Stability of Atoms in the Brown–Ravenhall Model

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March 28, 2022

Abstract

We consider the Brown–Ravenhall model of a relativistic atom with \(N\) electrons and a nucleus of charge \(Z\) and prove the existence of an infinite number of discrete eigenvalues for \(N \leq Z\). As an intermediate result we prove a HVZ–type theorem for these systems.

1 Introduction

A fundamental fact of quantum mechanics is that any stable state (a state which can exist infinitely long in time) of a quantum system corresponds to an eigenfunction of the Hamiltonian of this system. In particular, for an atom, which is known to be a stable system, this means that its lowest spectral point should be an eigenvalue. Hence the existence of an eigenvalue at the bottom of the spectrum of the Hamiltonian can be considered as one of the criteria of correctness of a mathematical model of an atom.

For multiparticle Schrödinger operators on the mathematically rigorous level the existence of discrete eigenvalues at the bottom of the spectrum was proved by T. Kato (for an atom with two electrons) \[15\] and G. Zhislin (in the general case) \[27\]. In the following 45 years these results were generalized in many different directions. The existence of ground states was proved for atoms in an external magnetic field (J. Avron, I. Herbst, B. Simon \[24\] and S. Vugalter, G. Zhislin \[23\]), for the Herbst operator (S. Vugalter, G. Zhislin \[26\]). The most recent development is the proof of the existence of a stable ground state in the Pauli–Fierz model, which describes an atom interacting with a quantized radiation field (V. Bach, J. Fröhlich, I. Sigal \[3\]; J.–M. Barbaroux, T. Chen, S. Vugalter \[5\]; E. Lieb, M. Loss \[19\]).

In the work at hand we prove the existence of an infinite number of discrete eigenvalues, which accumulate at the bottom of the essential spectrum for the Brown–Ravenhall model of an atom or a positive atomic ion. The Brown–Ravenhall operator is one of the models used by physicists and quantum–chemists to describe relativistic effects in atoms (for a discussion of physical accuracy of this model see \[18\]).
The mathematically rigorous study of this operator started with the work by W. Evans, P. Perry and H. Siedentop [7], who proved that the Brown–Ravenhall operator of a one–particle Coulomb system with the nuclear charge $Z$ is semi–bounded from below for $\alpha Z \leq 2 \left( \frac{\pi}{2} + \frac{1}{2} \right) - 1$, where $\alpha$ is the fine structure constant. Further results on the lower bound of the spectrum of this operator with one electron and one or several nuclei were obtained by C. Tix [20, 21] and A. Balinsky, W. Evans [4].

Although the questions of semiboundedness and self–adjointness of the Brown–Ravenhall operator are extremely important, its successful application requires much more detailed knowledge of its spectral properties. The goal of this paper is to establish some of them.

A way to prove the existence of a stable ground state of a multiparticle system was developed by G. Zhislin in [27] and consists of two steps. The first step is to prove a so–called HVZ–type theorem which establishes a criterion for the existence of a bound state. The second step is a construction of a trial function which satisfies this criterion. In the work at hand we follow the same strategy. First we prove a HVZ–type theorem (Theorem 1), showing that the bottom of the essential spectrum of the Brown–Ravenhall operator of an atomic system with $N$ electrons is determined by the bottom of the spectrum of the operator with $N - 1$ electrons. Then we construct a trial function with an expectation value of the energy less than the bottom of the essential spectrum (Theorem 2). Although we use the same strategy as in the original paper by G. Zhislin, the work at hand is technically very different from the works on Schrödinger operators. The main differences are caused by the nonlocality of the Brown–Ravenhall operator. Notice that the HVZ theorem was proved earlier by R. Lewis, H. Siedentop and S. Vugalter [15] for the Herbst–type operator, which is also non–local. The Brown–Ravenhall operator in contrast to the Herbst operator has, however, not only a non–local kinetic energy, but also a non–local potential energy. This leads to a large number of additional complications.

In Section 3 we prove several lemmata which allow us to estimate these non–local effects and to modify the method of [27] in such a way that it works also for the Brown–Ravenhall operator. Here the most important role is played by the estimates on the commutator of the projector on the positive spectral subspace of the Dirac operator with a smoothed characteristic function of a region in the configuration space (Lemma 1) and the decay of the integral kernel of this projector (Lemma 2).

When this work was in preparation, the authors received two preprints by D. Jakubaś–Amundsen [12, 11], where the HVZ theorem for the Brown–Ravenhall operator was proved in a different way and without taking the Pauli principle into account.
2 Preliminaries

The $N$–electron Brown–Ravenhall Hamiltonian is given by

$$H_N = \Lambda_N^+ \left( \sum_{n=1}^N \left( D_n - \frac{\alpha Z}{|x_n|} \right) + \sum_{n<j}^N \frac{\alpha}{|x_n - x_j|} \right) \Lambda_N^+. \quad (2.1)$$

Here $x_n \in \mathbb{R}^3$ is the position vector of the $n^{th}$ electron. The Dirac operator in the standard representation is given by

$$D = -i\alpha \cdot \nabla + \beta, \quad (2.2)$$

where $\alpha := (\alpha_1, \alpha_2, \alpha_3)$ and $\beta$ are the the four Dirac matrices, explicitly

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \quad k = 1, 2, 3,$$

$\sigma_k$ denoting the $k^{th}$ Pauli matrix

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

and

$$\beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

$D_n$ is the Dirac operator $D$ acting on the coordinates of the $n^{th}$ electron. $Z$ is the nuclear charge, $\alpha \approx 1/137$ is the fine structure constant, and

$$\Lambda_n^+ = \Lambda_+ \otimes \Lambda_n^{(n)}, \quad (2.3)$$

where $\Lambda_n^{(n)}$ is the projector onto the positive spectral subspace of $D_n$.

The underlying Hilbert space is $\mathcal{H}_N := \Lambda_+ \otimes \otimes_{n=1}^N \mathcal{H}_n$, where $\otimes$ stands for the antisymmetric tensor product of one–electron Hilbert spaces. The operator $\mathcal{H}_N$ is well defined as the operator corresponding to the semibounded closed form on $\Lambda_+ \otimes \otimes_{n=1}^N L^2(\mathbb{R}^3, \mathbb{C}^4)$ for

$$\alpha Z < \alpha Z_c = \frac{2}{\left( \frac{2}{\pi} + \frac{2}{\pi} \right)}.$$ \quad (2.4)

We always assume in the following that condition (2.4) is fulfilled.
The semiboundedness of $\mathcal{H}_N$ follows from the semiboundedness of the one-particle operators $\Lambda_+ \left( D - \frac{\alpha Z}{|x|} \right) \Lambda_+$ (see [7]) and the positivity of the two-particle interaction terms.

We denote the spectrum of an arbitrary selfadjoint operator $A$ by $\sigma(A)$. $[A, B] = AB - BA$ is the commutator of two operators. $B(R, x)$ is the open ball in $\mathbb{R}^d$ of radius $R > 0$ centered at $x$. $B(R) := B(R, 0)$. $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$ stand for the inner product and the norm in $L_2(\mathbb{R}^{3d}, \mathbb{C}^4)$, $d$ is usually clear by context. Let $E_{N-1} := \inf \sigma(\mathcal{H}_{N-1})$. Irrelevant constants are denoted by $C$. $I_\Omega$ is the indicator function of the set $\Omega$. The Fourier transform of $f$ is denoted by $\hat{f}$.

In auxiliary calculations it is sometimes convenient to consider the operator $\mathcal{P}_{2N}$ in the space $\Lambda_+^N \otimes \bigotimes_{n=1}^N L_2(\mathbb{R}^3, \mathbb{C}^4)$, i.e. without antisymmetrization. We use this extension without changing the notation.

The main result of this article are the following two theorems.

**Theorem 1** For any $N > 1$, we have

$$\sigma_{\text{ess}}(\mathcal{H}_N) = [E_{N-1} + 1, \infty). \tag{2.5}$$

**Theorem 2** Let $N \leq Z$. Then the operator $\mathcal{H}_N$ has infinitely many eigenvalues below the essential spectrum.

**Remark 1** Theorem 1 is an analogue of the HVZ theorem for multiparticle Schrödinger operators (see [6] and the original papers [27, 22, 10]). Analogous theorems were proved for the magnetic Schrödinger operator [24] and the Herbst operator [15].

**Remark 2** In contrast to the Schrödinger case the bottom of the essential spectrum of $\mathcal{H}_N$ is $E_{N-1} + 1$ and not $E_N$. This is related to the fact that in the Brown-Ravenhall model the spectrum of the free electron is $[1, \infty)$ instead of $[0, \infty)$.

**Remark 3** In the multiparticle Schrödinger case the existence of discrete eigenvalues was proved in [24] for $N = 2$, and in [27] for arbitrary $N$.

The proof of Theorem 1 is given in Sections 4 and 5. Theorem 2 is proved in Section 6. Section 3 contains some lemmata used in the subsequent sections.

## 3 Technical Lemmata

### 3.1 Commutator Estimate

The projector $\Lambda_+$ for the free one-particle Dirac operator is given by (see [19], formula 1.1.54)

$$\Lambda_+ = \frac{1}{2} + \frac{D}{2|D|} = \frac{1}{2} + F^{\ast} \frac{\alpha \cdot p + \beta}{2\sqrt{|p|^2 + 1}} F, \tag{3.1}$$
where \( \mathcal{F} \) is the Fourier transform. In the coordinate representation for \( f \in C_0^0(\mathbb{R}^3, \mathbb{C}^4) \) the operator \( \Lambda_+ \) acts as

\[
(\Lambda_+ f)(x) = \frac{f(x)}{2} + \frac{1}{4\pi^2} \int_{\mathbb{R}^3} \left( \frac{\beta K_1(|x-y|)}{|x-y|} + \frac{i\alpha \cdot (x-y)}{|x-y|^2} K_0(|x-y|) \right) f(y) dy \\
+ \frac{i}{2\pi^2} \lim_{\varepsilon \to 0^+} \int_{\mathbb{R}^3 \setminus B(\varepsilon, x)} \frac{\alpha \cdot (x-y)}{|x-y|^3} K_1(|x-y|) f(y) dy,
\]

(3.2)

where the limit on the r.h.s. is the limit in \( L_2(\mathbb{R}^3, \mathbb{C}^4) \) (see Appendix B). For convenience of the reader we state properties of the functions \( K_\nu, \nu = 1, 2, \) in Appendix A.

**Lemma 1** Let \( \chi \in C^2(\mathbb{R}^3) \). Then the norm of the operator

\[
[\chi, \Lambda_+] : L_2(\mathbb{R}^3, \mathbb{C}^4) \to H^1(\mathbb{R}^3, \mathbb{C}^4)
\]

satisfies

\[
\| [\chi, \Lambda_+] \|_{L_2(\mathbb{R}^3, \mathbb{C}^4) \to H^1(\mathbb{R}^3, \mathbb{C}^4)} \leq C(\| \nabla \chi \|_\infty + \| \partial^2 \chi \|_\infty).
\]

(3.3)

Here \( \| \partial^2 \chi \|_\infty = \max_{x \in \mathbb{R}^3} \left| \partial^2 \chi(x) \right| \).

In the proof of Lemma 1 we shall apply the following theorem, which we formulate here for convenience of the reader.

