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# The essential spectrum of relativistic multi-particle operators

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ABSTRACT. – We locate the essential spectrum of pseudo-relativistic electrons in the electric field of nuclei. Our result is the analogue of the well-known theorem of Hunziker, van Winter, and Zislin.

RÉSUMÉ. – Nous localisons le spectre essentiel des électrons pseudo-relativistes dans le potentiel électrique des noyaux. Notre résultat est l'analogue du théorème bien connu de Hunziker, van Winter et Zislin.

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## 1. INTRODUCTION

A fundamental result of non-relativistic quantum mechanics is a classical theorem of **H**unziker [6], van **W**inter [16], and **Z**islin [18], in the following referred to as the HWZ-Theorem. This theorem shows that the least point of the essential spectrum of a non-relativistic multi-particle operator (after the removal of the motion of the center of mass) is determined by two-cluster decompositions of the particles. Here we derive that result for a multi-particle, quasi-relativistic Hamiltonian of the type studied in Lieb and Yau [9] where questions concerning stability of relativistic matter in this context were resolved. We refer to that paper for further discussion concerning this model.

Consider $N+1$ particles at positions $r_\nu \in \mathbb{R}^3$, masses $m_\nu$, and momenta $k_\nu$. For interaction potentials $v_{\mu,\nu}$, $\mu, \nu = 0, 1, \ldots, N$, depending only on the difference of the coordinates of particle $\mu$ and particle $\nu$, the quasi-relativistic Hamiltonian of the type which we study here is

$$H := \sum_{\nu=0}^{N} \left(\sqrt{-c^2\hbar^2\Delta_\nu + m_\nu^2 c^4} - m_\nu c^2\right) + \sum_{0\le\mu<\nu\le N} v_{\mu,\nu}$$

where $c$ is the velocity of light.

Let $X := \{r \in \mathbb{R}^{3(N+1)} : \sum_{\nu=0}^{N} m_\nu r_\nu = 0\}$. One can change variables $r \mapsto x$ (with $k \mapsto p$) in order that $x_0$ may be the position of the center of mass, *i.e.*, $x_0 = M^{-1}\sum_{\nu=0}^{N} m_\nu r_\nu$ where $M := \sum_{\nu=0}^{N} m_\nu$ is the total mass. In general this change of variable is chosen in order that it may leave the subspaces $X$ and $X^\perp$ invariant and the momentum for the center of mass is always

$$P := p_0 = \sum_{\nu=0}^{N} k_\nu.$$

This is the case for either atomic coordinates, Jacobi coordinates, or clustered Jacobi coordinates (see Appendix A). The fundamental observation is that the total momentum commutes with the Hamiltonian.

We use here the change of variables

$$x_0 = \frac{1}{M}\sum_{\nu=0}^{N} m_\nu r_\nu, \tag{1}$$

$$x_\nu = r_\nu - r_0, \qquad \nu = 1, \ldots, N,$$

whose Jacobian is one, *cf.* Thirring [15], §4.6,4. For the variable change given by (1) we have that $k_\nu = \frac{m_\nu}{M}P + p_\nu$, $\nu = 1, \ldots, N$. The relativistic kinetic energy in momentum space

$$\sum_{\nu=0}^{N} \left(\sqrt{c^2|k_\nu|^2 + m_\nu^2 c^4} - m_\nu c^2\right)$$

consequently becomes

$$\hat{T} = \sqrt{c^2\left|\frac{m_0}{M}P - \Sigma_{\nu=1}^N p_\nu\right|^2 + m_0^2c^4} - m_0c^2 + \sum_{\nu=1}^{N}\left(\sqrt{c^2\left|\frac{m_\nu}{M}P + p_\nu\right|^2 + m_\nu^2c^4} - m_\nu c^2\right).$$

See Appendix A for more details. Note that our normalization of the Fourier transform in this section is given by

$$(U\phi)(p) := \hat{\phi}(p) = \frac{1}{(2\pi\hbar)^{d/2}}\int_{\mathbb{R}^d} e^{-\frac{i}{\hbar}p\cdot x}\phi(x)dx.$$

(In the next section we rescale in order that $\hbar = c = 1$.)

Heuristically, we can view things as follows: let

$$\psi_T(x) = \psi_0(x_0)\psi_R(x_1, \ldots, x_N) = e^{-\frac{i}{\hbar}\mathfrak{P}\cdot x_0}\psi_R(x_1, \ldots, x_N)$$

be a "generalized eigenfunction" of the total system,

$$H\psi_T = E\psi_T$$

where $\psi_T$ is typically called the total wave function and $\psi_R$ is called the reduced wave function.

In the familiar case of a non-relativistic operator, the motion of the center of mass separates off leaving a reduced Hamiltonian whose spectral points are easily related to the spectral points of the full Hamiltonian. Hence, it suffices to know the spectrum of the reduced Hamiltonian.

In the relativistic case, things are different. However, the most important fact, namely that the Hamiltonian commutes with the total momentum, remains unchanged. As before set

$$\psi_T(x_0, x_1, \ldots, x_N) = e^{-\frac{i}{\hbar}\mathfrak{P}\cdot x_0}\psi_R(x_1, \ldots, x_N), \qquad \mathfrak{P} \in \mathbb{R}^3.$$

Taking the Fourier transform

$$\hat{\psi}_T(p_0,\ldots,p_N)=\delta(\mathfrak{P}-p_0)\hat{\psi}_R(p_1,\ldots,p_N)$$

indicates that the kinetic energy is given by

$$\begin{aligned}
&\hat{T}\hat{\psi}_T(p_0,\ldots,p_N)\\
&=\left[\sum_{\nu=1}^{N}\sqrt{c^2\Big(\frac{m_\nu}{M}P+p_\nu\Big)^2+m_\nu^2c^4}-m_\nu c^2\right]\hat{\psi}_R\delta(\mathfrak{P}-p_0)\\
&\quad+\left[\sqrt{c^2\Big(\frac{m_0}{M}P-\sum_{\nu=1}^{N}p_\nu\Big)^2+m_0^2c^4}-m_0c^2\right]\hat{\psi}_R\delta(\mathfrak{P}-p_0)\\
&=\left[\sum_{\nu=1}^{N}\sqrt{c^2\Big(\frac{m_\nu}{M}\mathfrak{P}+p_\nu\Big)^2+m_\nu^2c^4}-m_\nu c^2\right]\hat{\psi}_R\delta(\mathfrak{P}-p_0)\\
&\quad+\left[\sqrt{c^2\Big(\frac{m_0}{M}\mathfrak{P}-\sum_{\nu=1}^{N}p_\nu\Big)^2+m_0^2c^4}-m_0c^2\right]\hat{\psi}_R\delta(\mathfrak{P}-p_0).
\end{aligned}$$

Therefore we have that

$$(\hat{T}U\psi_T)(p_0,\ldots,p_N)=\delta(\mathfrak{P}-p_0)\hat{T}_{\mathfrak{P}}(p)U\psi_R(p_1,\ldots,p_N)$$

where

$$\begin{aligned}
\hat{T}_{\mathfrak{P}}(p):=&\sum_{\nu=1}^{N}\left(\sqrt{c^2\Big(\frac{m_\nu}{M}\mathfrak{P}+p_\nu\Big)^2+m_\nu^2c^4}-m_\nu c^2\right)\\
&+\sqrt{c^2\Big(\frac{m_0}{M}\mathfrak{P}-\sum_{\nu=1}^{N}p_\nu\Big)^2+m_0^2c^4}-m_0c^2.
\end{aligned}$$

After the change of variables given in (1) the potential takes the form

$$(2)\quad V=\sum_{0\le\mu<\nu\le N}v_{\mu\nu}(r_\mu-r_\nu)=\sum_{\nu=1}^{N}v_{0\nu}(x_\nu)+\sum_{1\le\mu<\nu\le N}v_{\mu\nu}(x_\mu-x_\nu),$$

*i.e.*, it is a function of $x_1,\ldots,x_N$ only. Then for $H:=T+V$ in which $T:=U^{-1}\hat{T}U$ we have

$$H\psi_T=E\psi_T\iff e^{-i\mathfrak{P}\cdot x_0}H_{\mathfrak{P}}\psi_R=Ee^{-i\mathfrak{P}\cdot x_0}\psi_R\iff H_{\mathfrak{P}}\psi_R=E\psi_R$$

where $H_{\mathfrak{P}}:=T_{\mathfrak{P}}+V$. (Here $T_{\mathfrak{P}}:=U^{-1}\hat{T}_{\mathfrak{P}}U$ where-in slight abuse of notation-$U$ denotes also the Fourier transform in $p_1,\ldots,p_N$.) In effect, we are holding the momentum for the center of mass fixed at $\mathfrak{P} \in \mathbb{R}^3$. This means that it suffices to solve $H_{\mathfrak{P}}\psi_R = E\psi_R$ to solve $H\psi_T = E\psi_T$. This is the motivation for our study of $H_{\mathfrak{P}}$ . A mathematical treatment of a similar equivalence can be found in Simon [13], p. 196, Reed and Simon [12], §XIII.16, or-tailored for this situation-in Appendix B.

