r\,\mathrm{d}\,r'}{rr'}=\frac{i}{2}\int_{-\infty}^\infty\overline{F^\sharp}(s)G^\sharp(s)\Theta^\sharp(s)\,\mathrm{d}\,s,$$

where

$$\Theta^\sharp(s)=\frac{1}{\sqrt{2\pi}}\int_0^1p^{-\frac{1}{2}-is+l+1}\,\mathrm{d}\,p=\frac{1}{\sqrt{2\pi}}\big(\frac{1}{2}-is+l+1\big)^{-1}.$$

Similarly,

$$I_2=-\frac{i}{2}\int_{-\infty}^\infty F^\sharp(s)\overline{G^\sharp}(s)\ \overline{\Theta^\sharp}(s)\,\mathrm{d}\,s.$$

Hence, we can write

$$\big(\psi,\mathcal{K}\psi\big)=\gamma_c\int_{-\infty}^\infty\big(\overline{F^\sharp}(s),\ \overline{G^\sharp}(s)\big)\begin{pmatrix}\mathbf{Q}_l^\sharp(s) & \frac{i}{2}\Theta^\sharp(s)\\ -\frac{i}{2}\overline{\Theta^\sharp}(s) & \mathbf{Q}_{l+1}^\sharp(s)\end{pmatrix}\begin{pmatrix}F^\sharp(s)\\ G^\sharp(s)\end{pmatrix}\mathrm{d}\,s\ . \quad (3.14)$$

Since $\big(\psi,\mathcal{K}\psi\big)\ge 0$, the smooth $2\times 2-$matrix in (3.14) is pointwise non-negative, and hence so is the matrix

$$\begin{pmatrix}\mathbf{Q}_{l+1}^\sharp(s) & -\frac{i}{2}\Theta^\sharp(s)\\ \frac{i}{2}\overline{\Theta^\sharp}(s) & \mathbf{Q}_l^\sharp(s)\end{pmatrix}$$

since the two matrices have the same eigenvalues. Hence

$$\gamma_c\int_{-\infty}^\infty\big(\overline{F^\sharp}(s),\ \overline{G^\sharp}(s)\big)\begin{pmatrix}\mathbf{Q}_{l+1}^\sharp(s) & -\frac{i}{2}\Theta^\sharp(s)\\ \frac{i}{2}\overline{\Theta^\sharp}(s) & \mathbf{Q}_l^\sharp(s)\end{pmatrix}\begin{pmatrix}F^\sharp(s)\\ G^\sharp(s)\end{pmatrix}\mathrm{d}\,s\ \ge 0.$$

But this is precisely the right-hand of (3.13). Hence $\big(\psi, \mathcal{K}\psi\big) \leq \big(\psi, \tilde{\mathcal{K}}\psi\big)$ for all the $C_0^1(\mathbb{R}^3)$ functions ψ in $\mathcal{H}_{l,m}$ considered, and hence for all $\psi \in \mathcal{H}_{l,m}$ since $\mathcal{K}$ and $\tilde{\mathcal{K}}$ are bounded. Since $\mathcal{K}$ and $\tilde{\mathcal{K}}$ map $\mathcal{H}_{l,m}$ into itself, it follows that $\mathcal{K} \leq \tilde{\mathcal{K}}$ on $\mathcal{H}$ and hence the lemma is proved. □