**Theorem 3** (Stein [17], Chapter 2, sec. 3.2) Let \( K : \mathbb{R}^n \to \mathbb{C} \) be measurable such that

\[
|K(x)| \leq B|x|^{-n}, \quad x \neq 0,
\]

(3.4)

\[
\int_{|x| \geq 2|y|} |K(x-y) - K(x)| d^n x \leq B, \quad 0 < |y|,
\]

(3.5)

and

\[
\int_{R_1 < |x| < R_2} K(x) d^n x = 0, \quad \text{for all} \quad 0 < R_1 < R_2 < \infty.
\]

(3.6)

For an arbitrary \( f \in L_p(\mathbb{R}^n), 1 < p < \infty, \) let

\[
T_\varepsilon(f)(x) = \int_{|y| \geq \varepsilon} f(x-y) K(y) d^n y, \quad \varepsilon > 0.
\]

(3.7)

Then

\[
\| T_\varepsilon(f) \|_p \leq A_p \| f \|_p
\]

(3.8)

with \( A_p \) independent of \( f \) and \( \varepsilon \).
Remark 4 Inequality (3.8) shows that the operator \( T = \lim_{\varepsilon \to +0} T_\varepsilon \) exists as a bounded operator in \( L^p(\mathbb{R}^n) \) and its norm satisfies \( \|T\| \leq A_p \).

Proof of Lemma 1 Let us first prove that \([\chi, \Lambda+]\) is a bounded operator in \( L_2(\mathbb{R}^3, \mathbb{C}^4) \). For \( f \in C_0^1(\mathbb{R}^3, \mathbb{C}^4) \) formula (3.2) implies

\[
([\chi, \Lambda+]) (x) = \frac{1}{4\pi^2} \int \left( \frac{\beta K_1(|x-y|)}{|x-y|} + \frac{i \alpha \cdot (x-y) K_0(|x-y|)}{|x-y|^2} \right) (\chi(x) - \chi(y)) f(y) dy + \frac{i}{2\pi^2} \int \frac{\alpha \cdot (x-y)}{|x-y|^3} K_1(|x-y|) (\chi(x) - \chi(y)) f(y) dy.
\]

(3.9)

To complete the proof of Lemma 1 one has to show that

\[
\|([\chi, \Lambda+]) f\|_{L_2(\mathbb{R}^3, \mathbb{C}^4)} \leq C \|\nabla \chi\| \|\nabla f\|_{L_2(\mathbb{R}^3, \mathbb{C}^4)}.
\]

(3.10)

The differentiation of the first summand on the r.h.s. of (3.9) gives absolutely convergent integrals whose \( L_2 \)–norms are bounded by \( C \|\nabla \chi\| \|f\|_{L_2(\mathbb{R}^3, \mathbb{C}^4)} \). The differentiation of the second integral on the r.h.s. of (3.9) in the \( j \)th component of \( x \) gives for \( f \in C_0^1(\mathbb{R}^3, \mathbb{C}^4) \) (cf. Appendix B)

\[
\frac{i}{2\pi^2} \lim_{\varepsilon \to +0} \int_{\mathbb{R}^3 \setminus B(\varepsilon)} \left( \alpha_j \frac{K_1(|x-y|)}{|x-y|^3} - \frac{\alpha \cdot (x-y) (x_j - y_j) K_0(|x-y|)}{|x-y|^4} \right) (\chi(x) - \chi(y)) f(y) dy + \frac{i}{2\pi^2} \lim_{\varepsilon \to +0} \int_{\mathbb{R}^3 \setminus B(\varepsilon)} \frac{\alpha \cdot (x-y) K_1(|x-y|)}{|x-y|^3} \partial_j \chi(x) f(y) dy.
\]

(3.11)

The term

\[
- \frac{i}{2\pi^2} \int_{\mathbb{R}^3 \setminus B(\varepsilon)} \frac{\alpha \cdot (x-y) (x_j - y_j) K_0(|x-y|)}{|x-y|^4} (\chi(x) - \chi(y)) f(y) dy
\]
is bounded by $C\|\nabla \chi\|_\infty \|f\|$. The Taylor expansion of $\chi$ gives

$$\chi(x) - \chi(y) = (x_k - y_k) \partial_k \chi(x) - \frac{1}{2} (x_k - y_k)(x_l - y_l) \partial^2_{kl} \chi(z_{xy}), \quad z_{xy} \in [x, y]. \quad (3.12)$$

Here $[x, y]$ is the line segment connecting $x$ and $y$ and summations in $k$ and $l$ from 1 to 3 are assumed. Substituting $(3.12)$ into $(3.11)$ we arrive at

$$i \partial_k \chi(x) \lim_{\epsilon \to +0} \int_{\mathbb{R}^3 \setminus B(\epsilon)} \left( \alpha_j - \frac{4 \alpha \cdot (x - y)(x_j - y_j)}{|x - y|^2} \right) K_1(|x - y|) \frac{(x_k - y_k)}{|x - y|^3} f(y) dy$$

$$+ i \partial^2_{x_k} \chi(x) \lim_{\epsilon \to +0} \int_{\mathbb{R}^3 \setminus B(\epsilon)} \alpha \cdot (x - y) K_1(|x - y|) \frac{1}{|x - y|^3} f(y) dy$$

$$- \frac{i}{4\pi^2} \int \left( \alpha_j - \frac{4 \alpha \cdot (x - y)(x_j - y_j)}{|x - y|^2} \right) K_1(|x - y|) \frac{1}{|x - y|^3}$$

$$\times \frac{(x_k - y_k)(x_l - y_l)}{|x - y|^3} \partial^2_{kl} \chi(z_{xy}) f(y) dy. \quad (3.13)$$

To the first two integrals in $(3.13)$ we shall apply Theorem 3 with $n = 3$. Hypotheses $(3.4)$ and $(3.6)$ are obviously fulfilled. To prove that condition $(3.5)$ is also fulfilled we note that $(3.5)$ follows from the estimate

$$|\nabla K(x)| \leq B|x|^{-4} \quad (3.14)$$

(see [17], page 34). Inequality $(3.14)$ follows from $(3.2)$. Due to Theorem 3 the $L_2$–norms of the first two integrals in $(3.13)$ are bounded by $C\|f\|_{L_2(\mathbb{R}^3, C^1)}$. The last term in $(3.13)$ is a convolution with a function from $L_1(\mathbb{R}^3)$, whose $L_2$–norm due to the Young inequality can be estimated with

$$C\|\partial^2 \chi\|_\infty \|f\|_{L_2(\mathbb{R}^3, C^1)}.$$

This completes the proof of Lemma 1.

### 3.2 Non–local Properties of the Operator $\Lambda_+$

**Lemma 2** Let $\sup f \subset \Omega \subset \mathbb{R}^3$, $|\Omega| < \infty$, $x \in \mathbb{R}^3$, $d := \text{dist}(x, \Omega) > 0$. Then

$$| (\Lambda_+ f)(x) | \leq G(d)|\Omega|^{1/2}\|f\|_{L_2(\mathbb{R}^3, C^1)}, \quad (3.15)$$

where

$$G(d) = \frac{1}{4\pi^2} \left( \frac{K_1(d)}{d} + 3 \frac{K_0(d)}{d} + 6 \frac{K_1(d)}{d^2} \right). \quad (3.16)$$

**Proof.** The statement of Lemma 2 follows immediately from the Schwarz inequality and formula $(3.2)$, if we note that for $x \notin \sup f$ all integrals in $(3.2)$ converge absolutely. •
Remark 5 Notice that the functions $K_
u(d)$, $\nu = 0, 1$, and consequently $G(d)$, decay exponentially according to (3.19) as $d \to \infty$. Our proof of the HVZ theorem and of the existence of the discrete spectrum follows the same lines as in the original paper by G. Zhidlin [27] for the Schrödinger operator. The new obstacle which was overcome in the present work is the non–locality of the Brown–Ravenhall operator. Lemma 4 tells us that, although the operator $\Lambda_+$ is non–local, for a compactly supported function $f$ the function $\Lambda_+ f$ decays exponentially with the distance to the support of $f$.

3.3 Localization Error Estimate

Lemma 3 Any bounded function $\chi \in C^1(\mathbb{R}^d)$ with bounded derivatives is a multiplicator in $H^{1/2}(\mathbb{R}^d, C^k)$ for any $d, k \in \mathbb{N}$:

$$\|\chi u\|_{H^{1/2}(\mathbb{R}^d, C^k)} \leq C_d \cdot (\|\chi\|_{L_\infty(\mathbb{R}^d)} + \|\nabla \chi\|_{L_\infty(\mathbb{R}^d)}) \|u\|_{H^{1/2}(\mathbb{R}^d, C^k)},$$  \quad (3.17)

for all $u \in H^{1/2}(\mathbb{R}^d, C^k)$.

Proof of Lemma 3. We choose the norm in $H^{1/2}(\mathbb{R}^d, C^k)$ as (see [1], Theorem 7.48).

$$\|u\|_{H^{1/2}(\mathbb{R}^d, C^k)}^2 := \|u\|_{L_2(\mathbb{R}^d, C^k)}^2 + \iint \frac{|u(x) - u(y)|^2}{|x - y|^{d+1}} \, dx \, dy.$$ \quad (3.18)

Then

$$\|\chi u\|_{H^{1/2}(\mathbb{R}^d, C^k)}^2 = \|\chi u\|_{L_2(\mathbb{R}^d, C^k)}^2 + \iint \frac{|\chi(x)u(x) - \chi(y)u(y)|^2}{|x - y|^{d+1}} \, dx \, dy$$

$$\leq \|\chi\|_{L_\infty}^2 \|u\|_{L_2}^2 + \iint \left( \frac{|\chi(x)|^2 |u(x) - u(y)|^2}{|x - y|^{d+1}} + \frac{|\chi(x) - \chi(y)|^2 |u(y)|^2}{|x - y|^{d+1}} \right) \, dx \, dy$$

$$\leq \|\chi\|_{L_\infty}^2 \|u\|_{H^{1/2}}^2 + \sup_{y \in \mathbb{R}^d} \iint \frac{|\chi(x) - \chi(y)|^2}{|x - y|^{d+1}} \, dx \|u\|_{L_2}^2.$$  \quad (3.19)

The supremum on the r.h.s. of (3.19) can be estimated as

$$\sup_{y \in \mathbb{R}^d} \iint \frac{|\chi(x) - \chi(y)|^2}{|x - y|^{d+1}} \, dx \leq \sup_{y \in \mathbb{R}^d} \int_{B(1, y)} \frac{|\chi(x) - \chi(y)|^2}{|x - y|^{d+1}} \, dx$$ \quad (3.20)

$$+ \sup_{y \in \mathbb{R}^d} \int_{B(1, y)} \frac{|\chi(x) - \chi(y)|^2}{|x - y|^{d+1}} \, dx \leq |S_{d-1}|(\|\nabla \chi\|_{L_\infty}^2 + 4 \|\chi\|_{L_\infty}^2),$$

where $|S_{d-1}|$ is the area of $(d - 1)$–dimensional unit sphere. Substituting (3.20) into (3.19) and using the inequality $a^2 + b^2 \leq (a + b)^2$ for $a, b \geq 0$ we obtain (3.17).
Lemma 4 For any bounded function \( \chi \in \mathcal{C}^1(\mathbb{R}^{3N}) \) with bounded derivatives the operator \( [\chi, \Lambda_N] \) is bounded in \( H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4N}) \) and for any \( \psi \in H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4N}) \) we have

\[
\| [\chi, \Lambda_N^N] \psi \|_{H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4N})} \leq C_N (\| \nabla \chi \|_{L_{\infty}(\mathbb{R}^{3N})} + \| \partial^2 \chi \|_{L_{\infty}(\mathbb{R}^{3N})}) (1 + \| \nabla \chi \|_{L_{\infty}(\mathbb{R}^{3N})}) \| \psi \|_{H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4N})}.
\]

(3.21)

Proof. Successively commuting \( \chi \) with one–particle projections \( \Lambda_+^n \), \( n = 1, \ldots, N \) (see (2.3)) we obtain

\[
[\chi, \Lambda_N^N] = \sum_{n=1}^{N} \prod_{k=1}^{n-1} \Lambda_+^k \chi, \Lambda_+^{(n)} \prod_{l=n+1}^{N} \Lambda_+^l,
\]

(3.22)

where the empty products should be replaced by identity operators. According to (3.21), the operator \( \Lambda_+^n \) is bounded in \( H^{s}(\mathbb{R}^{3}, \mathbb{C}^{4}) \) for any \( s \in \mathbb{R} \). This, together with (3.22), and Lemmata 1 and 3, implies (3.21).