For later convenience we define another unitary transformation, namely the shift

$$(3) \qquad \tau_{\mathfrak{P}} : \phi(p) \mapsto \phi(\mathfrak{p} + p) \qquad \text{for } \mathfrak{p} := \left(\frac{\mathrm{m}_1}{\mathrm{M}}\mathfrak{P}, \ldots, \frac{\mathrm{m}_\mathrm{N}}{\mathrm{M}}\mathfrak{P}\right).$$

We write $\mu := \mathfrak{p} + p$ and set

$$(4) \qquad \hat{t}_{\mathfrak{P}}(\mu) : = \hat{T}_{\mathfrak{P}}(\mu - \mathfrak{p}) = \sum_{\nu=1}^{N}(\sqrt{c^2|\mu_\nu|^2 + m_\nu^2 c^4} - m_\nu c^2) + \sqrt{c^2|\mathfrak{P} - \sum_{\nu=1}^{N}\mu_\nu|^2 + m_0^2 c^4} - m_0 c^2.$$

Therefore the kinetic energy part of $H_{\mathfrak{P}}$ is given by $T_{\mathfrak{P}} = U^{-1}\tau_{\mathfrak{P}}^{-1}\hat{t}_{\mathfrak{P}}\tau_{\mathfrak{P}}U$.

The operator $H_{\mathfrak{P}}F = T_{\mathfrak{P}} + V$ is symmetric on $\mathfrak{S}$, the Schwartz space. We will henceforth assume that $V_-$ is relatively form-bounded with respect to $T_{\mathfrak{P}}$ with form-bound strictly less than 1. This implies that there exists a constant $M$ such that for all $\varphi \in \mathfrak{S}$

$$(5) \qquad \rho[\varphi] := (\varphi, H_{\mathfrak{P}}\varphi) \geq M(\varphi, \varphi).$$

The operator considered in this paper will be the Friedrichs extension of $H_{\mathfrak{P}}$ which we will-again in abuse of notation-also denote by $H_{\mathfrak{P}}$.

The goal is to investigate the spectral properties of $H_{\mathfrak{P}}$. The lowest spectral point of such an operator describing relativistic electrons and fixed nuclei interacting via Coulomb forces has been studied by Lieb and Yau [9]. Our main result is the localization of the essential spectrum for this operator analogous to the result of Hunziker, van Winter, and Zislin for non-relativistic Hamiltonians. However, because of the nonlocal nature of the operator and the critical nature of the Coulomb potential in combination with $\sqrt{-\hbar^2 c^2 \Delta + m^2 c^4}$, new estimates are required.

## 2. A RELATIVISTIC HWZ-THEOREM

The case of primary interest is that in which each $v_{\mu\nu}(r_\mu - r_\nu)$ is a Coulomb potential, *i.e.*, is a constant multiple of $\hbar c\alpha/|r_\mu - r_\nu|$ where $\alpha = e^2/\hbar c$ is the fine structure constant and $e$ is the charge of a particle. In this case we may simplify $H$ by rescaling $r = \hbar r'/c$ with $\phi(r) \to \phi(\hbar r'/c)(\hbar/c)^{3(N+1)/2} =: \psi(r')$. Then $(U\phi)(k) = \hat{\psi}(c^{-1}k)/c^{3(N+1)/2}$ where $\hat{f}$ here (and henceforth) denotes the Fourier transform of $f$ as given above by $U$, but with $\hbar = 1$. With these substitutions and $k = ck'$ the operator $H$ rescales to an operator in which only the term $c^2$ appears as a multiplicative constant. For this reason we confine our attention to the operator $H_{\mathfrak{P}}$ given above with $c$ and $\hbar$ set to 1.

For each $R > 0$, define

$$\Lambda_R(x; H_{\mathfrak{P}}) := \inf\{\rho[\varphi] : \varphi \in C_0^\infty(B(x;R)), \|\varphi\| = 1\} \tag{6}$$

in which $B(x;R)$ is the ball centered at $x \in \mathbb{R}^{3N}$ with radius $R$. The next estimate is central to the treatment here (*cf.* Agmon [1], Lemma 2.3).

LEMMA 1. – *For any $\epsilon > 0$ there exists $R_\epsilon > 0$ such that*

$$(\varphi, H_{\mathfrak{P}}\varphi) \geq \int_{\mathbb{R}^{3N}} (\Lambda_R(x; H_{\mathfrak{P}}) - \epsilon)|\varphi(x)|^2 dx$$

*for all $\varphi \in C_0^\infty(\mathbb{R}^{3N})$ and for any $R \geq R_\epsilon$.*

Before giving the proof of Lemma 1, we need to establish a few facts that are patterned after a similar treatment by Lieb and Yau [9].

PROPOSITION 1. – *Let $\varphi \in \mathfrak{S}(\mathbb{R}^{3N})$. Define for $1 \leq \alpha \leq N$*

$$G_\alpha(x,y) := \frac{m_0^2 K_2[m_0|x_\alpha - y_\alpha|]}{4\pi^2|x_\alpha - y_\alpha|^2} \prod_{j\neq\alpha} \delta((x_j - y_j) - (x_\alpha - y_\alpha)) \tag{7}$$

*where $K_2$ is a modified Bessel function of order 2 and*

$$F_\alpha(x,y) := \frac{m_\alpha^2 K_2[m_\alpha|x_\alpha - y_\alpha|]}{4\pi^2|x_\alpha - y_\alpha|^2} \prod_{j\neq\alpha} \delta(x_j - y_j). \tag{8}$$

*Then,*

$$(\varphi, T_{\mathfrak{P}}\varphi) = \sum_{\alpha=1}^{N} \int_{\mathbb{R}^{6N}} dxdy$$
$$\times \left\{ |\varphi(x) - \varphi(y)|^2 F_\alpha(x,y) + \frac{1}{N} G_\alpha(x,y)|\varphi(x) - e^{i\mathfrak{P}\cdot(x_\alpha - y_\alpha)}\varphi(y)|^2 \right\}.$$

*Proof.* – Since (with $\hbar = 1$)

$$(\varphi, T_{\mathfrak{P}}\varphi) = (\varphi, U^{-1}\tau_{\mathfrak{P}}^{-1}\hat{t}_{\mathfrak{P}}\tau_{\mathfrak{P}}U\varphi) = (\phi, \hat{t}_{\mathfrak{P}}\phi)$$

for $\phi(\mu) := (\tau_{\mathfrak{P}}U\varphi)(\mu)$ and $\hat{t}_{\mathfrak{P}}$ defined in (4), then it will suffice to work with $(\phi, \hat{t}_{\mathfrak{P}}\phi)$.

Let $\xi_\alpha = \mathfrak{P} - \sum_{j=1}^{N} \mu_j$ and $\xi_\nu = \mu_\nu$, for $\nu \neq \alpha$. Then

$$\left(\phi, \left[\left[\left|\mathfrak{P} - \sum_{j=1}^{N} \mu_j\right|^2 + m_0^2\right]^{\frac{1}{2}} - m_0\right]\phi\right) = \int_{\mathbb{R}^{3N}} d\xi \left(\sqrt{|\xi_\alpha|^2 + m_0^2} - m_0\right)|\phi_{\mathfrak{P}}(\xi)|^2$$

where

$$\phi_{\mathfrak{P}}(\xi) := \phi(\xi_1, \ldots, \xi_{\alpha-1}, \mathfrak{P} - \sum_{j=1}^{N}\xi_j, \xi_{\alpha+1}, \ldots, \xi_N).$$

Since

$$\phi_{\mathfrak{P}}(\xi) = \frac{1}{(2\pi)^{3N/2}} \int_{\mathbb{R}^{3N}} e^{-i\left(\sum_{j\neq\alpha} \xi_j \cdot x_j + (\mathfrak{P} - \sum_{j=1}^{N} \xi_j)\cdot x_\alpha\right)} \varphi(x)dx$$

then

$$\int_{\mathbb{R}^{3N}} d\xi e^{-t\sqrt{|\xi_\alpha|^2 + m_0^2}} |\phi_{\mathfrak{P}}(\xi)|^2$$
$$= \int_{\mathbb{R}^{6N}} dxdy \{G(t, |x_\alpha - y_\alpha|)e^{-i\mathfrak{P}\cdot(x_\alpha - y_\alpha)} \prod_{j\neq\alpha} \delta((x_j - y_j) - (x_\alpha - y_\alpha))\varphi(x)\overline{\varphi(y)}\}$$

(Lieb and Yau [9], (2.13)) in which we have set

$$G(t, |x - y|) := exp\left[-t\sqrt{|\xi|^2 + m_0^2}\right](x, y) = \frac{m_0^2 t}{2\pi^2} \frac{K_2(m_0\sqrt{|x-y|^2 + t^2})}{|x-y|^2 + t^2}.$$

It follows that

$$\frac{1}{t}\int_{\mathbb{R}^{3N}} d\xi e^{-t(\sqrt{|\xi_\alpha|^2 + m_0^2} - m_0)} |\phi_{\mathfrak{P}}(\xi)|^2$$
$$= \frac{m_0^2}{2\pi^2} \int_{\mathbb{R}^{3(N+1)}} dxdy_\alpha \varphi(x)\overline{\varphi(x - x(\alpha))}$$
$$\times \frac{K_2(m_0\sqrt{|x_\alpha - y_\alpha|^2 + t^2})}{|x_\alpha - y_\alpha|^2 + t^2} e^{-i\mathfrak{P}\cdot(x_\alpha - y_\alpha) + tm_0}$$

where

$$x(\alpha) := (x_\alpha - y_\alpha, \ldots, x_\alpha - y_\alpha). \tag{9}$$

Next note that

$$\int_{\mathbb{R}^{3N}} d\xi |\phi_{\mathfrak{P}}(\xi)|^2 = \int_{\mathbb{R}^{3N}} |\varphi(x)|^2 dx.$$