Lemma 3.3. *For all* $\psi \in \mathrm{L}^2(\mathbb{R}^3) \otimes \mathbb{C}^2$

$$\big(\psi, \tilde{\mathcal{K}}\psi\big) \leq \|\psi\|^2 .$$

Proof. First observe from (3.12) that since $\mathbf{Q}_0 \geq \mathbf{Q}_1 \geq \ldots \geq 0$, it is sufficient to prove the result for $\psi \in \mathcal{H}_{0,m}$. In (3.12), with $l = 0$, we may use Hilbert's double integral inequality given in [10, Section 9.3 (319)], since $\frac{1}{\sqrt{r}\sqrt{r'}}\mathbf{Q}_l\left(\frac{r^2+r'^2}{2rr'}\right)$ is homogeneous of degree -1. We have

$$\big(\psi, \tilde{\mathcal{K}}\psi\big) \leq \frac{\gamma_c}{2\pi}\left\{k_1 \int_0^\infty \big(\,|f(r)|^2 + \,|g(r)|^2\big)\,\mathrm{d}\,r + k_2 \int_0^\infty \big(\,|f(r)|^2 + \,|g(r)|^2\big)\,\mathrm{d}\,r\right\},$$

where

$$k_1 = \int_0^\infty \mathbf{Q}_0\left(\frac{1}{2}\left[r + \frac{1}{r}\right]\right)\frac{\mathrm{d}\,r}{r} = \int_0^\infty \ln\left|\frac{r+1}{r-1}\right|\frac{\mathrm{d}\,r}{r} = \frac{\pi^2}{2}$$

and

$$k_2 = \int_0^\infty \mathbf{Q}_1\left(\frac{1}{2}\left[r + \frac{1}{r}\right]\right)\frac{\mathrm{d}\,r}{r} = \int_0^\infty \left\{\frac{1}{2}\left(r + \frac{1}{r}\right)\ln\left|\frac{r+1}{r-1}\right| - 1\right\}\frac{\mathrm{d}\,r}{r} = 2.$$

Hence

$$\big(\psi, \tilde{\mathcal{K}}\psi\big) \leq \int_0^\infty \big(\,|f(r)|^2 + \,|g(r)|^2\big)\,\mathrm{d}\,r = \,\|\psi\|^2 .$$

and the lemma is proved. □

Lemma 3.4. *Let*

$$\psi(\mathbf{x}) = \sum_{(l,m,s)\in I} \frac{1}{r} f_{l,m,s}(r)\Omega_{l,m,s}(\omega)$$

$$\varphi(\mathbf{x}) = \frac{1}{r}\sqrt{\sum_{(l,m,s)\in I} \big|f_{l,m,s}(r)\big|^2}\;\Omega_{0,\frac{1}{2},\frac{1}{2}}, \quad \Omega_{0,\frac{1}{2},\frac{1}{2}} = \frac{1}{2\sqrt{\pi}}\begin{pmatrix}1\\0\end{pmatrix}.$$

Then

$$\|\psi\| = \,\|\varphi\|\,, \tag{3.15}$$

$$\big(\psi, \tilde{\mathcal{K}}\psi\big) \leq \big(\varphi, \tilde{\mathcal{K}}\varphi\big), \tag{3.16}$$

$$\int_{\mathbb{R}^3} \frac{1}{\sqrt{|\mathbf{x}|}}\,|\psi(\mathbf{x})|\,\mathrm{d}\,\mathbf{x} \leq \int_{\mathbb{R}^3} \frac{1}{\sqrt{|\mathbf{x}|}}\,|\varphi(x)|\,\mathrm{d}\,\mathbf{x}. \tag{3.17}$$

Proof. The equality (3.15) is obvious. With

$$\psi_{l,m}(\mathbf{x}) = \frac{1}{r} f_{l,m,\frac{1}{2}}(r)\Omega_{l,m,\frac{1}{2}}(\omega) + \frac{1}{r} f_{l,m,-\frac{1}{2}}(r)\Omega_{l+1,m,-\frac{1}{2}}(\omega)$$

we have from (3.12)

$$(\psi_{l,m}, \tilde{\mathcal{K}}\psi_{l,m}) \le \frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty \Big\{ \frac{1}{\sqrt{r}\sqrt{r'}}\big(|f_{l,m,\frac12}(r)|\,|f_{l,m,\frac12}(r')| + |f_{l,m,-\frac12}(r)|\,|f_{l,m,-\frac12}(r')|\big)\cdot \left(\mathbf{Q}_0\left(\frac{r^2+r'^2}{2rr'}\right) + \mathbf{Q}_1\left(\frac{r^2+r'^2}{2rr'}\right)\right)\Big\}\,\mathrm{d}\,r\,\mathrm{d}\,r'.$$