Lemma 5 There exists a constant \( C_{N,Z} \) depending on \( N \) and \( Z \) such that for any \( \psi \in \Lambda_+^N H^{1/2}(\mathbb{R}^{3}, \mathbb{C}^{4}) \)

\[
\langle \mathcal{H}_N \psi, \psi \rangle \geq C_{N,Z} \| \psi \|^2_{H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4N})}.
\]

(3.23)

Proof. For the one particle Brown–Ravenhall operator one has (see [21])

\[
\Lambda_+ \left( D - \frac{\alpha Z}{|x|} \right) \Lambda_+ \geq (1 - \alpha Z) \Lambda_+.
\]

(3.24)

Inequality (3.24) holds true for any \( Z \leq Z_c \) (cf. (2.4)). Using (3.24) with \( Z = Z_c \) we get

\[
\Lambda_+ \left( D - \frac{\alpha Z}{|x|} \right) \Lambda_+ \geq \frac{Z_c - Z}{Z_c} D \Lambda_+ + \frac{Z}{Z_c} (1 - \alpha Z_c) \Lambda_+ \geq \frac{Z_c - Z}{Z_c} D \Lambda_+.
\]

(3.25)

Now, since \( \sum_{n<j}^N \frac{\alpha}{|x_n - x_j|} > 0 \), \( Z < Z_c \), and \( \psi = \Lambda_+^N \psi \), using (3.25) we obtain

\[
\langle \mathcal{H}_N \psi, \psi \rangle \geq \left\langle \sum_{n=1}^N \left( D_n - \frac{\alpha Z}{|x_n|} \right) \psi, \psi \right\rangle \geq C_Z \left\langle \sum_{n=1}^N D_n \psi, \psi \right\rangle \geq C_{N,Z} \| \psi \|^2_{H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4N})},
\]

(3.26)

which is (3.23).
Lemma 6 Let \( \{\chi_a\}_{a \in A} \) be a partition of unity with the properties
\[
\chi_a \in C^2(\mathbb{R}^{3N}), \quad \chi_a \geq 0, \quad \sum_{a \in A} \chi_a^2 = 1.
\] (3.27)

Then for any \( \psi \in \Lambda^N_{N+1} \cap H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \) we have
\[
\left| \langle \mathcal{H}_N \psi, \psi \rangle - \sum_{a \in A} \langle \mathcal{H}_N \Lambda^N_{N+1} \chi_a \psi, \Lambda^N_{N+1} \chi_a \psi \rangle \right| 
\leq C_N Z \sum_{a \in A} \left( \| \nabla \chi_a \|_{L_\infty(\mathbb{R}^{3N})} + \| \partial^2 \chi_a \|_{L_\infty(\mathbb{R}^{3N})} \right) \left( 1 + \| \nabla \chi_a \|_{L_\infty(\mathbb{R}^{3N})} \right)^2 \langle \mathcal{H}_N \psi, \psi \rangle.
\] (3.28)

Proof. We write
\[
\langle \mathcal{H}_N \psi, \psi \rangle = \left( \sum_{n=1}^N \left( D_n - \frac{\alpha Z}{|x_n|} \right) + \sum_{n<j} \left( \frac{\alpha}{|x_n - x_j|} \right) \right) \sum_{a \in A} \chi_a^2 \Lambda^N_{N+1} \psi, \Lambda^N_{N+1} \psi \right)
= \sum_{a \in A} \left( \sum_{n=1}^N \left( D_n - \frac{\alpha Z}{|x_n|} \right) + \sum_{n<j} \left( \frac{\alpha}{|x_n - x_j|} \right) \right) \chi_a \Lambda^N_{N+1} \psi, \chi_a \Lambda^N_{N+1} \psi \right)
+ \sum_{a \in A} \left( \sum_{n=1}^N \left( D_n - \frac{\alpha Z}{|x_n|} \right) + \sum_{n<j} \left( \frac{\alpha}{|x_n - x_j|} \right) \right) [\chi_a, \Lambda^N_{N+1}] \psi, [\chi_a, \Lambda^N_{N+1}] \psi \right).
\] (3.29)

In the second line of (3.29) we used the relation
\[
\sum_{a \in A} \langle g, \nabla (\chi_a^2 g) \rangle = \sum_{a \in A} \langle \chi_a g, \nabla (\chi_a g) \rangle + \sum_{a \in A} \langle g, \nabla \left( \frac{\chi_a^2}{2} \right) g \rangle,
\] (3.30)
which holds for any \( g \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \). The last term in (3.30) is zero because of (3.27).

It remains to estimate the last two terms on the r.h.s. of (3.29). Since the sesquilinear form of \( \sum_{n=1}^N \left( D_n - \frac{\alpha Z}{|x_n|} \right) + \sum_{n<j} \left( \frac{\alpha}{|x_n - x_j|} \right) \) is bounded on \( H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4N}) \) (for the potential energy terms this follows from the Kato inequality), Lemmata 3
and (3.30) imply that
\[
\left| \left\langle \sum_{n=1}^{N} \left( D_n - \frac{\alpha Z}{|x_n|} \right) \right| + \sum_{n<j}^N \frac{\alpha}{|x_n - x_j|} \right| \left| \beta \right| \sum_{n=1}^N \left| \frac{1}{|x_n|} \right| \left| \alpha \right| \left| \beta \right| \left| \psi \right| \left| \chi \right| \left| \Lambda N^+ \right| \right| \leq \tilde{C}_{N,Z} \left( \left\| \nabla \chi a \right\|_{L^\infty(\mathbb{R}^3N)} + \left\| \partial^2 \chi a \right\|_{L^\infty(\mathbb{R}^3N)} \right) \right. 
\times \left( 1 + \left\| \nabla \chi a \right\|_{L^\infty(\mathbb{R}^3N)} \right)^2 \left\| \psi \right\|^2_{H^1/2(\mathbb{R}^3N,C^4N)}, \quad \text{for all } a \in \mathcal{A}.
\]

The relation (3.28) follows from (3.29), (3.31) and Lemma 5.

\section{Proof of Theorem 1: "Easy Part"}

We shall prove that
\[
\sigma_{ess}(H_N) \supseteq [E_{N-1} - 1, \infty),
\]
by construction of an appropriate Weyl sequence for $H_N$ at the point $E_{N-1} + \lambda$ for any $\lambda \geq 1$.

Since $H_N$ commutes with the projector $P_A$ onto the antisymmetric subspace, it suffices to find a Weyl sequence $\{\Psi_l\}_{l=1}^\infty \in \otimes_{n=1}^N L^2(\mathbb{R}^3, C^4)$ such that for $l$ big enough
\[
\left\| P_A \Psi_l \right\| > \delta_0, \quad \delta_0 > 0,
\]
where $\delta_0$ is independent of $l$.

For $j \in \mathbb{N}$ let
\[
\varphi_j \in P_j[H_{N-1}^{E_{N-1}, E_{N-1} + 1}](H_N) \delta N^{N-1}, \quad \left\| \varphi_j \right\|_{L_2(\mathbb{R}^3(N-1), C^4(N-1))} = 1.
\]

Here $P_j(H_{N-1})$ is the spectral projector of $H_{N-1}$ corresponding to the interval $J$.

We choose a vector $k \in \mathbb{R}^3$ with
\[
\sqrt{1 + |k|^2} = \lambda.
\]

Let $\chi \in C_0^\infty(\mathbb{R}^3)$ be a function with supp $\chi \subset \{ y \in \mathbb{R}^3 \mid 1 \leq |y| \leq 2 \}$,
$\left\| \chi \right\|_{L_2(\mathbb{R}^3)} = 1$. For $p \in \mathbb{R}^3$ we define a family of operators $\Lambda^+_p$ in $C^4$ by
\[
\Lambda^+_p := \frac{1}{2} + \frac{\alpha \cdot p + \beta}{2 \sqrt{|p|^2 + 1}}.
\]

Let $u(k) \in \text{Ran}(\Lambda^+_p)$ and $|u(k)| = 1$. Then (4.4) implies
\[
(\alpha \cdot k + \beta)u(k) = \lambda u(k).
\]
For a sequence \( 0 < R_j \nearrow \infty, \ j \in \mathbb{N} \) we define
\[
\psi_j(y) := R_j^{-3/2} \chi(R_j^{-1}y)e^{iky}u(k), \quad y \in \mathbb{R}^3, \ j \in \mathbb{N}.
\]
Assuming that
\[
R_{j+1} \geq 2R_j,
\]
we get
\[
\langle \psi_j, \psi_k \rangle = \delta_{jk}, \ j, k \in \mathbb{N}.
\]

**Lemma 7** For the sequence \( \{\psi_j\}_{j=1}^{\infty} \) we have
\[
\|\Lambda_+\psi_j - \psi_j\|_{L_2(\mathbb{R}^3,\mathbb{C}^1)} \rightarrow 0.
\]

**Proof.** Since the Fourier transform of \( \psi_j \) is
\[
\hat{\psi}_j(p) = R_j^{3/2} \hat{\chi}(R_j(p-k))u(k),
\]
one has
\[
\|\Lambda_+\psi_j - \psi_j\|_{L_2(\mathbb{R}^3,\mathbb{C}^1)} \leq \left\| (\Lambda_+(p) - 1)I_{B(R_j^{-1/2},k)}(p)R_j^{3/2} \hat{\chi}(R_j(p-k))u(k) \right\|_{L_2(\mathbb{R}^3,\mathbb{C}^1)}
\]
\[
+ \left\| (\Lambda_+(p) - 1)I_{\mathbb{R}^3 \setminus B(R_j^{-1/2},k)}(p)R_j^{3/2} \hat{\chi}(R_j(p-k))u(k) \right\|_{L_2(\mathbb{R}^3,\mathbb{C}^1)}.
\]
Obviously
\[
\left\| (\Lambda_+(p) - 1) - (\Lambda_+(k) - 1) \right\|_{\mathbb{C}^1 \rightarrow \mathbb{C}^1} \leq C|p-k|
\]
for \( C > 0 \) independent of \( k \). Hence one can estimate the first term in (11) by \( CR_j^{-1/2}\|\chi\|_{L_2(\mathbb{R}^3)} \). The second term in (11) is bounded by \( \|\hat{\chi}\|_{L_2(\mathbb{R}^3 \setminus B(R_j^{1/2}))} \), and consequently converges to zero, too.