Define $N(t)$ in order that

$$\int_{\mathbb{R}^3} dv \frac{K_2[m_0\sqrt{|v|^2+t^2}]}{|v|^2+t^2} = 4\pi t \int_0^\infty \frac{K_2[m_0 t\sqrt{r^2+1}]}{r^2+1} r^2 dr =: 4\pi t N(t).$$

Below, we need $\lim_{t\to 0} t^2 N(t)$. To this end we use

$$\lim_{z\to 0} K_\nu(z) = \frac{1}{2}\Gamma(\nu)\left(\frac{1}{2}z\right)^{-\nu}, \qquad \Re\nu > 0,$$

for $\nu$ fixed (Olver [10], Formula 9.6.9). Therefore,

$$\begin{aligned} \lim_{t\to 0} t^2 N(t) &= \int_0^\infty \lim_{t\to 0} t^2 K_2[m_0 t\sqrt{r^2+1}] \frac{r^2}{r^2+1} dr \\ &= \int_0^\infty \lim_{t\to 0} \frac{2t^2}{m_0^2 t^2 (r^2+1)} \frac{r^2}{r^2+1} dr \\ &= \frac{2}{m_0^2} \int_0^\infty \frac{r^2}{(r^2+1)^2} dr = \frac{\pi}{2m_0^2}. \end{aligned} \tag{10}$$

Next observe that

$$\begin{aligned} \frac{1}{t}\int_{\mathbb{R}^{3N}} d\xi |\phi_{\mathfrak{P}}(\xi)|^2 &= \frac{1}{t}\int_{\mathbb{R}^{3N}} |\varphi(x)|^2 dx \\ &= \frac{1}{2t(4\pi t N(t))} \int_{\mathbb{R}^{3(N+1)}} dx dy_\alpha \left[|\varphi(x)|^2 + |\varphi(x - x(\alpha))|^2\right] \\ &\quad \times \frac{K_2[m_0\sqrt{|x_\alpha - y_\alpha|^2 + t^2}]}{|x_\alpha - y_\alpha|^2 + t^2} \end{aligned} \tag{11}$$

where in order to deal with the term $\varphi(x - x(\alpha))$ we have used a change of variable

$$\begin{aligned} u_j &= x_j - (x_\alpha - y_\alpha), \qquad j = 1, \ldots, N, \\ v_\alpha &= x_\alpha - y_\alpha. \end{aligned} \tag{12}$$

Combining (11) with calculations above we have that

$$
\begin{aligned}
&\frac{1}{t}\int_{\mathbb{R}^{3N}} d\xi\Big(1-e^{-t(\sqrt{|\xi_\alpha|^2+m_0^2}-m_0)}\Big)\left|\phi_{\mathfrak{P}}(\xi)\right|^2\\
&=\frac{1}{2t(4\pi t N(t))}\int_{\mathbb{R}^{3(N+1)}} dx dy_\alpha\left[|\varphi(x)|^2+|\varphi(x-x(\alpha))|^2\right]\\
&\quad\times\frac{K_2[m_0\sqrt{|x_\alpha-y_\alpha|^2+t^2}]}{|x_\alpha-y_\alpha|^2+t^2}\\
&\quad-\frac{m_0^2}{2\pi^2}\int_{\mathbb{R}^{3(N+1)}} dx dy_\alpha \varphi(x)\overline{\varphi(x-x(\alpha))}\\
&\quad\times\frac{K_2(m_0\sqrt{|x_\alpha-y_\alpha|^2+t^2})}{|x_\alpha-y_\alpha|^2+t^2}e^{-i\mathfrak{P}\cdot(x_\alpha-y_\alpha)+tm_0}\\
&=\frac{m_0^2}{4\pi^2}\int_{\mathbb{R}^{3(N+1)}} dx dy_\alpha\frac{K_2[m_0\sqrt{|x_\alpha-y_\alpha|^2+t^2}]}{|x_\alpha-y_\alpha|^2+t^2}\\
&\quad\times\Bigg[\frac{\pi[|\varphi(x)|^2+|\varphi(x-x(\alpha))|^2]}{2m_0^2t^2N(t)}\\
&\qquad-2e^{-i\mathfrak{P}\cdot(x_\alpha-y_\alpha)+tm_0}\varphi(x)\overline{\varphi(x-x(\alpha))}\Bigg]
\end{aligned}
$$

By taking the limit as $t\to 0^+$ and using (7) we have that

$$
\begin{aligned}
(13)\quad &\left(\phi,\left(\left[\Big|\mathfrak{P}-\sum_{j=1}^{N}\mu_j\Big|^2+m_0^2\right]^{\frac{1}{2}}-m_0\right)\phi\right)\\
&=\lim_{t\to 0^+}\frac{1}{t}\int_{\mathbb{R}^{3N}} d\xi\Big(1-e^{-t(\sqrt{|\xi_\alpha|^2+m_0^2}-m_0)}\Big)\left|\phi_{\mathfrak{P}}(\xi)\right|^2\\
&=\frac{m_0^2}{4\pi^2}\int_{\mathbb{R}^{3(N+1)}} dx dy_\alpha|\varphi(x)-e^{i\mathfrak{P}\cdot(x_\alpha-y_\alpha)}\varphi(x-x(\alpha))|^2\\
&\quad\times\frac{K_2[m_0|x_\alpha-y_\alpha|]}{|x_\alpha-y_\alpha|^2}\\
&=\int_{\mathbb{R}^{6N}} dx dy|\varphi(x)-e^{-i\mathfrak{P}\cdot(x_\alpha-y_\alpha)}\varphi(y)|^2G_\alpha(x,y).
\end{aligned}
$$

A similar calculation shows that

$$
\begin{aligned}
(14)\quad &(\phi,(\sqrt{|\mu_\alpha|^2+{m_\alpha}^2}-m_\alpha)\phi)\\
&=\int_{\mathbb{R}^{6N}} dx dy|\varphi(x)-\varphi(y)|^2F_\alpha(x,y)\\
&=\frac{{m_\alpha}^2}{4\pi^2}\int_{\mathbb{R}^{3(N+1)}} dx dy_\alpha|\varphi(x)-\varphi(x',y_\alpha)|^2\frac{K_2[m_\alpha|x_\alpha-y_\alpha|]}{|x_\alpha-y_\alpha|^2}.
\end{aligned}
$$

The expression for $T_{\mathfrak{P}}$ now follows. □

PROPOSITION 2. – *Let $\chi$ be a real-valued Lipschitz continuous function on $\mathbb{R}^{3N}$ and $\varphi \in \mathfrak{S}(\mathbb{R}^{3N})$. Let $\tilde{G}_\alpha$ and $\tilde{F}_\alpha$ be bounded operators on $L^2(\mathbb{R}^{3N})$ with kernels*

$$\tilde{G}_\alpha(x,y) := G_\alpha(x,y)e^{i\mathfrak{P}\cdot(x_\alpha - y_\alpha)}(\chi(x)-\chi(y))^2$$

*and*

$$\tilde{F}_\alpha(x,y) := F_\alpha(x,y)(\chi(x)-\chi(y))^2$$

*relative to* (7) *and* (8). *Then for $1 \le \alpha \le N$ and $\hat{\psi}(\mu) := (\tau_{\mathfrak{P}}U(\chi\varphi))(\mu)$ defined in* (3) *(with $\hbar = 1$)*

$$\begin{aligned}&\left(\hat{\psi}, \left(\left[\left|\mathfrak{P} - \sum_{\nu=1}^{N}\mu_\nu\right|^2 + m_0^2\right]^{\frac{1}{2}} - m_0\right)\hat{\psi}\right)\\ &\quad = (\varphi, \tilde{G}_\alpha\varphi) + \frac{1}{2}\int_{\mathbb{R}^{6N}} dxdy|\varphi(x) - e^{i\mathfrak{P}\cdot(x_\alpha - y_\alpha)}\varphi(y)|^2\\ &\quad \times (\chi(x)^2 + \chi(y)^2)G_\alpha(x,y)\\ &\quad + \frac{1}{2}\int_{\mathbb{R}^{6N}} dxdy\big(|\varphi(x)|^2 - |\varphi(y)|^2\big)\big(\chi(x)^2 - \chi(y)^2\big)G_\alpha(x,y)\end{aligned}$$

*and*

$$\begin{aligned}&\left(\hat{\psi}, (\sqrt{|\mu_\alpha|^2 + m_\alpha^2} - m_\alpha)\hat{\psi}\right)\\ &\quad = (\varphi, \tilde{F}_\alpha\varphi) + \frac{1}{2}\int_{\mathbb{R}^{6N}} dxdy|\varphi(x) - \varphi(y)|^2(\chi(x)^2 + \chi(y)^2)F_\alpha(x,y)\\ &\quad + \frac{1}{2}\int_{\mathbb{R}^{6N}} dxdy\big(|\varphi(x)|^2 - |\varphi(y)|^2\big)\big(\chi(x)^2 - \chi(y)^2\big)F_\alpha(x,y).\end{aligned}$$

The proof follows from (13), (14), and direct calculation.

The proof of the next localization formula is a direct consequence of Propositions 1 and 2 (*cf.* Lieb and Yau [9], Theorem 9 (Localization of kinetic energy-general form)).