Hence

$$(\psi, \tilde{\mathcal{K}}\psi) = \sum_{l,m}(\psi_{l,m}, \tilde{\mathcal{K}}\psi_{l,m}) \le$$

$$\frac{\gamma_c}{2\pi}\sum_{(l,m,s)\in I}\int_0^\infty\int_0^\infty \frac{1}{\sqrt{r}\sqrt{r'}}|f_{l,m,s}(r)|\,|f_{l,m,s}(r')|\left[\mathbf{Q}_0\left(\frac{r^2+r'^2}{2rr'}\right) + \mathbf{Q}_1\left(\frac{r^2+r'^2}{2rr'}\right)\right]\mathrm{d}\,r\,\mathrm{d}\,r' \le$$

$$\frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty \frac{1}{\sqrt{rr'}}\Big(\sum_{(l,m,s)\in I}\big|f_{l,m,s}(r')\big|^2\Big)^{\frac12}\Big(\sum_{(l,m,s)\in I}\big|f_{l,m,s}(r)\big|^2\Big)^{\frac12}\left[\mathbf{Q}_0\left(\frac{r^2+r'^2}{2rr'}\right)+\mathbf{Q}_1\left(\frac{r^2+r'^2}{2rr'}\right)\right]\mathrm{d}\,r\,\mathrm{d}\,r' =$$

$$= (\varphi, \tilde{K}\varphi)$$

again by (3.12) with $g = 0$, $f = \big(\sum_{(l,m,s)\in I}\big|f_{l,m,s}\big|^2\big)^{1/2}$, $l = 0$ and $m = \frac12$.

Finally, if $\mathrm{d}\,\mu$ denotes the Haar measure on the orthogonal group $\mathrm{O}(3)$, we have for $g \in \mathrm{O}(3)$

$$\begin{aligned}
\int_{\mathbb{R}^3}\frac{1}{\sqrt{|\mathbf{x}|}}|\psi(\mathbf{x})|\,\mathrm{d}\,\mathbf{x} &= \int_{\mathbb{R}^3}\frac{1}{\sqrt{|\mathbf{x}|}}|\psi(g\mathbf{x})|\,\mathrm{d}\,\mathbf{x} \\
&=: I(g) \\
&= \int_{\mathrm{O}(3)} I(g)\,\mathrm{d}\,\mu(g) \\
&= \int_{\mathbb{R}^3}\frac{1}{\sqrt{|\mathbf{x}|}}\,\mathrm{d}\,\mathbf{x}\,\Big(\int_{\mathrm{O}(3)}|\psi(g\mathbf{x})|\,\mathrm{d}\,\mu(g)\Big) \\
&\le \int_{\mathbb{R}^3}\frac{1}{\sqrt{|\mathbf{x}|}}\Big(\int_{\mathrm{O}(3)}|\psi(g\mathbf{x})|^2\,\mathrm{d}\,\mu(g)\Big)^{\frac12}\mathrm{d}\,\mathbf{x} \\
&= \frac{1}{2\sqrt{\pi}}\int_{\mathbb{R}^3}\frac{1}{\sqrt{|\mathbf{x}|}}\Big(\frac{1}{r^2}\sum_{(l,m,s)\in I}\big|f_{l,m,s}(r)\big|^2\Big)^{\frac12}\mathrm{d}\,\mathbf{x} \\
&= \int_{\mathbb{R}^3}\frac{1}{\sqrt{|\mathbf{x}|}}|\varphi(\mathbf{x})|\,\mathrm{d}\,\mathbf{x}.
\end{aligned}$$