Now we are ready to define the desired Weyl sequence. Let
\[
\Psi_j(x,x_N) := \varphi_j(x) \otimes \psi_j(x_N),
\]
\[
x = (x_1, \ldots, x_{N-1}) \in \mathbb{R}^{3(N-1)}, \ x_N \in \mathbb{R}^3, \ j \in \mathbb{N}.
\]
Recall that \( \varphi_j \) is a vector function with \( 4(N-1) \) components and \( \psi_j \) is a vector function with 4 components.

**Lemma 8** The sequence \( \{\Psi_j\}_{j=1}^{\infty} \) has the following properties:
(i) \( \|\Lambda_+^N\Psi_j\|_{j \rightarrow \infty} \rightarrow 1, \)
(ii) \( |\langle \Lambda_+^N\Psi_j, \Lambda_+^N\Psi_k \rangle| \rightarrow 0, \ k \neq j, \ k, j \rightarrow \infty, \)
(iii) \( \| (\mathcal{H}_N - E_{N-1} - \lambda)\Lambda_+^N\Psi_j \|_{j \rightarrow \infty} \rightarrow 0. \)
Proof of Lemma 8. Relations \((i)\) and \((ii)\) follow from Lemma 7 and relation \((4.9)\).

Let us prove \((4.13)\). We have

\[
(\mathcal{H}_N - E_{N-1} - \lambda)\Lambda^N_{+}\Psi_j
\]

\[
= (\mathcal{H}_N - E_{N-1})\Lambda^N_{+}\Psi_j + \Lambda^N_{+}\left((D_N - \lambda) - \frac{\alpha Z}{|x_N|} + \sum_{n=1}^{N-1} \frac{\alpha}{|x_n - x_N|}\right)\Lambda^N_{+}\Psi_j.
\]

(4.14)

The operator \(\mathcal{H}_N - 1\) acts on the function \(\varphi_j\) only.

The first term in \((4.14)\) tends to zero in norm according to \((4.3)\).

Since \(\Lambda^N_{+}\) commutes with \(D_N\) we have

\[
\|(D_N - \lambda)\Lambda^N_{+}\Psi_j\|_{L_2(\mathbb{R}^{3N},\mathcal{L}^N)} \leq \|(D_N - \lambda)\Psi_j\|_{L_2(\mathbb{R}^{3N},\mathcal{L}^N)}
\]

\[
\leq \|R_j^{-3/2} \alpha \cdot \nabla_{x_N} \chi(R_j^{-1}x_N)u(k)\|_{L_2(\mathbb{R}^3,\mathcal{L}^N)} \xrightarrow{j \to \infty} 0.
\]

(4.15)

In the second inequality of \((4.15)\) we have used \((4.6)\).

To prove \((4.13)\) it suffices now to show that

\[
\left\| \Lambda^N_{+}\left(-\frac{\alpha Z}{|x_N|} + \sum_{n=1}^{N-1} \frac{\alpha}{|x_n - x_N|}\right)\Lambda^N_{+}\Psi_j \right\| \xrightarrow{j \to \infty} 0.
\]

(4.16)

Let

\[
\eta_1 \in C_0^\infty(\mathbb{R}^3), \quad \eta_1(x) \equiv \begin{cases} 1, & x \in B(1/2), \\ 0, & x \in \mathbb{R}^3 \setminus B(3/4), \end{cases} \quad \eta_j(x) := \eta_1(x/R_j), \quad j \in \mathbb{N}.
\]

We estimate now the term in \((4.16)\) corresponding to the interaction with the nucleus.

\[
\left\| \Lambda^N_{+}\left(-\frac{\alpha Z}{|x_N|} + \sum_{n=1}^{N-1} \frac{\alpha}{|x_n - x_N|}\right)\Lambda^N_{+}\Psi_j \right\| \leq \alpha Z \left( \frac{\eta_j(x_N)}{|x_N|} \right)(\Lambda_{+}\psi_j)(x_N)
\]

\[
+ \left\| \frac{(1 - \eta_j(x_N))}{|x_N|} \right(\Lambda_{+}\psi_j)(x_N) \right\|.
\]

(4.17)

For the first term in \((4.17)\) the Hardy inequality and the commutativity of \(\Lambda_{+}\) with \(\nabla\) imply

\[
\left\| \frac{\eta_j(x_N)}{|x_N|} \right(\Lambda_{+}\psi_j)(x_N) \right\| \leq 2\|\nabla \eta_j\|_{L_\infty(\mathbb{R}^3)} \|\Lambda_{+}\psi_j\| + 2\|\Lambda_{+}\nabla \psi_j\|_{L_2(B(3R_j/4))}.
\]

(4.18)

The first term in \((4.18)\) decays as \(R_j \to \infty\), since it is bounded by

\[
2\|\nabla \eta_1\|_{L_\infty(\mathbb{R}^3)} R_j^{-1}. \quad \text{Applying Lemma 2 to the second term on the r.h.s. of \((4.18)\),}
\]

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we arrive at
\[ \| \Lambda_+ \nabla \psi_j \|_{L^2(B(3R_j/4))} \leq \left( \frac{4\pi}{3} \left( \frac{3R_j}{4} \right)^3 \right)^{1/2} \| \Lambda_+ \nabla \psi_j \|_{L^\infty(B(3R_j/4))} \]
\[ \leq \left( \frac{4\pi}{3} \left( \frac{3R_j}{4} \right)^3 \right)^{1/2} G(R_j/4) \left( \frac{4\pi}{3} (2R_j)^3 \right)^{1/2} \| \nabla \psi_j \|_{L^2(\mathbb{R}^3)}. \] (4.19)

The last factor in (4.19) is bounded uniformly in \( j \). The function \( G \) and consequently the r.h.s. of (4.19) decays exponentially as \( R_j \to \infty \). We can estimate the second term in (4.20) by \( 2\alpha Z/R_j \). Hence the r.h.s. of (4.17) tends to 0 as \( R_j \to \infty \).

Let us turn to the interaction between the \( N^{th} \) and the \( n^{th} \) electrons. We have
\[ \left\| \Lambda_+^N \frac{\alpha}{|x_n - x_N|} \Lambda_+^N \Psi_j \right\| \leq \left\| \frac{\alpha \rho_{\varphi_j} (x_n)}{|x_n - x_N|} (\Lambda_+ \psi_j)(x_N) \right\|_{\{ |x_n| \geq R_j/4 \}} \]
\[ + \left\| \frac{\alpha \rho_{\varphi_j} (x_n)}{|x_n - x_N|} \eta_j(x_N) (\Lambda_+ \psi_j)(x_N) \right\|_{\{ |x_n| < R_j/4 \}} \]
\[ + \left\| \frac{\alpha \rho_{\varphi_j} (x_n)}{|x_n - x_N|} (1 - \eta_j(x_N)) (\Lambda_+ \psi_j)(x_N) \right\|_{\{ |x_n| < R_j/4 \}}, \] (4.20)

where
\[ \rho_{\varphi_j}(x_n) = \int_{\mathbb{R}^{3(N-2)}} |\varphi_j(x_1, \ldots, x_{N-1})|^2 \, dx_1 \cdots dx_{n-1} dx_{n+1} \cdots dx_{N-1} \] (4.21)

if \( N > 2 \), and \( \rho_{\varphi_j} = |\varphi_j|^2 \) if \( N = 2 \); \( \| \rho_{\varphi_j} \|_{L^2(\mathbb{R}^3)} = 1 \). By the Hardy inequality the first term in (4.20) can be estimated as
\[ \left\| \frac{\alpha \rho_{\varphi_j} (x_n)}{|x_n - x_N|} (\Lambda_+ \psi_j)(x_N) \right\|_{\{ |x_n| \geq R_j/4 \}} \leq 2\alpha \| \nabla \psi_j \| \| \rho_{\varphi_j} \|_{L^2(\mathbb{R}^3 \setminus B(R_j/4))}. \] (4.22)

For the second term in (4.20) analogously to (4.16) and (4.19) we have
\[ \left\| \frac{\alpha \rho_{\varphi_j} (x_n)}{|x_n - x_N|} \eta_j(x_N) (\Lambda_+ \psi_j)(x_N) \right\|_{\{ |x_n| < R_j/4 \}} \leq 2\alpha \| \nabla \eta_j \|_{L^\infty(\mathbb{R}^3)} R_j^{-1} \]
\[ + 2\alpha \left( \frac{4\pi}{3} \left( \frac{3R_j}{4} \right)^3 \right)^{1/2} G(R_j/4) \left( \frac{4\pi}{3} (2R_j)^3 \right)^{1/2} \| \nabla \psi_j \|_{L^2(\mathbb{R}^3)}. \] (4.23)

Finally, the last term on the r.h.s. of (4.20) can be estimated by \( 4\alpha/R_j \), since on the domain of integration \( |x_n - x_N| > R_j/4 \).

Combining these estimates, we arrive at (4.13). Lemma S is proved. •

Our next goal is to prove that the functions \( \{ \Psi_j \}_{j=1}^\infty \) can be antisymmetrized without violation of the condition (4.2) at least for \( j \) big enough.
Let
\[(T_{kN}\Psi_j)(x_1, \ldots, x_N) := \varphi(x_1, \ldots, x_{k-1}, x_k, x_{k+1}, \ldots, x_{N-1}) \otimes \psi_j(x_k), \quad k = 1, \ldots, N - 1, \quad T_{NN}\Psi_j := -\Psi_j, \quad j \in \mathbb{N}. \tag{4.24}\]

The operator \(T_{kN}\) permutes the \(k^{th}\) and the \(N^{th}\) electrons. The functions \(P_A\Psi_j\) are given by
\[(P_A\Psi_j)(x_1, \ldots, x_N) = \frac{-1}{\sqrt{N}} \sum_{k=1}^{N-1} T_{kN}A_j^N\Psi_j(x_1, \ldots, x_N), \quad j \in \mathbb{N}. \tag{4.25}\]

For the norms of these functions we have
\[
\|P_A\Psi_j\|^2 = \frac{1}{N} \sum_{k=1}^{N-1} T_{kN}\varphi_j(x_1, \ldots, x_{N-1})(\Lambda_+\psi_j)(x_N), \quad j \in \mathbb{N},
\]
\[
\geq 1 - \frac{N - 1}{2} \left| \langle \varphi_j(x_1, \ldots, x_{N-1}) (\Lambda_+\psi_j)(x_N), (\Lambda_+\psi_j)(x_1) \varphi_j(x_2, \ldots, x_N) \rangle \right|,
\tag{4.26}\]
where the scalar products are taken in \(\bigotimes_{n=1}^{N} L_2(\mathbb{R}^3, \mathbb{C}^4)\). To estimate the inner product on the r. h. s. of (4.26), we write
\[
\left| \langle \varphi_j(x_1, \ldots, x_{N-1}) (\Lambda_+\psi_j)(x_N), (\Lambda_+\psi_j)(x_1) \varphi_j(x_2, \ldots, x_N) \rangle \right|
\leq \left| \langle (1 - I_{B(R_j/2)}(x_1)) \varphi_j(x_1, \ldots, x_{N-1}) (\Lambda_+\psi_j)(x_N), (\Lambda_+\psi_j)(x_1) \varphi_j(x_2, \ldots, x_N) \rangle \right|
\]
\[
+ \left| \langle \varphi_j(x_1, \ldots, x_{N-1}) (\Lambda_+\psi_j)(x_N), I_{B(R_j/2)}(x_1)(\Lambda_+\psi_j)(x_1) \varphi_j(x_2, \ldots, x_N) \rangle \right|.
\tag{4.27}\]

The first term on the r. h. s. of (4.27) tends to zero since
\[
\left\| (1 - I_{B(R_j/2)}(x_1)) \varphi_j(x_1, \ldots, x_{N-1}) \right\|_{L^2(\mathbb{R}^{N-1}, C^{(N-1)})} \text{ does. The second one also vanishes, because by Lemma 2}
\]
\[
\left\| I_{B(R_j/2)}(x_1)(\Lambda_+\psi_j)(x_1) \right\|_{R_j \to \infty} \to 0.
\]

This completes the proof of (4.1).