COROLLARY 1 (Localization formula). – *Let $\{\chi_\nu\}_{\nu=1}^K$ be real-valued Lipschitz continuous functions on $\mathbb{R}^{3N}$ such that $\sum_{\nu=1}^K \chi_\nu(x)^2 \equiv 1$. Let $L_K : L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$ be the bounded operator with kernel*

$$\begin{aligned}&L_K(x,y)\\ &\quad := \left(\sum_{\alpha=1}^{N}\left[F_\alpha(x,y) + \frac{1}{N}G_\alpha(x,y)e^{i\mathfrak{P}\cdot(x_\alpha - y_\alpha)}\right]\right)\sum_{\nu=1}^{K}(\chi_\nu(x) - \chi_\nu(y))^2\end{aligned}$$

*for $G_\alpha$ and $F_\alpha$ given by* (7) *and* (8). *Then for all $\varphi \in \mathfrak{S}(\mathbb{R}^{3N})$*

$$(\varphi, T_{\mathfrak{P}}\varphi) = \sum_{\nu=1}^{K}((\chi_\nu\varphi), T_{\mathfrak{P}}(\chi_\nu\varphi)) - (\varphi, L_K\varphi).$$

We are now in a position to give a proof which we promised.

*Proof of Lemma* 1. – Choose a real-valued function $\zeta \in C_0^\infty(B(0;\frac{1}{2}))$ normalized as an element of $L^2(\mathbb{R}^{3N})$ and extended as zero to the whole of $\mathbb{R}^{3N}$. For each $z \in \mathbb{R}^{3N}$ and $R > 0$ define

$$\zeta_{R,z}(x) := \zeta\big((x-z)R^{-1}\big), \qquad x \in \mathbb{R}^{3N}.$$

Then, $\zeta_{R,z} \in C_0^\infty(B(z;\frac{R}{2}))$,

$$\int_{\mathbb{R}^{3N}} |\zeta_{R,z}(x)|^2 dx = R^{3N}, \qquad \text{and} \quad |\nabla_x \zeta_{R,z}(x)|^2 \leq \frac{C}{R^2}$$

for some constant $C > 0$.

Set

$$\mathfrak{J}_\alpha(x,y) := |\varphi(x)-\varphi(y)|^2 F_\alpha(x,y) + \frac{1}{N}G_\alpha(x,y)|\varphi(x) - e^{i\mathfrak{P}\cdot(x_\alpha - y_\alpha)}\varphi(y)|^2$$

and

$$\mathfrak{K}_\alpha(x,y) := (|\varphi(x)|^2 - |\varphi(y)|^2)\Big(F_\alpha(x,y) + \frac{1}{N}G_\alpha(x,y)\Big).$$

It follows from Proposition 1 that the kinetic energy is given as

$$(\varphi, T_{\mathfrak{P}}\varphi) = \sum_{\alpha=1}^{N}\int_{\mathbb{R}^{6N}} dxdy\,\mathfrak{J}_\alpha(x,y).$$

According to Proposition 2 and Corollary 1 with $\chi_1 := \zeta_{R,z}$

$$\begin{aligned}(15)\qquad &(\zeta_{R,z}\varphi, T_{\mathfrak{P}}(\zeta_{R,z}\varphi)) - (\varphi, L_1\varphi)\\ &= \frac{1}{2}\sum_{\alpha=1}^{N}\int_{\mathbb{R}^{6N}} dxdy[(\zeta_{R,z}(x)^2 + \zeta_{R,z}(y)^2)\mathfrak{J}_\alpha(x,y)\\ &+ (\zeta_{R,z}(x)^2 - \zeta_{R,z}(y)^2)\mathfrak{K}_\alpha(x,y)].\end{aligned}$$

Consequently,

$$\begin{aligned}(16)\qquad & \Lambda_{R/2}(z;H_{\mathfrak{P}})\int_{B(z;R/2)}|\zeta_{R,z}(x)\varphi(x)|^2dx-(\varphi,L_1\varphi)\\ &\le\frac{1}{2}\sum_{\alpha=1}^{N}\int_{\mathbb{R}^{6N}}dxdy(\zeta_{R,z}(x)^2+\zeta_{R,z}(y)^2)\mathfrak{J}_\alpha(x,y)\\ &+\frac{1}{2}\sum_{\alpha=1}^{N}\int_{\mathbb{R}^{6N}}dxdy(\zeta_{R,z}(x)^2-\zeta_{R,z}(y)^2)\mathfrak{K}_\alpha(x,y)\\ &+(\zeta_{R,z}\varphi,V\zeta_{R,z}\varphi).\end{aligned}$$

We have that $\Lambda_R(x;H_{\mathfrak{P}})\le\Lambda_{R/2}(z;H_{\mathfrak{P}})$ for $x\in B(z;R/2)$. Using this fact in (16) and integrating over $z$ gives the inequality

$$\begin{aligned}(17)\qquad & R^{3N}\int_{\mathbb{R}^{3N}}\Lambda_R(x;H_{\mathfrak{P}})|\varphi(x)|^2dx-\int_{\mathbb{R}^{3N}}dz(\varphi,L_1\varphi)\\ &\le R^{3N}((\varphi,T_{\mathfrak{P}}\varphi)+(\varphi,V\varphi))\end{aligned}$$

by Proposition 1.

Now we examine

$$\begin{aligned}\int_{\mathbb{R}^{3N}}dz(\varphi,L_1\varphi)&=\int_{\mathbb{R}^{9N}}dzdxdy\sum_{\alpha=1}^{N}\left[F_\alpha(x,y)+\frac{1}{N}G_\alpha(x,y)e^{i\mathfrak{P}\cdot(x_\alpha-y_\alpha)}\right]\\ &\times(\zeta_{R,z}(x)-\zeta_{R,z}(y))^2\varphi(x)\overline{\varphi(y)}.\end{aligned}$$

For $(x',y_\alpha)=(x_1,\ldots,y_\alpha,\ldots,x_N)$ and $\xi$ some point between $x$ and $(x',y_\alpha)$ in $\mathbb{R}^{3N}$

$$\begin{aligned}&\int_{\mathbb{R}^{9N}}dzdxdyF_\alpha(x,y)(\zeta_{R,z}(x)-\zeta_{R,z}(y))^2\varphi(x)\overline{\varphi(y)}\\ &=\frac{m_\alpha^2}{4\pi^2}\int_{\mathbb{R}^{6N+3}}dzdxdy_\alpha\frac{K_2[m_\alpha|x_\alpha-y_\alpha|]}{|x_\alpha-y_\alpha|^2}\\ &\times(\zeta_{R,z}(x)-\zeta_{R,z}(x',y_\alpha))^2\varphi(x)\overline{\varphi(x',y_\alpha)}\end{aligned}$$

$$\leq \frac{C_m}{R^2} \int_{\mathbb{R}^{6N+3}} dz dx dy_\alpha \frac{K_2[m_\alpha |x_\alpha - y_\alpha|]}{|x_\alpha - y_\alpha|^2}$$
$$\times \left|(\nabla\zeta)\big((\xi - z)R^{-1}\big)\chi_{B(\xi;R/2)}(z)\right|^2$$
$$\times |x_\alpha - y_\alpha|^2 \varphi(x)\overline{\varphi(x', y_\alpha)}$$
$$\leq C'_m R^{3N-2} \int_{\mathbb{R}^{3(N+1)}} dx dy_\alpha K_2[m_\alpha |x_\alpha - y_\alpha|] \varphi(x)\overline{\varphi(x', y_\alpha)}$$
$$\leq C'_m R^{3N-2} \left[\int_{\mathbb{R}^6} dx_\alpha dy_\alpha K_2[m_\alpha |x_\alpha - y_\alpha|] \int_{\mathbb{R}^{3(N-1)}} dx' |\varphi(x', x_\alpha)|^2\right]^{\frac{1}{2}}$$
$$\times \left[\int_{\mathbb{R}^6} dx_\alpha dy_\alpha K_2[m_\alpha |x_\alpha - y_\alpha|] \int_{\mathbb{R}^{3(N-1)}} dx' |\varphi(x', y_\alpha)|^2\right]^{\frac{1}{2}}$$
$$= C'_m R^{3N-2} \int_{\mathbb{R}^3} du K_2[m_\alpha |u|] \|\varphi\|^2,$$

and for $\xi'$ between $x$ and $x - x(\alpha)$, $x(\alpha)$ defined in (9),

$$\mathcal{G}_\alpha := \left|\int_{\mathbb{R}^{9N}} dz dx dy G_\alpha(x, y) e^{i\mathfrak{P}\cdot(x_\alpha - y_\alpha)} \big(\zeta_{R,z}(x) - \zeta_{R,z}(y)\big)^2 \varphi(x)\overline{\varphi(y)}\right|$$
$$= \left|\frac{m_0^2}{4\pi^2} \int_{\mathbb{R}^{6N+3}} dz dx dy_\alpha \frac{K_2[m_0 |x_\alpha - y_\alpha|]}{|x_\alpha - y_\alpha|^2} e^{i\mathfrak{P}\cdot(x_\alpha - y_\alpha)} \right.$$
$$\left. \times \big(\zeta_{R,z}(x) - \zeta_{R,z}(x - x(\alpha))\big)^2 \varphi(x)\overline{\varphi(x - x(\alpha))}\right|$$
$$\leq \frac{C_M N}{R^2} \int_{\mathbb{R}^{6N+3}} dz dx dy_\alpha K_2[m_0 |x_\alpha - y_\alpha|]$$
$$\times |(\nabla\zeta)\big((\xi' - z)R^{-1}\big)\chi_{B(\xi';R/2)}(z)|^2 |\varphi(x)||\varphi(x - x(\alpha))|.$$