The proof is therefore complete. □

Proof of Theorem 3.1

In view of Lemmas 3.2-3.4 and change of scale, it is enough to prove (3.1) with $\mathcal{K}$ replaced by $\tilde{\mathcal{K}}$ and ψ of the form

$$\psi(\mathbf{x}) = \frac{f(r)}{r}\Omega_{0,\frac12,\frac12}(\omega),$$

with $f \geq 0$ and $\operatorname{supp} f \subset B(\mathbf{0},1)$, that is, from (3.12)

$$\begin{aligned}
\left(\psi, \tilde{\mathcal{K}}\psi\right) \quad &\equiv \quad \frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty \frac{f(r)f(r')}{\sqrt{r}\sqrt{r'}}\left[\mathbf{Q}_0\left(\frac{r^2+r'^2}{2rr'}\right)+\mathbf{Q}_1\left(\frac{r^2+r'^2}{2rr'}\right)\right]\mathrm{d}\,r\,\mathrm{d}\,r' \\
&\leq \quad \int_0^1 |f(r)|^2\,\mathrm{d}\,r \;-\; C\left(2\sqrt{\pi}\int_0^1 \sqrt{r}f(r)\,\mathrm{d}\,r\right)^2. \qquad (3.18)
\end{aligned}$$

Define

$$\tilde{f}(r) := \begin{cases} f(r) & ,\quad r\in[0,1] \\ \frac{1}{r}f\left(\frac{1}{r}\right) & ,\quad r>1. \end{cases}$$

Then

$$2\int_0^1 |f(r)|^2\,\mathrm{d}\,r \;=\; \int_0^\infty |\tilde{f}(r)|^2\,\mathrm{d}\,r \qquad (3.19)$$

and, from Lemma 3.3,

$$\begin{aligned}
&\frac{\gamma_c}{2\pi}\int_0^\infty\int_0^\infty \frac{\tilde{f}(r)\tilde{f}(r')}{\sqrt{r}\sqrt{r'}}\left[\mathbf{Q}_0\left(\frac{r^2+r'^2}{2rr'}\right)+\mathbf{Q}_1\left(\frac{r^2+r'^2}{2rr'}\right)\right]\mathrm{d}\,r\,\mathrm{d}\,r' \\
&\qquad\qquad\leq \int_0^\infty |\tilde{f}(r)|^2\,\mathrm{d}\,r = 2\int_0^1 |f(r)|^2\,\mathrm{d}\,r. \qquad (3.20)
\end{aligned}$$

The left-hand side can be written as

$$\begin{aligned}
&2\gamma_c\left\{\frac{1}{2\pi}\int_0^1\int_0^1 \frac{f(r)f(r')}{\sqrt{r}\sqrt{r'}}\left[\mathbf{Q}_0\left(\frac{r^2+r'^2}{2rr'}\right)+\mathbf{Q}_1\left(\frac{r^2+r'^2}{2rr'}\right)\right]\mathrm{d}\,r\,\mathrm{d}\,r'\right. \\
&\qquad\left.+\frac{1}{2\pi}\int_0^1\int_1^\infty \frac{f(r)f(1/r')}{\sqrt{r}\;r'\sqrt{r'}}\left[\mathbf{Q}_0\left(\frac{r^2+r'^2}{2rr'}\right)+\mathbf{Q}_1\left(\frac{r^2+r'^2}{2rr'}\right)\right]\mathrm{d}\,r\,\mathrm{d}\,r'\right\} \\
&= 2\gamma_c\left(J_1+J_2\right)
\end{aligned}$$