5 Proof of Theorem \[\square\] “Hard Part”

We shall prove that
\[
\inf \sigma_{ess}(\mathcal{H}_N) \geq E_{N-1} + 1. \tag{5.1}\]
Together with (4.1) this gives (2.5).
5.1 Partition of Unity

For a function \( \chi \in C^\infty(\mathbb{R}^3, [0, 1]) \) with \( \chi|_{B(1)} \equiv 0 \) and \( \chi|_{\mathbb{R}^3 \setminus B(2)} \equiv 1 \), let

\[
\tilde{\chi}_a := \chi(x_a), \quad a = 1 \ldots N, \quad \tilde{\chi}_0 := \prod_{a=1}^{N} (1 - \tilde{\chi}_a).
\]

Let

\[
\varphi(x) := \sum_{a=0}^{N} \tilde{\chi}_a^2(x).
\]

Obviously, there exists a constant \( \delta > 0 \) such that for any \( x \in \mathbb{R}^{3N} \) we have \( \delta < \varphi(x) < \delta^{-1} \). For \( R > 0 \) we define a partition of unity

\[
\chi_a(x) := \frac{\tilde{\chi}_a(x/R)}{\sqrt{\varphi(x/R)}}, \quad x \in \mathbb{R}^{3N}, \quad a = 0, \ldots, N. \tag{5.2}
\]

It is clear that the partition (5.2) satisfies all the hypotheses (3.27) of Lemma 6. Moreover, for \( a \neq 0 \) the functions \( \chi_a \) are symmetric under all permutations of the electrons which do not include the \( a^{th} \) one. We also note that the derivatives of \( \chi_a \) decay as \( R \) tends to infinity:

\[
\| \nabla \chi_a \|_\infty \leq CR^{-1}, \quad \| \partial^2 \chi_a \|_\infty \leq CR^{-2}, \quad a = 0, \ldots, N. \tag{5.3}
\]

5.2 Estimates Outside the Compact Region

For \( \varepsilon > 0 \) we choose \( R = R(\varepsilon) \) big enough so that the following conditions hold:

(i)

\[
\bar{C}_{N,Z} \sum_{a \in \mathcal{A}} \left( \| \nabla \chi_a \|_{L_\infty(\mathbb{R}^{3N})} + \| \partial^2 \chi_a \|_{L_\infty(\mathbb{R}^{3N})} \right) \left( 1 + \| \nabla \chi_a \|_{L_\infty(\mathbb{R}^{3N})} \right)^2 < \varepsilon, \tag{5.4}
\]

where \( \bar{C}_{N,Z} \) is the constant in (3.28),

(ii)

\[
\frac{\alpha Z}{R} < \varepsilon(1 - \alpha Z), \tag{5.5}
\]

(iii) For any \( \psi \in \Lambda^N \bigoplus_{n=1}^{N} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \) and \( a = 1, \ldots, N \)

\[
\left| \left( E_{N-1} + 1 - \frac{\alpha Z}{|x_a|} \right) [A^N_+, \chi_a] \psi, [A^N_+, \chi_a] \psi \right| + \left| \left( E_{N-1} + 1 - \frac{\alpha Z}{|x_a|} \right) \chi_a \psi, [A^N_+, \chi_a] \psi \right| < \frac{\varepsilon N}{N} \langle H_N \psi, \psi \rangle. \tag{5.6}
\]

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The possibility to fulfill (5.6) choosing \( R \) big enough follows from the Kato inequality and Lemmata 3, 4, and 5.

We now estimate from below the quadratic form of \( H_N \) on a function \( \psi \) from \( \Lambda^N_{+} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \). Recall that \( \Lambda^N_{+} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \) is the form domain of \( H_N \).

By Lemma 6 and (5.4)

\[
\langle H_N \psi, \psi \rangle \geq \sum_{a=0}^{N} \langle H_N \Lambda^N_{+} \chi_a \psi, \Lambda^N_{+} \chi_a \psi \rangle - \epsilon \langle H_N \psi, \psi \rangle.
\] (5.7)

For \( a = 1, \ldots, N \) we have

\[
\langle H_N \Lambda^N_{+} \chi_a \psi, \Lambda^N_{+} \chi_a \psi \rangle = \left( \langle H_{N-1} + D_a - \frac{\alpha Z}{|x_a|} + \sum_{k \neq a} \frac{\alpha}{|x_a - x_k|} \rangle \Lambda^N_{+} \chi_a \psi, \Lambda^N_{+} \chi_a \psi \right),
\] (5.8)

where \( H_{N-1} \) acts on the coordinates of all electrons except the \( a^{th} \) one. The inequalities \( H_{N-1} \geq E_{N-1}, \Lambda^N_{+} D_a \Lambda^N_{+} \geq 1 \), and \( \sum_{k \neq a} \frac{\alpha}{|x_a - x_k|} > 0 \) for \( a = 1, \ldots, N \) imply

\[
\langle H_N \Lambda^N_{+} \chi_a \psi, \Lambda^N_{+} \chi_a \psi \rangle \geq \langle (E_{N-1} + 1 - \frac{\alpha Z}{|x_a|}) \Lambda^N_{+} \chi_a \psi, \Lambda^N_{+} \chi_a \psi \rangle
\]

\[
= \langle (E_{N-1} + 1 - \frac{\alpha Z}{|x_a|}) \chi_a \psi, \chi_a \psi \rangle + \langle (E_{N-1} + 1 - \frac{\alpha Z}{|x_a|}) \Lambda^N_{+} \chi_a \psi, \Lambda^N_{+} \chi_a \psi \rangle
\]

\[
+ \langle (E_{N-1} + 1 - \frac{\alpha Z}{|x_a|}) \chi_a \psi, [\Lambda^N_{+} \chi_a \psi] \rangle.
\] (5.9)

Since on supp \( \chi_a \) we have \(|x_a| \geq R\), from the relations (5.5), (5.6), and (5.9) we conclude

\[
\langle H_N \Lambda^N_{+} \chi_a \psi, \Lambda^N_{+} \chi_a \psi \rangle \geq (E_{N-1} + 1) \langle \chi_a \psi, \chi_a \psi \rangle
\]

\[
- \frac{\epsilon}{N} \langle H_N \psi, \psi \rangle - \epsilon (1 - \alpha Z) \|\psi\|^2, \quad a = 1, \ldots, N.
\] (5.10)

Using (3.24), we arrive at

\[
\langle H_N \psi, \psi \rangle \geq \sum_{n=1}^{N} \left( D_n - \frac{\alpha Z}{|x_n|} \right) \psi, \psi \rangle \geq N (1 - \alpha Z) \|\psi\|^2.
\] (5.11)

Due to (5.7), (5.10), and (5.11)

\[
(1 + 3\epsilon) \langle H_N \psi, \psi \rangle \geq (E_{N-1} + 1) \sum_{a=1}^{N} \langle \chi_a \psi, \chi_a \psi \rangle + \langle H_N \Lambda^N_{+} \chi_0 \psi, \Lambda^N_{+} \chi_0 \psi \rangle.
\] (5.12)
5.3 Estimate Inside the Compact Region

Our next goal is to estimate from below the quadratic form of the operator \( H_N \Lambda^N_+ \) on the function \( \chi_0 \psi \) supported in \([-2R, 2R]^3N\).

**Lemma 9** For \( M > 0 \) let \( W_M := \{ p \in \mathbb{R}^{3N} \mid |p_i| \leq M, i = 1, \ldots, 3N \} \), \( \bar{W}_M := \mathbb{R}^{3N} \setminus W_M \). There exists a finite set \( Q_M \) of functions in \( L_2(\mathbb{R}^{3N}) \) such that for any function \( f \in L_2(\mathbb{R}^{3N}) \) with \( \text{supp} f \subset [-2R, 2R]^3N \), \( f \perp Q_M \) holds

\[
\| \tilde{f} \|_{L_2(\bar{W}_M)} \geq \frac{1}{2} \| \tilde{f} \|_{L_2(\mathbb{R}^{3N})}.
\]  

(5.13)

The proof of Lemma 9 is analogous to the proof of Theorem 7 in [25] and will be given in the Appendix C for convenience.

It follows from (3.25) that for any \( M > 0 \)

\[
\langle \mathcal{H}_N \Lambda^N_+ \chi_0 \psi, \Lambda^N_+ \chi_0 \psi \rangle = \left\langle \left( \sum_{n=1}^{N} \left( D_n - \frac{\alpha Z}{|x_n|} \right) + \sum_{n<j} \frac{\alpha}{|x_n - x_j|} \right) \Lambda^N_+ \chi_0 \psi, \Lambda^N_+ \chi_0 \psi \right\rangle \geq \frac{Z_c - Z}{Z_c} \left( \sum_{n=1}^{N} D_n I_{\bar{W}_M} \Lambda^N_+ \chi_0 \psi, \Lambda^N_+ \chi_0 \psi \right).
\]  

(5.14)

Here \( I_{\bar{W}_M} \) is the operator of multiplication by the characteristic function of \( \bar{W}_M \) in momentum space.

We choose

\[
M := \sqrt{\frac{8Z_c(E_{N-1} + 1)}{Z_c - Z}} - 1
\]  

(5.15)

and assume henceforth that \( f := \chi_0 \psi \) is orthogonal to the set \( Q_M \) defined in Lemma 9. Since in momentum space the operator \( D \) acts on functions from \( \Lambda_+ L_2(\mathbb{R}^3, \mathbb{C}^4) \) as multiplication by \( \sqrt{|k|^2 + 1} \), we have

\[
\left\langle \sum_{n=1}^{N} D_n I_{\bar{W}_M} \Lambda^N_+ \chi_0 \psi, \Lambda^N_+ \chi_0 \psi \right\rangle \geq \sqrt{M^2 + 1} \| I_{\bar{W}_M} \Lambda^N_+ \chi_0 \psi \|^2.
\]  

(5.16)

Inequalities (5.14) and (5.16) imply

\[
\langle \mathcal{H}_N \Lambda^N_+ \chi_0 \psi, \Lambda^N_+ \chi_0 \psi \rangle \geq \frac{Z_c - Z}{Z_c} \sqrt{M^2 + 1} \| I_{\bar{W}_M} \Lambda^N_+ \chi_0 \psi \|^2 \\
\geq \frac{Z_c - Z}{Z_c} \sqrt{M^2 + 1} \left( \| I_{\bar{W}_M} \chi_0 \psi \| - \frac{1}{2} \| I_{\bar{W}_M} [\Lambda^N_+, \chi_0] \psi \| \right)^2 \\
\geq \frac{Z_c - Z}{Z_c} \sqrt{M^2 + 1} \left( \| I_{\bar{W}_M} \chi_0 \psi \|^2 - \frac{1}{2} \| I_{\bar{W}_M} [\Lambda^N_+, \chi_0] \psi \|^2 \right) \\
\geq 4(E_{N-1} + 1) \| I_{\bar{W}_M} \chi_0 \psi \|^2 \\
- 8(E_{N-1} + 1) \| [\Lambda^N_+, \chi_0] \|^2_{L_2(\mathbb{R}^{3N}, \mathbb{C}^{4N})} \| \psi \|^2.
\]  