Estimating the gradient term yields

$$\mathcal{G}_\alpha \leq C'_M N R^{3N-2} \int_{\mathbb{R}^{3(N+1)}} dx dy_\alpha K_2[m_0 |x_\alpha - y_\alpha|] |\varphi(x)||\varphi(x - x(\alpha))|$$
$$\leq C'_M N R^{3N-2} \left[\int_{\mathbb{R}^6} dx_\alpha dy_\alpha K_2[m_0 |x_\alpha - y_\alpha|] \int_{\mathbb{R}^{3(N-1)}} dx' |\varphi(x', x_\alpha)|^2\right]^{\frac{1}{2}}$$
$$\times \left[\int_{\mathbb{R}^6} dx_\alpha dy_\alpha K_2[m_0 |x_\alpha - y_\alpha|] \int_{\mathbb{R}^{3(N-1)}} dx' |\varphi(x - x(\alpha))|^2\right]^{\frac{1}{2}}.$$

Now we use the variable change (12) to show that

$$\mathcal{G}_\alpha \leq C'_M N R^{3N-2}\left[\int\!\!\int_{\mathbb{R}^6} dx_\alpha dy_\alpha K_2[m_0|x_\alpha - y_\alpha|]\int_{\mathbb{R}^{3(N-1)}} dx'|\varphi(x', x_\alpha)|^2\right]^{\frac{1}{2}}$$
$$\times\left[\int\!\!\int_{\mathbb{R}^{3(N+1)}} dv_\alpha du K_2[m_0|v_\alpha|]|\varphi(u)|^2\right]^{\frac{1}{2}}$$
$$= C'_M N R^{3N-2}\int_{\mathbb{R}^3} dv K_2[m_0|v|]\|\varphi\|^2.$$

Hence we have that $\int_{\mathbb{R}^{3N}} dz(\varphi, L_1\varphi) \leq CR^{3N-2}\|\varphi\|^2$, since $\int_{\mathbb{R}^3} du(K_2[m_\alpha|u|] + K_2[m_0|u|]) < \infty$ which follows since $K_2[z] \sim \frac{1}{8z^2}$ as $z \to 0$ (Olver [10], Formula 9.6.9) and $K_2[z] \sim \sqrt{\frac{\pi}{2z}}e^{-z}$ as $z \to \infty$ (Olver [10], Formula 9.7.2). The lemma now follows by using these facts in inequality (17) and choosing $R_\epsilon := R$ sufficiently large. □

Define

$$\Lambda(H_{\mathfrak{P}}) := \inf\left\{\frac{\rho[\varphi]}{\|\varphi\|^2} : \varphi \in C_0^\infty(\mathbb{R}^{3N}), \varphi \neq 0\right\}$$
$$\Sigma(H_{\mathfrak{P}}) := \sup\left\{\inf\left\{\frac{\rho[\varphi]}{\|\varphi\|^2} : \varphi \in C_0^\infty(\mathbb{R}^{3N}\setminus K), \varphi \neq 0\right\} : K \subset\subset \mathbb{R}^{3N}\right\}.$$

An important question is whether or not $\Sigma(H_{\mathfrak{P}}) = \inf \sigma_e(H_{\mathfrak{P}})$, a question that has been answered in the positive by Persson [11], Theorem 2.1, for Schrödinger operators with potentials that are bounded from below at infinity.

PROPOSITION 3. – *If $V_-$ is relatively form bounded with respect to $T_{\mathfrak{P}}$ with form-bound strictly less than 1, then* $\Sigma(H_{\mathfrak{P}}) = \inf \sigma_e(H_{\mathfrak{P}})$.

*Proof.* – The proof that $\inf \sigma_e(H_{\mathfrak{P}}) \leq \Sigma(H_{\mathfrak{P}})$ is a consequence of the spectral theorem, see, e.g., [1], pp 50, 51.

For the reverse inequality, we apply Lemma 1 to note that given $\epsilon > 0$ there exists $R_\epsilon > 0$ such that

$$(\phi, H_{\mathfrak{P}}\phi) \geq \int_{\mathbb{R}^{3N}} (\Lambda_R(x; H_{\mathfrak{P}}) - \epsilon)|\varphi(x)|^2 dx$$

for all $\varphi \in C_0^\infty(\mathbb{R}^{3N})$ and for any $R \geq R_\epsilon$. For $R$ so chosen it follows from (6) that

$$\lim_{|x|\to\infty} \inf \Lambda_R(x; H_{\mathfrak{P}}) \geq \Sigma(H_{\mathfrak{P}}).$$

Choose $\alpha > 0$ sufficiently large in order that

$$\Lambda_R(x; H_{\mathfrak{P}}) \geq \Sigma(H_{\mathfrak{P}}) - \frac{\epsilon}{2}, \qquad |x| \geq \alpha.$$

Since $\Lambda_R(x; H_{\mathfrak{P}}) \geq \Lambda(H_{\mathfrak{P}}) > -\infty$ for all $x$, then there is some constant $C > 0$ such that

$$\Lambda_R(x; H_{\mathfrak{P}}) \geq \Sigma(H_{\mathfrak{P}}) - C, \qquad |x| \leq \alpha.$$

Choose a real-valued nonnegative function $\chi \in C_0^\infty(\mathbb{R}^{3N})$ such that $\chi(x) \geq C$ in $B(0; \alpha)$. Define

$$\rho_\chi[\varphi] := \rho[\varphi] + \int_{\mathbb{R}^{3N}} \chi(x)|\varphi(x)|^2 dx, \qquad \varphi \in (\mathbb{R}^{3N}),$$

then $H_{\mathfrak{P}} + \chi$ is the associated operator. Since

$$\rho_\chi[\varphi] \geq (\Sigma(H_{\mathfrak{P}}) - \epsilon)\|\varphi\|^2, \qquad \varphi \in (\mathbb{R}^{3N}),$$

according to Weyl (Reed and Simon [12], §XIII.4, Corollary 4) it suffices to show that $W := (H_{\mathfrak{P}} + \lambda)^{-\frac{1}{2}}\chi(H_{\mathfrak{P}} + \lambda)^{-\frac{1}{2}}$ is compact for a sufficiently large $\lambda$. In fact we will show that $W$ is in some trace ideal $\mathfrak{S}_p$ for some $p \in (0, \infty)$: since $V_-$ is relatively form-bounded with respect to $T_{\mathfrak{P}}$ with form-bound strictly less than 1, the operator $(T_{\mathfrak{P}} + \lambda)^{\frac{1}{2}}(H_{\mathfrak{P}} + \lambda)^{-\frac{1}{2}}$ is bounded for sufficiently large $\lambda$. Consequently this holds also for its adjoint which can be shown to be $(H_{\mathfrak{P}} + \lambda)^{-\frac{1}{2}}(T_{\mathfrak{P}} + \lambda)^{\frac{1}{2}}$. Therefore, we have for $p$ sufficiently large

$$\begin{aligned}
(18)\qquad \|W\|_p &\leq \|[(H_{\mathfrak{P}} + \lambda)^{-\frac{1}{2}}(T_{\mathfrak{P}} + \lambda)^{\frac{1}{2}}][(T_{\mathfrak{P}} + \lambda)^{-\frac{1}{2}}\chi^{\frac{1}{2}}] \\
&\qquad [\chi^{\frac{1}{2}}(T_{\mathfrak{P}} + \lambda)^{-\frac{1}{2}}][(T_{\mathfrak{P}} + \lambda)^{\frac{1}{2}}(H_{\mathfrak{P}} + \lambda)^{-\frac{1}{2}}]\|_p \\
(19)\qquad &\leq \mathrm{const}\|\chi^{\frac{1}{2}}(\mathrm{T}_{\mathfrak{P}} + \lambda)^{-\frac{1}{2}}\|_{\mathrm{p}/2}^2 \\
(20)\qquad &\leq \mathrm{const}\|\chi^{\frac{1}{2}}\|_{2\mathrm{p}}^2\|\mathrm{T}_{\mathfrak{P}}\|_{2\mathrm{p}}^2 < \infty
\end{aligned}$$

using the Hölder inequality from (18) to (19) and [14], Theorem 4.1, from (19) to (20). □

Recall $V$ given in (2)

$$V = \sum_{0 \leq \mu < \nu \leq N} v_{\mu\nu}(r_\mu - r_\nu) = \sum_{\nu=1}^{N} v_{0\nu}(x_\nu) + \sum_{1 \leq \mu < \nu \leq N} v_{\mu\nu}(x_\mu - x_\nu).$$

We assume that

(21) each $v_{\mu\nu} : \mathbb{R}^3 \to \mathbb{R}$ is in $L^2_{\text{loc}}(\mathbb{R}^3)$ and $v_{\mu\nu}(s) \to 0$ as $|s| \to \infty$.

Undoubtedly weaker conditions may be imposed upon the potential (cf Cycon *et al.*, [4], (3.4) and (3.5)), but (21) includes the important case of a Coulomb potential, which is the primary concern in this paper.