say. We have

$$\begin{aligned}
J_2 &= \frac{1}{2\pi}\int_0^1\int_0^1 \frac{f(r)f(r')}{\sqrt{r}\sqrt{r'}}\left[\mathbf{Q}_0\left(\frac{1}{2}\left[rr'+\frac{1}{rr'}\right]\right)+\mathbf{Q}_1\left(\frac{1}{2}\left[rr'+\frac{1}{rr'}\right]\right)\right]\mathrm{d}\,r\,\mathrm{d}\,r' \\
&\geq \frac{1}{2\pi}\int_0^1\int_0^1 \sqrt{r}f(r)\sqrt{r'}f(r')\left[\frac{1}{rr'}\mathbf{Q}_0\left(\frac{1}{2}\left[rr'+\frac{1}{rr'}\right]\right)\right]\mathrm{d}\,r\,\mathrm{d}\,r' \\
&\geq \frac{1}{\pi}\int_0^1\int_0^1 \sqrt{r}f(r)\sqrt{r'}f(r')\,\mathrm{d}\,r\,\mathrm{d}\,r' \qquad (3.21)
\end{aligned}$$

since $\inf\limits_{0\le u\le 1}\left[\frac{1}{u}\ln\left(\frac{1+u}{1-u}\right)\right]=2$. Hence from (3.20) and(3.21),

$$2\int\limits_0^1 |f(r)|^2\,\mathrm{d}\,r \ge 2\big(\psi,\tilde{K}\psi\big)+2\gamma_c\left(\frac{1}{\pi}\int\limits_0^1\int\limits_0^1 \sqrt{r}f(r)\sqrt{r'}f(r')\,\mathrm{d}\,r\,\mathrm{d}\,r'\right),$$

whence

$$\begin{aligned}\big(\psi,\tilde{\mathcal{K}}\psi\big) &\le \|\psi\|^2-\frac{\gamma_c}{\pi}\left(\int\limits_0^1\sqrt{r}f(r)\,\mathrm{d}\,r\right)^2\\ &= \|\psi\|^2-C\left(\int\limits_{\mathbb{R}^3}|\psi(\mathbf{x})|\,\frac{\mathrm{d}\,\mathbf{x}}{\sqrt{|\mathbf{x}|}}\right)^2\end{aligned}$$

with $C=\frac{\gamma_c}{4\pi^2}=\frac{1}{\pi^3+4\pi}$.

$\square$

4. Proof of the main theorem

Now that we have available Theorem 3.1, we are able to proceed along similar lines to those in [4]. The argument in [4], based on their Lemma 2.3, to justify the sufficiency of taking $Z_k=Z_c$ for all k, continues to hold for us.

We shall prove that when $\alpha Z_k=\alpha Z=\gamma_c$, $k=1,\dots,K$, there exist constants A and C such that

$$\big(\psi,\ \mathbf{B}^0_{1,K}\big(\underline{Z},\ \underline{R}\big)\psi\big)\ge -A\gamma_c\sum_{j\ne k}\frac{1}{|R_j-R_k|}\|\psi\|^2+CK\|\psi\|^2 \tag{4.1}$$

for all $\psi\in\Lambda_+Q_4(|\mathbf{p}|)$.

We have

$$\begin{aligned}V(\mathbf{x}) &:= \sum_{k=1}^K\left\{\frac{\alpha Z_k}{|\mathbf{x}-R_k|}-A\gamma_c\sum_{j\ne k}\frac{1}{|R_j-R_k|}\right\}\\ &\le \left(\sum_{k=1}^K V_k^2(\mathbf{x})\right)\\ &\le \left(\sum_{k=1}^K V_k(\mathbf{x})\right)^2\\ &=: U(\mathbf{x}),\end{aligned} \tag{4.2}$$

where

$$V_k^2(\mathbf{x}):=\gamma_c\left[\frac{1}{|\mathbf{x}-R_k|}-A\sum_{j\ne k}\frac{1}{|R_j-R_k|}\right]_+,$$

and the subscript $+$ denotes the positive part. Hence, (4.1)is satisfied if

$$\big(\psi,\ D_0\psi\big)\ge\big(\psi,\ U\psi\big)+CK\|\psi\|^2. \tag{4.3}$$

We now translate the problem to one for 2-spinors, using (2.1). In view of Lemma 2.1, (4.3) will follow if we can prove that for all $\varphi \in Q_2(|\mathbf{p}|)$

$$\Big(\varphi, \big[\,|\mathbf{p}| - \frac{1}{2}\big(U + \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|} U \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|}\big)\big]\,\varphi\Big) \geq 0. \tag{4.4}$$