(5.17)
In the last step we used our choice of \(M\) (see (5.13)). Since \(\Lambda_+ \psi\) is a bounded operator in \(L_2(\mathbb{R}^3, \mathbb{C}^4)\), and
\[
\|[\chi_0, \Lambda_N^+]\|_{L_2(\mathbb{R}^3, \mathbb{C}^4)} \leq C(\|\nabla \chi_0\| \infty + \|\partial^2 \chi_0\| \infty)
\]
by Lemma 1 and the relation (5.22), we can choose \(R\) big enough, so that
\[
8|E_{N-1} + 1|\|\Lambda_N^+ \psi\|_{L_2(\mathbb{R}^3, \mathbb{C}^4)} \leq \varepsilon. \tag{5.18}
\]
For the first term on the r.h.s. of (5.17) Lemma 9 implies
\[
4\|I_{W_\delta} \chi_0 \psi\| \geq \|\chi_0 \psi\|^2. \tag{5.19}
\]
As a consequence of (5.17)–(5.19), we have
\[
\langle H_N \Lambda_N^+ \chi_0 \psi, \Lambda_N^+ \chi_0 \psi \rangle \geq (E_{N-1} + 1)\|\chi_0 \psi\|^2 - \varepsilon \|\psi\|^2. \tag{5.20}
\]

5.4 Completion of the Proof

By (5.12) and (5.20)
\[
(1 + 3\varepsilon)\langle H_N \psi, \psi \rangle \geq (E_{N-1} + 1) \sum_{a=0}^N \langle \chi_a \psi, \chi_a \psi \rangle - \varepsilon \|\psi\|^2 = (E_{N-1} + 1 - \varepsilon)\|\psi\|^2 \tag{5.21}
\]
for any \(\varepsilon > 0\) and any \(\psi\) in the form domain of \(H_N\) orthogonal to the finite set of functions (cardinality of this set depends on \(\varepsilon\)). This implies the discreteness of the spectrum of \(H_N\) below \(E_{N-1} + 1\) and thus (5.1).

6 Existence of Eigenvalues

1. To prove the infiniteness of the discrete spectrum of \(H_N\) it suffices to construct for a given \(Q \in \mathbb{N}\) a \(Q\)-dimensional subspace \(\mathcal{M}\) such that for any \(\Psi \in \mathcal{M}\) we have
\[
\langle H_N \Psi, \Psi \rangle < (E_{N-1} + 1)\|\Psi\|^2.
\]

Using induction on \(N\) and the well–known existence of the ground state of \(H_1\), we can assume that \(H_{N-1}\) has a ground state \(\phi\). Let \(\psi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^4)\) be a function with \(\operatorname{supp} \bar{\psi} \subset B(N - \frac{4}{3}) \setminus B(N - \frac{2}{3})\), whose 3rd and 4th components are identical to zero. Let \(\|\bar{\psi}\|_{L_2(\mathbb{R}^3, \mathbb{C}^4)} = 1\). Let
\[
\psi_m(y) := R_m^{-3/2} \bar{\psi}\left(\frac{y}{R_m}\right), \quad R_m := 2^m R, \quad m = 1, \ldots Q. \tag{6.1}
\]
The parameter \(R\) will be chosen later. Note that \(\Lambda_+ \psi_m \neq 0\) for large \(R\) due to (5.11) and the choice of the components of \(\bar{\psi}\).
We consider the quadratic form of $H_N$ on linear combinations of the form

$$\sum_{m=1}^{Q} c_m \sum_{k=1}^{N} T_{kN}(\phi \otimes \Lambda_{\psi_m}).$$

(6.2)

Here $T_{kN}$ for $k < N$ is the operator permuting the $k^{th}$ and the $N^{th}$ electrons, $T_{NN} := -1$. In the tensor product $\phi \otimes \Lambda_{\psi_m}$ the function $\phi$ is assumed to depend on $x_1, \ldots, x_{N-1}$, and $\psi_m$ depends on $x_N$. The functions $\tilde{H}_N$ are antisymmetric in all variables.

It suffices to show that on the functions (6.2) the quadratic form of $\tilde{H}_N := H_N - E_{N-1} - 1$

is negative for any choice of the coefficients $\{c_m\}_{m=1}^{Q}$.

Using the permutation symmetry of $\phi$ and $\tilde{H}_N$, we can write

$$\langle \tilde{H}_N \sum_{m=1}^{Q} c_m \sum_{k=1}^{N} T_{kN}(\phi \otimes \Lambda_{\psi_m}), \sum_{n=1}^{Q} c_n \sum_{l=1}^{N} T_{lN}(\phi \otimes \Lambda_{\psi_n}) \rangle$$

$$= \sum_{m=1}^{Q} |c_m|^2 \sum_{k,l=1}^{N} \langle \tilde{H}_N T_{kN}(\phi \otimes \Lambda_{\psi_m}), T_{lN}(\phi \otimes \Lambda_{\psi_m}) \rangle$$

$$+ 2 \sum_{n < m} c_m c_n \sum_{k,l=1}^{N} \langle \tilde{H}_N T_{kN}(\phi \otimes \Lambda_{\psi_m}), T_{lN}(\phi \otimes \Lambda_{\psi_n}) \rangle$$

(6.3)

$$\leq \sum_{m=1}^{Q} |c_m|^2 \left\{ N \langle \tilde{H}_N (\phi \otimes \Lambda_{\psi_m}), \phi \otimes \Lambda_{\psi_m} \rangle \right.$$  

$$\left. + \frac{N(N-1)}{2} \sum_{n=1}^{Q} \left| \langle \tilde{H}_N (\phi \otimes \Lambda_{\psi_m}), T_{1N}(\phi \otimes \Lambda_{\psi_n}) \rangle \right| \right.$$  

$$\left. + N \sum_{n \neq m}^{Q} \left| \langle \tilde{H}_N (\phi \otimes \Lambda_{\psi_m}), \phi \otimes \Lambda_{\psi_n} \rangle \right| \right\}.$$

Our strategy is to show that the first term on the r.h.s. of (6.3) is negative and of the order $R^{-1}$ as $R \to \infty$, whereas the other terms decay more rapidly.

2. For the first term on the r.h.s. of (6.3) we have

$$\langle \tilde{H}_N (\phi \otimes \Lambda_{\psi_m}), \phi \otimes \Lambda_{\psi_m} \rangle$$

$$= \langle (D - 1)\Lambda_{\psi_m}, \Lambda_{\psi_m} \rangle - \langle \frac{\alpha Z}{|x|} \Lambda_{\psi_m}, \Lambda_{\psi_m} \rangle$$

(6.4)

$$+ \sum_{i < N} \frac{\alpha}{|x_i - x_N|} \rho_\phi(x_i)(\Lambda_{\psi_m})(x_N), \rho_\phi(x_i)(\Lambda_{\psi_m})(x_N) \rangle.$$
with $\rho_\phi$ defined in (4.21).

We start with the lower bound on the first term on the r.h.s. of (6.4). Recall that $\psi_1$ has the last two components equal to zero, thus relations (6.1), (2.2), and (3.1) imply

$$\langle (D\Lambda_+ - \Lambda_+)\psi_m, \psi_m \rangle = \langle \left(\frac{1}{2} + \frac{\sqrt{|q|^2 + R_m^2}}{2R_m} - \frac{1}{2} \frac{R_m}{2\sqrt{|q|^2 + R_m^2}}\right)\hat{\psi}_1(q), \hat{\psi}_1(q) \rangle = \langle \left(\frac{|q|^2}{2R_m\sqrt{|q|^2 + R_m^2}}\right)\hat{\psi}_1(q), \hat{\psi}_1(q) \rangle \leq \frac{1}{2R_m^2} \|q|\hat{\psi}_1(q)\|^2. \quad (6.5)$$

Here $q$ is the momentum dual to $y$ in (6.1). The norm in (6.5) is finite, since $\hat{\psi}_1 \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^4)$.

To estimate the interaction of an electron with the nucleus we choose

$$\delta := \frac{1}{10N - 8}. \quad (6.6)$$

Obviously,

$$- \langle \frac{\alpha Z}{|x|} \Lambda_+ \psi_m, \Lambda_+ \psi_m \rangle = - \langle \frac{\alpha Z}{|x|} I_{B(ZR_m)} \Lambda_+ \psi_m, \Lambda_+ \psi_m \rangle - \langle \frac{\alpha Z}{|x|} (1 - I_{B(ZR_m)}) \Lambda_+ \psi_m, \Lambda_+ \psi_m \rangle \leq - \frac{\alpha}{R_m} \|\Lambda_+ \psi_m\|^2 - \left\| (1 - I_{B(ZR_m)}) \Lambda_+ \psi_m \right\|^2 + \frac{\alpha}{R_m} \|\Lambda_+ \psi_m\|^2 \leq - \frac{(1 - \delta)\alpha}{R_m} \|\Lambda_+ \psi_m\|^2 + \frac{(2 + \delta^{-1})\alpha}{R_m} \|\Lambda_+ \psi_m\|^2. \quad (6.7)$$

Lemma 2 implies

$$\| (1 - I_{B(ZR_m)}) \Lambda_+ \psi_m \|^2 \leq \int_{ZR_m} 4\pi r^2 G^2 \left( r - \left( N - \frac{1}{5} \right) R_m \right)^4 \left( N - \frac{1}{5} \right)^3 R_m^3 \|\psi_m\|^2 dr$$

$$\leq \frac{16\pi^2}{3} \left( N - \frac{1}{5} \right)^3 R_m^3 \int_{ZR_m} G^2 \left( r - \left( N - \frac{1}{5} \right) R_m \right) r^2 dr,$$

which is a function decaying faster than any power of $R_m$.

Now we turn to estimating the electron-electron interaction. We split the
corresponding quadratic form into three integrals:

\[
\left\langle \frac{\alpha}{|x_i - x_N|} \rho_\phi(x_i)(\Lambda + \psi_m)(x_N), \rho_\phi(x_i)(\Lambda + \psi_m)(x_N) \right\rangle
= \alpha \left( \int_{|x| \geq R_m/5} \int_{|y| < (N-3/5)R_m} \int_{|x| < R_m/5} \right) \frac{|\rho_\phi(x)|^2}{|x - y|} (\Lambda + \psi_m)(y)^2 \left| \frac{\partial}{\partial x} \right| \left| \frac{\partial}{\partial y} \right| dxdy \tag{6.8}
\]

\(= I_1 + I_2 + I_3\).