As defined in [4] a *cluster decomposition* is a set $\mathbf{a} := \{\mathbf{C_1}, \ldots, \mathbf{C_k}\}$ whose elements are nonempty, mutually disjoint sets $C_1, \ldots, C_k$ with union equal to $\{0, 1, \ldots, N\}$. We set $\#\mathbf{a} := \mathbf{k}$ and $\mathbf{a}$ is called a *k-cluster*. We write $(\mu\nu) \subset \mathbf{a}$ if, and only if $\{\mu, \nu\} \subset C_j$ for some $j$, $1 \leq j \leq k$. Otherwise we write $(\mu\nu) \not\subset \mathbf{a}$ to indicate that $\mu$ and $\nu$ belong to different sets. For a cluster decomposition $\mathbf{a}$, the *inter-cluster interaction* is defined by

$$I_{\mathbf{a}} := \sum_{(\mu\nu)\not\subset\mathbf{a}} v_{\mu\nu}, \qquad 0 \leq \mu < \nu \leq N,$$

and the *internal Hamiltonian* is given by

$$H_{\mathfrak{P}}(\mathbf{a}) := H_{\mathfrak{P}} - I_{\mathbf{a}} = T_{\mathfrak{P}} + \sum_{(\mu\nu)\subset\mathbf{a}} v_{\mu\nu}.$$

THEOREM 1. The Relativistic HWZ-Theorem. – *For a cluster decomposition* $\mathbf{a}$, *define* $\Sigma(\mathbf{a}) := \inf \sigma(H_{\mathfrak{P}}(\mathbf{a}))$ *and* $\Sigma := \min_{\#\mathbf{a}=2} \Sigma(\mathbf{a})$. *If* (21) *holds and* $V_-$ *is relatively form bounded with respect to* $T_{\mathfrak{P}}$ *with form-bound strictly less than 1, then* $\sigma_e(H_{\mathfrak{P}}) = [\Sigma, \infty)$.

*Proof.* – In the terminology used in the proof of the HWZ-Theorem for a non-relativistic system we divide the proof into the "hard part" and the "easy part".

"Hard part": Let $\{J_{\mathbf{a}}\}$ be a partition of unity indexed by all two-cluster decompositions $\mathbf{a}$ with the following properties:

(i) $\{J_{\mathbf{a}}\}_{\#\mathbf{a}=2} \subset C^1(\mathbb{R}^{3(N+1)})$;

(ii) $\sum_{\#\mathbf{a}=2} J^2_{\mathbf{a}}(r) \equiv 1$, $r \in \mathbb{R}^{3(N+1)}$;

(iii) each function $J_{\mathbf{a}}$ is homogeneous of degree zero for $|r| > 1$; and

(iv) there exists a constant $C > 0$ such that

$$\text{supp} J_{\mathbf{a}} \cap \{r : |r| > 1\} \subset \{r : |r_\mu - r_\nu| \geq C|r| \text{ for all } (\mu\nu) \not\subset \mathbf{a}\}.$$

The *Ruelle-Simon partition of unity*, Cycon et al [4], satisfies these properties as well as a partition of unity given in [17]. When restricted to $(x_1, \ldots, x_N) \in \mathbb{R}^{3N}$ in (1) with fixed $x_0 = \mathfrak{x}_0$, this partition of unity will satisfy the properties required of $\{\chi_\nu\}_{\nu=1}^K$ in Corollary 1. Henceforth, each $J_{\mathbf{a}} = J_{\mathbf{a}}(\mathfrak{x}_0, x_1, \ldots, x_N) =: J_{\mathbf{a}}(\mathfrak{x}_0; x)$ and $x = (x_1, \ldots, x_N)$.

Using Corollary 1 we have that

$$(22)\quad (\varphi, H_{\mathfrak{P}}\varphi) = \sum_{\#\mathbf{a}=2} \big((J_{\mathbf{a}}\varphi, H_{\mathfrak{P}}(\mathbf{a})J_{\mathbf{a}}\varphi) + (J_{\mathbf{a}}\varphi, I_{\mathbf{a}}J_{\mathbf{a}}\varphi)\big) - (\varphi, L\varphi)$$

for $L$ corresponding to the operator $L_K$ in Corollary 1 with kernel

$$L(x,y) := \left(\sum_{\alpha=1}^{N}\left[F_\alpha(x,y) + \frac{1}{N}G_\alpha(x,y)e^{i\mathfrak{P}\cdot(x_\alpha - y_\alpha)}\right]\right) \times \sum_{\#\mathbf{a}=2}(J_{\mathbf{a}}(\mathfrak{x}_0; x) - J_{\mathbf{a}}(\mathfrak{x}_0; y))^2.$$

By Proposition 3 it will suffice to show that

$$(23)\quad \lim_{R\to\infty}\inf\{\rho[\varphi] : \varphi \in C_0^\infty(\mathbb{R}^{3N}\setminus B(0;R)), \|\varphi\| = 1\} = \lim_{R\to\infty}\inf \times \left\{\sum_{\#\mathbf{a}=2}(J_{\mathbf{a}}\varphi, H_{\mathfrak{P}}(\mathbf{a})J_{\mathbf{a}}\varphi) : \varphi \in C_0^\infty(\mathbb{R}^{3N}\setminus B(0;R)), \|\varphi\| = 1\right\}.$$

It follows from (21) and property (iv) that $I_{\mathbf{a}}J_{\mathbf{a}} \to 0$ as $|x| \to \infty$ since $|x| \to \infty$ implies that $|r| \to \infty$. Recall that the variable change (1) gives the identities $x_\nu = r_\nu - r_0$, $\nu = 1, \ldots, N$, and $x_\mu - x_\nu = r_\mu - r_\nu$, $1 \le \mu < \nu \le N$. As a consequence the second term on the right side of the identity (22) will approach zero as $R \to \infty$.

For the error term in (22) note that for some constant $C' > 0$

$$|J_{\mathbf{a}}(\mathfrak{x}_0; x) - J_{\mathbf{a}}(\mathfrak{x}_0; y)| \le C'\big|(\mathfrak{x}_0; x)/|(\mathfrak{x}_0; x)| - (\mathfrak{x}_0; y)/|(\mathfrak{x}_0; y)|\big| \le 2C'|x - y|/|x|,$$

since each $J_{\mathbf{a}} \in C^1$ is homogeneous of degree zero. This implies that

$$|(\varphi, L\varphi)| \le C'' \int_{\mathbb{R}^{6N}} dx dy \sum_{\alpha=1}^{N}\left|F_\alpha(x,y) + \frac{1}{N}G_\alpha(x,y)e^{i\mathfrak{P}\cdot(x_\alpha - y_\alpha)}\right| \times |x|^{-2}|x - y|^2|\varphi(x)||\varphi(y)|.$$

Now we proceed in a manner similar to the last part of the proof of Lemma 1. For $(x', y_\alpha) = (x_1, \dots, y_\alpha, \dots, x_N)$ and $\varphi \in C_0^\infty(\mathbb{R}^{3N} \setminus B(0; R))$

$$\begin{aligned}
&\int_{\mathbb{R}^{6N}} dxdy F_\alpha(x,y) \frac{|x-y|^2}{|x|^2} |\varphi(x)||\varphi(y)| \\
&\quad = \frac{m_\alpha^2}{4\pi^2} \int_{\mathbb{R}^{3(N+1)}} dxdy_\alpha \frac{K_2[m_\alpha |x_\alpha - y_\alpha|]}{|x|^2} |\varphi(x)||\varphi(x', y_\alpha)| \\
&\quad \le C_m R^{-2} \int_{\mathbb{R}^{3(N+1)}} dxdy_\alpha K_2[m_\alpha |x_\alpha - y_\alpha|] |\varphi(x)||\varphi(x', y_\alpha)| \\
&\quad \le C'_m R^{-2} \int_{\mathbb{R}^3} du K_2[m_\alpha |u|] \|\varphi\|^2
\end{aligned}$$

and similarly

$$\begin{aligned}
&\int_{\mathbb{R}^{6N}} dxdy |G_\alpha(x,y) e^{i\mathfrak{P}\cdot(x_\alpha - y_\alpha)}| |x|^{-2} |x-y|^2 |\varphi(x)||\varphi(y)| \\
&\quad \le \frac{C_M N}{R^2} \int_{\mathbb{R}^{3N+3}} dxdy_\alpha K_2[m_0 |x_\alpha - y_\alpha|] |\varphi(x)||\varphi(x - x(\alpha))| \\
&\quad \le C'_M N R^{-2} \int_{\mathbb{R}^3} dv K_2[m_0 |v|] \|\varphi\|^2.
\end{aligned}$$

We conclude that for some constant $C > 0$

$$|(\varphi, L\varphi)| \le C R^{-2} \|\varphi\|^2.$$

Therefore (23) follows and the proof of the "hard part" is complete.