Clearly, $\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|}$ commutes with $U + \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|} U \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|} =: \tilde{U}$ and if L is the operator $\varphi(x_1, x_2, x_3) \to \sigma_3\varphi(x_1, x_2, -x_3)$ we have $L(\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|}) = -(\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|})L$, and $L\tilde{U} = \tilde{\tilde{U}}L$, where $\tilde{\tilde{U}}$ coincides with $\tilde{U}$ with a minus sign inserted before the third components of the R_k. Thus we need only prove (4.4) for $\varphi \in P_+Q_2(|\mathbf{p}|)$, where P_+ is the projection onto the eigenspace at 1 for $\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|}$. Thus, it is sufficient to prove that for all $\varphi \in Q_2(|\mathbf{p}|)$

$$\big(\varphi,\ |\mathbf{p}|\,\varphi\big) \geq \big(\varphi,\ P_+UP_+\varphi\big),$$

or, equivalently, for all $u \in \mathcal{H}$,

$$\|u\|^2 \geq \Big(u, \frac{1}{\sqrt{|\mathbf{p}|}} P_+UP_+ \frac{1}{\sqrt{|\mathbf{p}|}} u\Big). \tag{4.5}$$

With $\mathrm{T} := \frac{1}{\sqrt{|\mathbf{p}|}} P_+\sqrt{U}$, (4.5) becomes

$$\big(u, \mathrm{T}\,\mathrm{T}^*\,u\big) \leq \|u\|^2,$$

and so $\|\mathrm{T}^*\| \leq 1$, which in turn gives

$$\big(u, \mathrm{T}^*\,\mathrm{T}\,u\big) \leq \|u\|^2 \ , \quad u \in \mathcal{H},$$

or

$$\Big(u,\ \sqrt{U} P_+ \frac{1}{|\mathbf{p}|} \sqrt{U}\ u\Big) \leq \|u\|^2 \ , \quad u \in \mathcal{H}. \tag{4.6}$$

The functions V_k are supported in balls $B(R_k, t_k)$, where

$$t_k^{-1} = A \sum_{j \neq k} \frac{1}{|R_j - R_k|}. \tag{4.7}$$

Hence

$$|R_j - R_k| - (t_j + t_k) \geq \big(1 - \frac{2}{A}\big)|R_j - R_k| \tag{4.8}$$

so that the balls are disjoint if $A > 2$.

Let χ_k denotes the characteristic functions of $B(R_k, t_k)$. Then $V_k^2(\mathbf{x}) = V_k^2(\mathbf{x})\chi_k(\mathbf{x}) \leq \big(\gamma_c/|\mathbf{x} - R_k|\big)$ and

$$\sqrt{U(\mathbf{x})} \leq \gamma_c^{\frac{1}{2}} \sum_{k=1}^{K} \big\{\, |\mathbf{x} - R_k|^{-\frac{1}{2}}\, \chi_k(\mathbf{x})\big\}.$$