From the Kato inequality (see [14], inequality V.5.33; see also [9])

\[
\int_{\mathbb{R}^3} |x|^{-1} |u(x)|^2 dx \leq \frac{\pi}{2} \int_{\mathbb{R}^3} |k|^2 |\hat{u}(k)|^2 dk, \quad \forall u \in H^{1/2}(\mathbb{R}^3) \tag{6.9}
\]

it follows that

\[
I_1 \leq \frac{\pi \alpha}{2R_m} \| \rho_\phi \|^2_{L_2(\mathbb{R}^3 \setminus B(R_m/5))} \| q^{1/2} \|_{L_2(\mathbb{R}^3)}^2. \tag{6.10}
\]

Using Lemma 2 we arrive at

\[
I_2 \leq \frac{4\pi \alpha}{3} \left( N - \frac{1}{5} \right) R_m^3 C^2 \left( \frac{R_m}{5} \right) \| \Lambda + \psi_m \|^2 \int_{|x| < \frac{2R_m}{5}} \int_{|y| < (N-3/5)R_m} \frac{1}{|x - y|} dydx. \tag{6.11}
\]

Here

\[
\int_{|y| < (N-3/5)R_m} \frac{1}{|x - y|} dy \leq \int_{|y| < (N-3/5)R_m} \frac{1}{|y|} dy \leq 2\pi \left( N - \frac{3}{5} \right)^2 R_m^2.
\]

Obviously, the r.h.s.'s of (6.10) and (6.11) decay faster than \(R_m^{-1}\). Finally, for \(I_3\) we have

\[
I_3 \leq \frac{\alpha}{(N - \frac{4}{5}) R_m} \| \Lambda + \psi_m \|^2. \tag{6.12}
\]

Combining (6.4) — (6.12), for large \(R\) we get

\[
\langle \tilde{H}_N (\phi \otimes \Lambda + \psi_m), \phi \otimes \Lambda + \psi_m \rangle \\
\leq \alpha \left( \frac{N - 1}{(N - \frac{4}{5})} - 1 + \delta \right) \| \Lambda + \psi_m \|^2 R_m^{-1} + o(R^{-1}). \tag{6.13}
\]

The coefficient at \(R_m^{-1}\) is negative due to (6.6).
where for the electrostatic terms we have used the Hardy inequality, the fact that 
$
\alpha > 0
$
commutes with the gradient and the equality 
$\|\Lambda_+\|_{L_2(\mathbb{R}^3, C^1)} = 1$. 

Let us prove now that the second term on the r.h.s. of (6.3) decays faster than 
$R^{-1}$. 

$\langle \tilde{H}_N (\phi \otimes \Lambda_+ \psi_m), T_{1N} (\phi \otimes \Lambda_+ \psi_n) \rangle$

\[
= \langle \left( (H_{N-1} - E_{N-1}) + (D_N - 1) - \frac{\alpha Z}{|x_N|} + \sum_{j=1}^{N-1} \frac{\alpha}{|x_j - x_N|} \right) 
\times \phi(x_1, \ldots, x_{N-1})(\Lambda_+ \psi_m)(x_N), (\Lambda_+ \psi_n)(x_1) \phi(x_2, \ldots, x_N) \rangle
\]

\[= \langle \left( (D_N - 1) - \frac{\alpha Z}{|x_N|} + \sum_{j=1}^{N-1} \frac{\alpha}{|x_j - x_N|} \right) 
\times \phi(x_1, \ldots, x_{N-1})(\Lambda_+ \psi_m)(x_N), (\Lambda_+ \psi_n)(x_1) \phi(x_2, \ldots, x_N) \rangle \quad (6.14)
\]

where $H_{N-1}$ acts on the first $N-1$ electrons.

We introduce a cut-off function

$\chi \in C_0^\infty(\mathbb{R}^3)$, $\chi(x) = \begin{cases} 1, & |x| \leq 1/4, \\ 0, & |x| \geq 1/2, \end{cases}$ $\chi_n(x) := \chi\left(\frac{x}{R_n}\right)$. (6.15)

One has

\[
\left| \langle \left( (D_N - 1) - \frac{\alpha Z}{|x_N|} + \sum_{j=1}^{N-1} \frac{\alpha}{|x_j - x_N|} \right) 
\times \phi(x_1, \ldots, x_{N-1})(\Lambda_+ \psi_m)(x_N), (\Lambda_+ \psi_n)(x_1) \phi(x_2, \ldots, x_N) \rangle \right|
\]

\[
\leq \left| \langle \phi(x_1, \ldots, x_{N-1}) - \frac{\alpha Z}{|x_N|} + \sum_{j=1}^{N-1} \frac{\alpha}{|x_j - x_N|} \right) 
\times (\Lambda_+ \psi_m)(x_N), \chi_n(x_1)(\Lambda_+ \psi_n)(x_1) \phi(x_2, \ldots, x_N) \rangle \right|
\]

\[
+ \left| \langle (1 - \chi_n(x_1)) \phi(x_1, \ldots, x_{N-1}) - \frac{\alpha Z}{|x_N|} + \sum_{j=1}^{N-1} \frac{\alpha}{|x_j - x_N|} \right) 
\times (\Lambda_+ \psi_m)(x_N), (\Lambda_+ \psi_n)(x_1) \phi(x_2, \ldots, x_N) \rangle \right|
\]

\[
\leq \left( \| (D_N - 1) \Lambda_+ \psi_m \|_{L_2(\mathbb{R}^3, C^1)} + 2\alpha (Z + N - 1) \| \psi_m \|_{L_2(\mathbb{R}^3, C^1)} \right)
\times \left( \| \chi_n \Lambda_+ \psi_n \|_{L_2(\mathbb{R}^3, C^1)} + \left( \| (1 - \chi_n(x_1)) \phi(x_1, \ldots, x_{N-1}) \|_{L_2(\mathbb{R}^3, C^1)} \right)^{N-1} \right).
\]

(6.16)

where for the electrostatic terms we have used the Hardy inequality, the fact that 
$\Lambda_+$ commutes with the gradient and the equality 
$\|\Lambda_+\|_{L_2(\mathbb{R}^3, C^1)} \to L_2(\mathbb{R}^3, C^1) = 1$. 

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Since only the first two components of $\psi_m$ are nonzero, we calculate

$$\|(D - 1)\Lambda_+\psi_m\|^2$$

$$= \langle (\alpha \cdot p + \beta - 1)(\alpha \cdot p + \beta - 1)\langle p\rangle + \alpha \cdot p + \beta \rangle \psi_m(p)\rangle \psi_m(p) \rangle$$

$$= \langle |p|^2\left(\frac{1}{2} - \frac{1}{2|p|^2 + 1}\right)\psi_m(p)\rangle \psi_m(p) \rangle$$

$$= \langle \left|q^2\right|\frac{1}{2} - \frac{R_m}{2|q|^2 + R_m^2}\left|\psi(q)\right| \psi(q) \rangle \leq \frac{1}{2R_m^2} \|\left|q\right| \psi(q)\|^2.$$  \hspace{1cm} (6.17)

Thus the first factor on the r.h.s. of (6.16) decays as $\|\nabla \psi_m\|$, which is of order $R^{-1}$. The first term in the second factor of (6.16) is an exponentially decaying function of $R$ due to Lemma 2 and the support properties of $\psi_n$ and $\chi_n$. The second one also goes to zero as $R \to \infty$. We conclude that the second term on the r.h.s. of (6.16) decays faster than $R^{-1}$.

4. We proceed to the estimate of the last term on the r.h.s. of (6.3). The key tool here is Lemma 2. We use the relation

$$\langle \hat{H}_N(\phi \otimes \Lambda_+\psi_m), \phi \otimes \Lambda_+\psi_n \rangle$$

$$= \langle (D - 1)\Lambda_+\psi_m, \Lambda_+\psi_n \rangle - \frac{\alpha Z}{|x\rangle} \Lambda_+\psi_m, \Lambda_+\psi_n \rangle$$

$$+ \sum_{i< N} \frac{\alpha}{|x_i - x_N|} \rho_\phi(x_i)(\Lambda_+\psi_m)(x_N), \rho_\phi(x_i)(\Lambda_+\psi_n)(x_N).$$  \hspace{1cm} (6.18)

For the kinetic energy term we have

$$\|\langle (D\Lambda_+ - \Lambda_+)\psi_m, \Lambda_+\psi_n \rangle \| = \|\langle \Lambda_+\psi_m, (D - 1)\psi_n \rangle \|$$

$$\leq \|\Lambda_+\psi_m\|_{L_2(supp \psi_n)} \| (D - 1)\psi_n \|.$$  \hspace{1cm} (6.19)

Notice that the norm $\|(D - 1)\psi_n\|$ is bounded uniformly in $n$ and $R$.

Since

$$\text{supp} \psi_k \subset B(2^k R(N - \frac{1}{5})) \setminus B(2^k R(N - \frac{2}{5}))$$

for $k = 1, \ldots, Q$,

Lemma 2 implies the exponential decay of $\|\Lambda_+\psi_m\|_{L_2(supp \psi_n)}$, and hence of the r.h.s. of (6.19), in $R$.

Let $B_m$ be the ball with the radius $\frac{1}{2}(R_m + R_m)$ centered at the origin. For the interaction with the nucleus one has

$$\langle -\frac{\alpha Z}{|x_N|} \Lambda_+\psi_m, \Lambda_+\psi_n \rangle$$

$$= \alpha Z \int_{B_m} \int_{\mathbb{R}^3 \setminus B_m} \frac{1}{|x_N|} \left(\Lambda_+\psi_n\right)^*(x_N)(\Lambda_+\psi_m)(x_N) dx_N.$$  \hspace{1cm} (6.20)
Without loss of generality assume \( n > m \). By Lemma 2,
\[
\|\Lambda + \psi_n\|_{L^2(B_{mn})} \leq Ce^{-\delta R} \tag{6.21}
\]
for some \( C > 0 \) and \( \delta > 0 \) independent of \( m \) and \( n \).

By the Hardy inequality
\[
\left\| \frac{1}{|x_N|} \Lambda + \psi_m \right\| \leq 2 \| \nabla (\Lambda + \psi_m) \| \leq C_1 |R_m|^{-1}. \tag{6.22}
\]
Together with (6.21) this implies
\[
\left| \int_{B_{mn}} \frac{1}{|x_N|} (\Lambda + \psi_n)^*(x_N)(\Lambda + \psi_m)(x_N) dx_N \right| \leq Ce^{-\delta R}. \tag{6.23}
\]
Similarly, in \( \mathbb{R}^3 \setminus B_{mn} \) the estimates (6.21), (6.22), and (6.23) hold if we replace everywhere \( m \leftrightarrow n \) and \( B_{mn} \) by \( \mathbb{R}^3 \setminus B_{mn} \).

It follows that
\[
\left| \langle \frac{\alpha Z}{|x|} \Lambda + \psi_m, \Lambda + \psi_n \rangle \right| \leq Ce^{-\delta R}. \tag{6.24}
\]
The last term in (6.18), which describes the electron–electron interaction, can be estimated analogously to (6.20) — (6.24). Together with (6.19) and (6.24) this implies
\[
\left| \langle \tilde{H}_N (\phi \otimes \Lambda + \psi_m), \phi \otimes \Lambda + \psi_n \rangle \right| \leq Ce^{-\delta R},
\]
which completes the proof of Theorem 2.

A  Some Properties of the Bessel Functions \( K_\nu \)

The modified Bessel (McDonald) functions are related to the Hankel functions by the formula
\[
K_\nu(z) = \frac{\pi}{2} e^{\pi(\nu+1)/2} H^{(1)}_\nu(iz).
\]
These functions are positive and decaying for \( z \in (0, \infty) \). Their asymptotics are (see [8] 8.446, 8.447.3, 8.451.6)
\[
K_\nu(z) = \sqrt{\frac{\pi}{2z}} e^{-z} \left( 1 + O\left( \frac{1}{z} \right) \right), \quad z \to +\infty;
\]
\[
K_0(z) = -\log z (1 + o(1)), \quad K_1(z) = \frac{1}{z} (1 + o(1)), \quad z \to +0. \tag{A.1}
\]
The derivatives of these functions are (see [8] 8.486.12, 8.486.18)
\[
K_0'(z) = -K_1(z), \quad K_1'(z) = -K_0(z) - \frac{1}{z} K_1(z), \quad z \in (0, \infty). \tag{A.2}
\]
B Coordinate Representation for the Operator $\Lambda_+$

**Lemma 10** Let $f \in L_2(\mathbb{R}^3, \mathbb{C}^4) \cap C^1_0(\mathbb{R}^3, \mathbb{C}^4)$ be a function in the coordinate representation. Then for $\Lambda_+ f$ formula \((3.2)\) holds.