"Easy part": Let $\lambda > \Sigma$. Our goal is to prove that $\lambda \in \sigma_e(H_\mathfrak{P})$. Let $\mathbf{a} = \{C_1, C_2\}$ be a 2-cluster decomposition such that $\Sigma = \Sigma(\mathbf{a})$ and set $\ell_1 = \#C_1$ and $\ell_2 = \#C_2$. For particles in these respective clusters we will define operators $H_{\mathfrak{P}_1}^{C_1}$ and $H_{\mathfrak{P}_2}^{C_2}$ much like we did for $H_\mathfrak{P}$ with $\mathfrak{P}_j = \sum_{\nu \in C_j} k_\nu$, $j = 1, 2$, in which the transformation matrices corresponding to $A$ described in Appendix A will be denoted as $A_j$, $j = 1, 2$. We view the change of variables in momenta according to the following scheme:

$$\begin{pmatrix} p_0 \\ p_1 \\ \vdots \\ p_N \end{pmatrix} \xrightarrow{A^t} \begin{pmatrix} k_0 \\ k_1 \\ \vdots \\ k_N \end{pmatrix} \xrightarrow{U_1} \begin{pmatrix} k'_1 \\ \vdots \\ k'_{\ell_1} \\ k''_1 \\ \vdots \\ k''_{\ell_2} \end{pmatrix} \xrightarrow{B} \begin{pmatrix} P_1 \\ p'_1 \\ \vdots \\ p'_{\ell_1 - 1} \\ P_2 \\ p''_1 \\ \vdots \\ p''_{\ell_2 - 1} \end{pmatrix} \xrightarrow{U_2} \begin{pmatrix} P \\ p'_1 \\ \vdots \\ p'_{\ell_1 - 1} \\ Q \\ p''_1 \\ \vdots \\ p''_{\ell_2 - 1} \end{pmatrix} \tag{24}$$

where $A$ is given by (1), $U_1$ and $U_2$ are products of elementary matrices,

$$B := \begin{pmatrix} (A_1^t)^{-1} & 0 \\ 0 & (A_2^t)^{-1} \end{pmatrix},$$

$P = P_1 + P_2$, and $Q := P_1 - P_2$. (That is, $k'_{\nu+1} = \frac{m'_\nu}{M_1} P_1 + p'_\nu$, $\nu = 1, \ldots, \ell_1 - 1$, where $M_1 = \sum_{\nu \in C_1} m_\nu$, and each $k''_\nu$ is given similarly. Note that $\det(A_j) = 1$, $j = 1, 2$.) We have that the transformation $S := U_2 B U_1 A^t : (p_0, p_1, \ldots, p_N)^t \mapsto (P, p', Q, p'')^t$ with $p' := (p'_1, \ldots, p'_{\ell_1 - 1})$, $p'' := (p''_1, \ldots, p''_{\ell_2 - 1})$, and $\det(S) = \det(U_2) = -8$. The kinetic energy terms

$$\hat{T}^{C_1}_{\mathfrak{P}_1} = \sum_{\nu=1}^{\ell_1 - 1} \left( \left( \frac{m'_\nu}{M_1} \mathfrak{P}_1 + p'_\nu \right)^2 + {m'_\nu}^2 \right)^{\frac{1}{2}} - m'_\nu + \left( \left( \frac{m'_0}{M_1} \mathfrak{P}_1 - \sum_{\nu=1}^{\ell_1 - 1} p'_\nu \right)^2 + {m'_0}^2 \right)^{\frac{1}{2}} - m'_0$$

$$\hat{T}^{C_2}_{\mathfrak{P}_2} = \sum_{\nu=1}^{\ell_2 - 1} \left( \left( \frac{m''_\nu}{M_2} \mathfrak{P}_2 + p''_\nu \right)^2 + m''^2_\nu \right)^{\frac{1}{2}} - m''_\nu + \left( \left( \frac{m''_0}{M_2} \mathfrak{P}_2 - \sum_{\nu=1}^{\ell_2 - 1} p''_\nu \right)^2 + m''^2_0 \right)^{\frac{1}{2}} - m''_0$$

are used to derive $H^{C_1}_{\mathfrak{P}_1}$ and $H^{C_2}_{\mathfrak{P}_2}$. The potentials for these operators are

$$V_{C_1} := \sum_{\mu,\nu \in C_1} v_{\mu,\nu} \qquad \text{and} \qquad V_{C_2} := \sum_{\mu,\nu \in C_2} v_{\mu,\nu}.$$

We also need the Hamiltonian in the coordinates $p', p'', Q$. Its kinetic energy $\tilde{T}_{\mathfrak{P}}$ is the multiplication operator

(25) $$\tilde{T}_{\mathfrak{P}}(p', p'', Q) = \frac{1}{8} \Bigg[ \sum_{\nu=1}^{\ell_1 - 1} \left( \left( \frac{m'_\nu}{2M_1} (\mathfrak{P} + Q) + p'_\nu \right)^2 + {m'_\nu}^2 \right)^{\frac{1}{2}} - m'_\nu + \left( \left( \frac{m'_0}{2M_1} (\mathfrak{P} + Q) - \sum_{\nu=1}^{\ell_1 - 1} p'_\nu \right)^2 + {m'_0}^2 \right)^{\frac{1}{2}} - m'_0$$
$$+ \sum_{\nu=1}^{\ell_2 - 1} \left( \left( \frac{m''_\nu}{2M_2} (\mathfrak{P} - Q) + p''_\nu \right)^2 + m''^2_\nu \right)^{\frac{1}{2}} - m''_\nu + \left( \left( \frac{m''_0}{2M_2} (\mathfrak{P} - Q) - \sum_{\nu=1}^{\ell_2 - 1} p''_\nu \right)^2 + m''^2_0 \right)^{\frac{1}{2}} - m''_0 \Bigg].$$

First we prove that $\lambda \in \sigma(H_{\mathfrak{P}}(\mathbf{a}))$. The $\min\sigma(H_{\mathfrak{P}_j}^{C_j})$ is a continuous function of $\mathfrak{P}_j$ and it tends to $\infty$ as $|\mathfrak{P}_j| \to \infty$. Consequently, we can choose $\mathfrak{P}_1$ and $\mathfrak{P}_2$ such that

$$\lambda = \min\sigma(H_{\mathfrak{P}_1}^{C_1}) + \min\sigma(H_{\mathfrak{P}_2}^{C_2}).$$

Denote $\lambda_1 = \min\sigma(H_{\mathfrak{P}_1}^{C_1})$ and $\lambda_2 = \min\sigma(H_{\mathfrak{P}_2}^{C_2})$. Choose normalized $\phi_j \in C_0^\infty(\mathbb{R}^{3(\ell_j-1)})$, $j = 1, 2$, such that

$$\|(H_{\mathfrak{P}_j}^{C_j} - \lambda_j)\phi_j\| < \frac{\epsilon}{4}, \qquad j = 1,\ 2.$$

Note that $\hat{\phi}_1$ is a function of $p'$ and $\hat{\phi}_2$ is a function of $p''$ derived in (24). Choose $f \in C_0^\infty(B(0;1))$ with $\|f\| = 1$. Now we define $\psi_n$ such that its transform $\tilde{\psi}_n$ in the $p', p'', Q$, coordinates is

$$\tilde{\psi}_n(p', p'', Q) := \hat{\phi}_1(p')\hat{\phi}_2(p'')f_n(Q)$$

where $f_n(Q) := n^{\frac{3}{2}} f(n(Q - (\mathfrak{P}_1 - \mathfrak{P}_2)))$. Note that $f_n(Q)$ vanishes outside $B(\mathfrak{P}_1 - \mathfrak{P}_2; \frac{1}{n})$ and $\|f_n\| = 1$.

To complete the proof it suffices to show that $\|(H_{\mathfrak{P}} - \lambda)\psi_n\| \to 0$ as $n \to \infty$. Note that

$$\begin{aligned}\|(H_{\mathfrak{P}} - \lambda)\psi_n\| &\le \|I_{\mathbf{a}}\psi_n\| + \|(H_{\mathfrak{P}}(\mathbf{a}) - \lambda)\psi_n\| \\ &= \|I_{\mathbf{a}}\psi_n\| + \|(\tilde{T}_{\mathfrak{P}}(p', p'', Q) \\ &\quad + U_{C_1}V_{C_1}U_{C_1}^{-1} + U_{C_2}V_{C_2}U_{C_2}^{-1} - \lambda_1 - \lambda_2)\tilde{\psi}_n\|\end{aligned}$$

where $U_{C_1}$ and $U_{C_2}$ are the Fourier transforms in $p'$ and $p''$ respectively. Since $f_n$ is supported in $B := B(\mathfrak{P}_1 - \mathfrak{P}_2; \frac{1}{n})$,

$$\tilde{T}_{\mathfrak{P}}(p', p'', Q)\tilde{\psi}_n = \tilde{T}_{\mathfrak{P}}(p', p'', Q)\chi_B(Q)\tilde{\psi}_n$$

and $\max_{Q\in S} |\nabla_Q \tilde{T}| < \infty$. It follows that

$$\begin{aligned}&\|(\tilde{T}_{\mathfrak{P}}(p', p'', Q) + U_{C_1}V_{C_1}U_{C_1}^{-1} + U_{C_2}V_{C_2}U_{C_2}^{-1} - \lambda_1 - \lambda_2)\tilde{\psi}_n\| \\ &\le \|(\tilde{T}_{\mathfrak{P}}(p', p'', \mathfrak{P}_1 - \mathfrak{P}_2) + U_{C_1}V_{C_1}U_{C_1}^{-1} \\ &\quad + U_{C_2}V_{C_2}U_{C_2}^{-1} - \lambda_1 - \lambda_2)\tilde{\psi}_n\| + \frac{C'}{n}\end{aligned}$$

for some $C' > 0$. But

$$\tilde{T}_{\mathfrak{P}}(p', p'', \mathfrak{P}_1 - \mathfrak{P}_2) = \frac{1}{8}\hat{T}_{\mathfrak{P}_1}^{C_1}(p') + \frac{1}{8}\hat{T}_{\mathfrak{P}_2}^{C_2}(p'')$$

by (25). Therefore,

$$8\|(H_{\mathfrak{P}}-\lambda)\psi_n\| \le \|I_{\mathbf{a}}\psi_n\|+\sum_{j=1}^{2}\|(H_{\mathfrak{P}_j}^{C_j}-\lambda_j)\hat{\phi}_j\|+\frac{C'}{n} \le \|I_{\mathbf{a}}\psi_n\|+\frac{\epsilon}{2}+\frac{C'}{n}.$$