Thus, we need to prove that for all $u \in \mathcal{H}$

$$\begin{aligned}
\|u\|^2 &\geq \gamma_c \sum_{j,k=1}^{K} \Big(u,\ \chi_j(\mathbf{x}) \frac{1}{\big|\mathbf{x}-R_j\big|^{\frac{1}{2}}} P_+ \frac{1}{|\mathbf{p}|} P_+ \chi_k(\mathbf{x}) \frac{1}{\big|\mathbf{x}-R_k\big|^{\frac{1}{2}}} \Big) \\
&= \gamma_c \sum_{j=1}^{K} \Big(u,\ \chi_j(\mathbf{x}) \frac{1}{\big|\mathbf{x}-R_j\big|^{\frac{1}{2}}} P_+ \frac{1}{|\mathbf{p}|} P_+ \chi_j(\mathbf{x}) \frac{1}{\big|\mathbf{x}-R_j\big|^{\frac{1}{2}}} \Big) \\
&+ \gamma_c \sum_{j\neq k} \Big(u,\ \chi_j(\mathbf{x}) \frac{1}{\big|\mathbf{x}-R_j\big|^{\frac{1}{2}}} P_+ \frac{1}{|\mathbf{p}|} P_+ \chi_k(\mathbf{x}) \frac{1}{\big|\mathbf{x}-R_k\big|^{\frac{1}{2}}} \Big) \\
&= I_1 + I_2
\end{aligned}$$

say. By Theorem 3.1, with $C = (\pi^3 + 4\pi)^{-1}$,

$$I_1 \leq \sum_{j=1}^{K} \Big\{ \|\chi_j u\|^2 - \frac{C}{t_j^2} \big(\int \frac{1}{|\mathbf{x}-R_j|^{\frac{1}{2}}} \, |(\chi_j u)(\mathbf{x})| \, \mathrm{d}\,\mathbf{x} \big)^2 \Big\}.$$

In I_2

$$P_+ \frac{1}{|\mathbf{p}|} P_+ = \frac{1}{2} \Big(\frac{1}{|\mathbf{p}|} + \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|^2} \Big);$$

$\frac{1}{|\mathbf{p}|}$ has kernel $\frac{1}{2\pi^2|\mathbf{x}-\mathbf{y}|^2}$, and from (3.2), $\frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{|\mathbf{p}|^2} \leq \frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|} \frac{1}{|\mathbf{p}|} \frac{\mathbf{x}\cdot\boldsymbol{\sigma}}{|\mathbf{x}|}$ whose kernel is bounded by $\frac{1}{2\pi^2|\mathbf{x}-\mathbf{y}|^2}$. Thus

$$\begin{aligned}
I_2 &\leq \frac{\gamma_c}{2\pi^2} \sum_{j\neq k} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{1}{|\mathbf{x}-R_j|^{\frac{1}{2}}} \, |(\chi_j u)(\mathbf{x})| \, \frac{1}{|\mathbf{x}-\mathbf{y}|^2} \frac{1}{|\mathbf{y}-R_k|^{\frac{1}{2}}} \, |(\chi_k u)(\mathbf{y})| \, \mathrm{d}\,\mathbf{x} \, \mathrm{d}\,\mathbf{y} \\
&\leq \frac{\gamma_c}{2\pi^2} \big[1 - \frac{2}{A}\big]^{-2} \sum_{j\neq k} \big|R_j - R_k\big|^{-2} m_j m_k
\end{aligned}$$

by (4.8), where

$$m_j := \int_{\mathbb{R}^3} \frac{\chi_j \, |u(\mathbf{x})|}{|\mathbf{x}-R_j|^{\frac{1}{2}}} \, \mathrm{d}\,\mathbf{x}.$$

Thus

$$\begin{aligned}
I_1 + I_2 &\leq \|u\|^2 - C \sum_{j=1}^{K} \frac{1}{t_j^2} m_j^2 + \frac{\gamma_c}{2\pi^2} \big[1 - \frac{2}{A}\big]^{-2} \sum_{j\neq k} \big|R_j - R_k\big|^{-2} \frac{1}{2} \big(m_j^2 + m_k^2 \big) \\
&\leq \|u\|^2
\end{aligned}$$

if

$$\frac{C}{t_j^2} - \frac{\gamma_c}{2\pi^2} \big[1 - \frac{2}{A}\big]^{-2} \sum_{j\neq k} \big|R_j - R_k\big|^{-2} \geq 0$$