**Proof.** We start with the operator $2\Lambda_+ - 1$, which is due to \((3.1)\) the multiplication by the matrix function $\frac{\alpha \cdot p + \beta}{\sqrt{|p|^2 + 1}}$ in the momentum space. It can be factorized as $A \cdot B$ with

$$A := (\alpha \cdot p + \beta)(|p|^2 + 1)^{-3/2}.$$  

In coordinate representation $B : L_2(\mathbb{R}^3, \mathbb{C}^4) \to H^3(\mathbb{R}^3, \mathbb{C}^4)$ is a bounded integral operator. Its kernel is given by the convergent integral

$$B(x, y) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{i p \cdot (x - y)} \frac{1}{(|p|^2 + 1)^{3/2}} dp = \frac{1}{2\pi^2} K_0(|x - y|).$$

In configuration space $A$ is the differential operator $(-i\alpha \cdot \nabla + \beta)(-\Delta + 1)$ mapping $H^3(\mathbb{R}^3, \mathbb{C}^4)$ onto $L_2(\mathbb{R}^3, \mathbb{C}^4)$. Thus with the help of \((A.2)\) for any $f \in L_2(\mathbb{R}^3, \mathbb{C}^4) \cap C^1_0(\mathbb{R}^3, \mathbb{C}^4)$ we get

$$\left( (2\Lambda_+ - 1)f \right)(x) = (-i\alpha \cdot \nabla + \beta)(-\Delta + 1) \frac{1}{2\pi^2} \int_{\mathbb{R}^3} K_0(|x - y|) f(y) dy$$

$$= (-i\alpha \cdot \nabla + \beta) \frac{1}{2\pi^2} \int_{\mathbb{R}^3} \frac{K_1(|x - y|)}{|x - y|} f(y) dy \quad (B.1)$$

$$= (-i\alpha \cdot \nabla + \beta) \frac{1}{2\pi^2} \int_{\mathbb{R}^3} \frac{K_1(|y|)}{|y|} f(x - y) dy.$$ 

The term with $\beta$ defines a function from $L_2(\mathbb{R}^3, \mathbb{C}^4)$, because $|\cdot|^{-1} K_1(|\cdot|) \in L_1(\mathbb{R}^3)$. We rewrite the gradient term on the r. h. s. of \((B.1)\) as

$$-i\alpha \cdot \nabla_x \frac{1}{2\pi^2} \int_{\mathbb{R}^3} \frac{K_1(|y|)}{|y|} f(x - y) dy$$

$$= \frac{i}{2\pi^2} \left( \int_{\mathbb{R}^3 \setminus B(\varepsilon)} + \int_{B(\varepsilon)} \right) \frac{K_1(|y|)}{|y|} \alpha \cdot \nabla_y (f(x - y)) dy. \quad (B.2)$$
The second integral on the r.h.s. of (B.2) can be estimated as

\[ \left| \frac{i}{2\pi^2} \int_{B(\varepsilon)} \frac{K_1(|y|)}{|y|} \alpha \cdot \nabla_y (f(x - y)) dy \right| \leq \frac{3}{2\pi^2} \|\nabla f\|_\infty \int_{B(\varepsilon)} \frac{K_1(|y|)}{|y|} dy, \tag{B.3} \]

where the r.h.s. of (B.3) tends to zero as \( \varepsilon \to 0 \). For the first integral on the r.h.s. of (B.2) the integration by parts gives

\[ \frac{i}{2\pi^2} \int_{R^3 \setminus B(\varepsilon)} \frac{K_1(|y|)}{|y|} \alpha \cdot \nabla_y (f(x - y)) dy = -\frac{i}{2\pi^2} \int_{R^3 \setminus B(\varepsilon)} \alpha \cdot \nabla_y \left( \frac{K_1(|y|)}{|y|} \right) f(x - y) dy + \frac{iK_1(\varepsilon)}{2\pi^2} \int_{\partial B(\varepsilon)} \alpha \cdot \frac{y}{|y|} f(x - y) dy. \tag{B.4} \]

We can rewrite the second integral on the r.h.s. of (B.4) as the sum of two integrals, using the Taylor expansion \( f(x - y) = f(x) - \nabla f(z) \cdot y \) with \( z \) lying on the segment connecting \( x \) and \( y \). The integral containing \( f(x) \) vanishes, because \( \alpha \cdot \frac{y}{|y|} \) is odd. The integral with \( \nabla f(z) \cdot y \) is different from zero only for \( x \) in the compact region

\[ \Omega := \{ x \in \mathbb{R}^3, \text{ dist } \{ x, \text{ supp } f \} \leq \varepsilon \}. \]

For \( x \in \Omega \) we have

\[ \left| \frac{iK_1(\varepsilon)}{2\pi^2} \int_{\partial B(\varepsilon)} \left( \alpha \cdot \frac{y}{|y|} \right) (\nabla f(z) \cdot y) dy \right| \leq \frac{3K_1(\varepsilon)}{2\pi^2} \|\nabla f\|_\infty 4\pi \varepsilon^2. \tag{B.5} \]

Hence the last term on the r.h.s. of (B.4) converges to zero in the \( L_2 \)-norm. Together with (B.1) — (B.4) and (A.2) this proves Lemma 10.

**C Proof of Lemma 9**

Let \( f \in L_2(\mathbb{R}^3) \), \( \text{supp} f \subset [-2R, 2R]^3 \). Then

\[ f(x) = \sum_{k \in \mathbb{Z}_+^3} c_k \prod_{i=1}^{3N} \varphi_k(x_i), \]

where

\[ \varphi_k(x) = \begin{cases} \frac{1}{\sqrt{2R}} \sin \left( \pi k \left( \frac{x}{2} + \frac{x}{4R} \right) \right), & x \in [-2R, 2R], \\ 0, & x \notin [-2R, 2R], \end{cases} \]

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$c_k$ are the Fourier coefficients of $f|_{-2R,2R}^{3N}$.

For the Fourier transform of $f$ we have

$$\hat{f}(p) = \sum_{k \in \mathbb{Z}^{3N}} c_k \prod_{i=1}^{3N} \hat{\varphi}_{k_i}(p_i), \quad (C.1)$$

where

$$\hat{\varphi}_k(p) = \frac{4\sqrt{\pi} R e^{i\pi(k-1)}}{\pi^2 k^2 - 16p^2 R^2}. \quad (C.2)$$

Let

$$L := \frac{1536 R N M}{\pi^3} + 1. \quad (C.3)$$

Assume that $f$ is orthogonal to the linear span of $L^{3N}$ functions

$$\left\{ \prod_{i=1}^{3N} \varphi_{k_i}(x_i), \quad k_i \in [0, L - 1] \cap \mathbb{Z}, \quad i = 1, \ldots, 3N \right\}.$$ 

Then the summation in (C.1) can be restricted to

$$k \in \bigcup_{j=1}^{3N} \gamma_j, \quad \gamma_j := \bigcap_{l=1}^{j-1} \{ k \in \mathbb{Z}^{3N}_+ | k_l < L \} \cap \{ k \in \mathbb{Z}^{3N}_+ | k_j \geq L \}.$$ 

Obviously $\| \hat{f} \|^2_{L_2(\mathbb{R}^{3N})} = \sum_{k \in \mathbb{Z}^{3N}_+} |c_k|^2$. On the other hand,

$$\| \hat{f} \|^2_{L_2(W_M)} \leq \sum_{j=1}^{3N} \left\| \sum_{k \in \gamma_j} c_k \prod_{i=1}^{3N} \varphi_{k_i}(p_i) \right\|_{L_2(\{|p_i| \leq M\})}^2$$

$$= \sum_{j=1}^{3N} \left( \sum_{k,k' \in \gamma_j} \langle c_k, c_{k'} \rangle \int_{-M}^{M} \varphi_{k_j}(p_j) \overline{\varphi_{k'_j}(p_j)} dp_j \prod_{i \neq j}^{3N} \int_{-M}^{M} \varphi_{k_i}(p_i) \overline{\varphi_{k'_i}(p_i)} dp_i \right)^{1/2}$$

$$= \sum_{j=1}^{3N} \left( \sum_{k_i=1}^{L} \sum_{k'_i=1}^{L} \sum_{k_j \geq L} \sum_{k'_j \geq L} \langle c(k_1, \ldots, k_j, \ldots, k_{3N}), c(k_1, \ldots, k'_j, \ldots, k_{3N}) \rangle \int_{-M}^{M} \varphi_{k_j}(p) \overline{\varphi_{k'_j}(p)} dp \right)^{1/2}.$$ 

Since

$$k_j, k'_j \geq L > \frac{4\sqrt{2} MR}{\pi}, \quad (C.4)$$

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we estimate
\[
\left| \int_{-M}^{M} \varphi_{k_j}(p) \overline{\varphi_{k'_j}(p)} dp \right| \lesssim 16\pi R k_j k'_j \int_{-M}^{M} \frac{1}{\pi^2 k_j^2 - 16p^2 R^2} \left| \frac{2}{\pi^2 k_j^2} \varphi_{k_j}(p) \overline{\varphi_{k'_j}(p)} dp \right|
\]
\[
\lesssim 16\pi R k_j k'_j \cdot 2M \cdot \frac{2}{\pi^2 k_j^2} \cdot \frac{2}{\pi^2 k'_j^2} = \frac{128RM}{\pi^3 k_j k'_j}.
\]

Applying the Schwarz inequality, we arrive at
\[
\left| \sum_{k_j, k'_j = L}^{\infty} \langle c(k_1, \ldots, k_{3N}), c(k_1', \ldots, k_{3N}) \rangle \int_{-M}^{M} \varphi_{k_j}(p) \overline{\varphi_{k'_j}(p)} dp \right|
\]
\[
\lesssim \frac{128RM}{\pi^3} \sum_{k'_j = L}^{\infty} |c(k_1, \ldots, k_{3N})|^2 \cdot \sum_{k_j = L}^{\infty} k_j^{-2}
\]
\[
\lesssim \frac{128RM}{\pi^3(L-1)} \sum_{k'_j = L}^{\infty} |c(k_1, \ldots, k_{3N})|^2.
\]

Therefore
\[
\| \hat{f} \|_{L^2(W_M)} \lesssim \sum_{j=1}^{3N} \left( \frac{128RM}{\pi^3(L-1)} \sum_{k \in \gamma_j} |c_k|^2 \right)^{1/2}
\]
\[
\lesssim \sqrt{\frac{384RM}{\pi^3(L-1)}} \| \hat{f} \|_{L^2(\mathbb{R}^{3N})} = \frac{1}{2} \| \hat{f} \|_{L^2(\mathbb{R}^{3N})}.
\]

Acknowledgement. This work was supported by the EU Network "Analysis and Quantum" (HPRN–CT–2002–00277). S. M. was supported by the DFG grant SI 348/12–2, S. V. was supported by the DFG grant WE-1964/2.

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