for all j. On substituting (4.7), the last inequality is satisfied if

$$A^2 \geq 2 \Big(1 - \frac{2}{A} \Big)^{-2},$$

that is $A \geq 2 + \sqrt{2}$.We have therefore established (4.1), and can take $A = 2 + \sqrt{2}$. Consequently, we have

$$\mathbf{B}_{1,K}\big(\underline{Z},\ \underline{R}\big) \geq -2A\gamma_c \sum_{j<k} \frac{1}{\big|R_k - R_j\big|} + \alpha Z_c^2 \sum_{j<k} \frac{1}{\big|R_k - R_j\big|} + CK \geq CK$$

if $2\alpha[2+\sqrt{2}] \leq \gamma_c$, that is $\alpha \leq \frac{2\pi}{(\pi^2+4)(2+\sqrt{2})} \approx 0.1327$; this includes the physical value of α. The proof is therefore complete. $\square$

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References

[1] A.A. Balinsky and W.D. Evans, *On the virial theorem for the relativistic operator of Brown and Ravenhall, and the absence of embedded eigenvalues*,to appear in Lett. Math. Phys.

[2] G.E. Brown and D.G. Ravenhall, *On the interaction of two electrons*, Proc. Roy. Soc. London A **208** (1952), pp. 552-559.

[3] V.I. Burenkov and W.D. Evans, *On the evaluation of the norm of an integral operator associated with the stability of one-electron atoms*, to appear in Proc. Roy. Soc. Edinburgh.

[4] I. Daubechies and E.H. Lieb, *One-electron relativistic molecules with Coulomb Interaction*, Commun. Math. Phys **90** (1983), pp. 497-510.

[5] W.D. Evans, P. Perry and H. Siedentop, *The spectrum of relativistic one-electron atoms according to Bethe and Salpeter*, Commun. Math. Phys. **178** (1996), pp. 733-746.

[6] S. Flügge, *Practical Quantum Mechanics I*, volume 177 of *Grundlehren der mathematischen Wissenschaften*, Springer-Verlag, Berlin, 1 edition, 1982.

[7] W. Greiner, *Relativistic Quantum Mechanics*, volume 3 of *Theoretical Physics – Text and Excercise Books*, Springer, Berlin, 1 edition, 1990.

[8] M. Griesemer and H. Siedentop, *A minimax principle for the eigenvalues in spectral gaps*, to appear in Journ. London Math. Soc.

[9] G. Hardekopf and J. Sucher, *Critical coupling constants for relativistic wave equations and vacuum breakdown in quantum electrodynamics*, Phys. Rev. A, **31(4)** (April 1985), pp. 2020–2029.

[10] G.H. Hardy, J.E. Littlewood and G. Polya, *Inequalities*, 2 edition, Cambridge, 1952.

[11] I. Herbst, *Spectral theory of the operator* $(p^2+m^2)^{1/2} - Ze^2/r$, Commun. Math. Phys. **53** (1977), pp. 285-294.

[12] W. Magnus, F. Oberhettinger and R. Soni, *Formulas and theorems for the special functions of mathematical physics*, Springer Verlag, New York 1966.

[13] A. Messiah, *Mécanique Quantique*, volume 1, Dunod, Paris, 2 edition, 1969.

[14] Irene A. Stegun, Legendre functions. In Milton Abramowitz and Irene A. Stegun, editors, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, chapter 8, pages 331–353, Dover Publications, New York, 1965.

[15] C. Tix, *Strict positivity of a relativistic Hamiltonian due to Brown and Ravenhall*, Bull. London Math. Soc., **30** (1998), pp. 283-290

[16] C. Tix, *Self-adjointness and spectral properties of a pseudo-relativistic Hamiltonian due to Brown and Ravenhall*, Preprint mp-arc/97-441.

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