We need only to show that $\|I_{\mathbf{a}}\psi_n\| \to 0$ as $n \to \infty$. Choose $C > 0$ so large that $|x_\mu - x_\nu| > C$ implies that $|v_{\mu\nu}(x_\mu - x_\nu)| < \epsilon$. Then

$$\begin{aligned}\|v_{\mu\nu}(x_\mu - x_\nu)\psi_n\|^2 = &\int_{|x_\mu - x_\nu|<C} |v_{\mu\nu}(x_\mu - x_\nu)\psi_n(x)|^2 dx \\ &+ \int_{|x_\mu - x_\nu|\ge C} |v_{\mu\nu}(x_\mu - x_\nu)\psi_n(x)|^2 dx.\end{aligned}$$

The second term in the right-hand side of the last equation is less than $\epsilon$. The first term is also less than $\epsilon$ since $v_{\mu\nu} \in L^2_{\text{loc}}(\mathbb{R}^3)$; $\max|\psi_n| \to 0$ as $n \to \infty$; and the region $\Omega$, where $|x_\mu - x_\nu| < C$, $\phi_1 \ne 0$, and $\phi_2 \ne 0$, is compact. This completes the proof. □

## 3. COULOMB SYSTEMS

We wish to extend our results above so that they are also applicable to a Coulomb system of electrons and one or several nuclei. Since the Coulomb singularities are border-line concerning the relative boundedness, we will have to use an elaborate result of Lieb and Yau [9] to verify our assumptions. Moreover we will have to take into account the symmetry of the Hamiltonian, since this influences the spectrum in an essential way. This latter consideration is well known in the non-relativistic case (Zislin [19], Jörgens and Weidmann [7], Balslev [2, 3]). Here we consider the relativistic case, but only for bosons and fermions.

For the sake of simplicity we consider only a system of $N_n$ identical nuclei, which are assumed to be bosons, of mass $M$ and charge $Z$, and $N_e$ electrons of mass $m$ *without regard for spin.* (The reader will see that extensions to more general cases are straightforward.) Then $N + 1 = N_n + N_e$. Let $S_k$ denote the symmetric group of $k$ elements for a positive integer $k$. We are interested in the subgroup $S$ of $S_{N+1}$ which permutes only the indices of identical elements, *i.e.*,

$$S := S_{N_n} \times S_{N_e} = \{\sigma = (\sigma_1, \sigma_2) : \sigma_1 \in S_{N_n}, \sigma_2 \in S_{N_e}\}.$$

To be definitive we assume initially that $r_0, \dots, r_{N_n-1}$, represent the positions of the nuclei and $s_1, \dots, s_{N_e}$, represent the positions of the electrons with associated momenta $k_{r_\mu}, k_{s_\nu}$. For each $\sigma \in S$ let $\epsilon(\sigma) = -1$ if $\sigma_2$ is an odd permutation and $\epsilon(\sigma) = 1$ if $\sigma_2$ is an even permutation, i.e., decomposable into an even or odd number of transpositions. For any $f \in L^2(\mathbb{R}^{3(N+1)})$ define $(\sigma f)(r,s) := f(\sigma^{-1}(r,s)) = f(\sigma_1^{-1}r, \sigma_2^{-1}s)$, $\sigma \in S$. Let $\mathcal{S} := \{f : \sigma f = \epsilon(\sigma) f \text{ for all } \sigma \in \mathrm{S}\}$. Define

$$f_{\mathcal{S}}(r,s) := \frac{1}{|S|} \sum_{\sigma \in S} \epsilon(\sigma)(\sigma f)(r,s), \qquad \text{for } f \in L^2(\mathbb{R}^{3(N+1)})$$

in which $|S| = 3(N+1)!$. Then, $f_{\mathcal{S}} \in \mathcal{S}$ and since $(r,s) \mapsto \sigma(r,s)$ is a linear isometry on $\mathbb{R}^{3(N+1)}$ (endowed with the usual Euclidean norm) it follows that the map $\Pi_{\mathcal{S}} : f \mapsto f_{\mathcal{S}}$ is a projection of $L^2(\mathbb{R}^{3(N+1)})$ onto the closed subspace $\mathcal{S} \cap L^2(\mathbb{R}^{3(N+1)})$. Note also that $U\Pi_{\mathcal{S}} f = \Pi_{\mathcal{S}} U f$ (where $U : f \mapsto \hat{f}$) since $(\hat{\sigma f})(k_r, k_s) = (\sigma^{-1}\hat{f})(k_r, k_s)$. Hence, we can consider symmetry properties of domain elements in momenta variables without loss of generality.

Let $\mathfrak{S}_{\mathcal{S}}(\mathbb{R}^{3(N+1)}) := \mathcal{S} \cap \mathfrak{S}(\mathbb{R}^{3(N+1)})$. This is the set of all functions in Schwartz space that also satisfy the required symmetry in the momenta variables $k_r, k_s$. Define

$$\tilde{\mathfrak{S}}_{\mathcal{S}}(\mathbb{R}^{3N}) := \{f : f(p_1, \dots, p_N) = g(\mathfrak{P}, p_1, \dots, p_N) \text{ for } g \in \mathfrak{S}_{\mathcal{S}}(\mathbb{R}^{3(N+1)})\}$$

where $\mathfrak{P} = \sum k_r + \sum k_s$ and $p_1, \dots, p_N$ are related to $k_r, k_s$, by (24). Now $H_{\mathfrak{P}}$ with the required symmetry restrictions is given as in (5) by

$$\rho[\varphi] := (\varphi, H_{\mathfrak{P}}\varphi), \qquad U\varphi \in \tilde{\mathfrak{S}}_{\mathcal{S}}(\mathbb{R}^{3N}). \tag{26}$$

Denote the $L^2$-closure of $\tilde{\mathfrak{S}}_{\mathcal{S}}(\mathbb{R}^{3N})$ by $L^2_{\mathcal{S}}(\mathbb{R}^{3N})$.

Let $\mathbf{a}$ be some 2-cluster decomposition of $\{0, 1, \dots, N\}$ into disjoint, nonempty sets $\{C_1, C_2\}$. Let $S_{\mathbf{a}}$ denote the subgroup of $S$ consisting of permutations in $S$ that exchange elements only within $C_1$ and only within $C_2$leaving the sets $C_1$ and $C_2$ unchanged. The projection $\Pi_{\mathcal{S}_{\mathbf{a}}}$ is defined as $\Pi_{\mathcal{S}}$ above with $S_{\mathbf{a}}$ replacing $S$. The projection $\Pi_{\mathcal{S}_{\mathbf{a}}}$ acts only on the subspace of functions of $p', p''$, which are called the "internal coordinates". (Recall from (24) that $p'_\nu = k'_{\nu+1} - \frac{m'_\nu}{M_1} \sum_{\mu=1}^{|C_1|} k'_\mu$, $\nu = 1, \dots, |C_1| - 1$, and similarly for $p''$. Therefore functions of $p'$ and $p''$ remain functions of $p'$ and $p''$ under the projection $\Pi_{\mathcal{S}_{\mathbf{a}}}$.) For $U : f \rightarrow \hat{f}$ the operator $(H^{C_1}_{\mathfrak{P}_1} \otimes 1 + 1 \otimes H^{C_2}_{\mathfrak{P}_2}) U^{-1} \Pi_{\mathcal{S}_{\mathbf{a}}}$ is defined as above. The candidate for the minimal point of the essential spectrum of $H_{\mathfrak{P}}$ is

$$\Sigma_{\mathfrak{P}} := \min_{\mathbf{a}} \{ \min \sigma[(H^{C_1}_{\mathfrak{P}_1} \otimes 1 + 1 \otimes H^{C_2}_{\mathfrak{P}_2}) U^{-1} \Pi_{\mathcal{S}_{\mathbf{a}}}] : \mathbf{a} = \{C_1, C_2\}, \mathfrak{P} = \mathfrak{P}_1 + \mathfrak{P}_2 \}. \tag{27}$$

The results of §2 leading to Theorem 1 now follow with obvious modifications. We refer to a similar treatment for non-relativistic operators in [5] for further details which may be used here. In the proof of the "Hard part" of Theorem 1 the functions $\{J_{\mathbf{a}}\}$ in the *Ruelle-Simon partition of unity* must be chosen in order that each $J_{\mathbf{a}}\varphi \in \tilde{\mathfrak{S}}_S(\mathbb{R}^{3N})$ for $\varphi \in \tilde{\mathfrak{S}}_S(\mathbb{R}^{3N})$. It suffices that each $J_{\mathbf{a}}$ be symmetric, *i.e.*, $J_{\mathbf{a}} = \sigma J_{\mathbf{a}}$ for all $\sigma \in S$. The "Hard part" of the proof of Theorem 1 follows with $\Sigma = \Sigma_{\mathfrak{P}}$.

Next we indicate the revisions which are needed in the proof of Theorem 1, the "Easy part". Let $\mathbf{a} = \{C_1, C_2\}$ be a 2-cluster for which the minimum occurs, *i.e.*, $\Sigma = \Sigma_{\mathfrak{P}}$ as given in (27) with $\mathfrak{P}_1$ and $\mathfrak{P}_2$ chosen in order that $\mathfrak{P} = \mathfrak{P}_1 + \mathfrak{P}_2$. Let $\lambda > \Sigma$. Corresponding to the sequence $\{\psi_n\}$ constructed in the proof of Theorem 1, we must show here that we can construct such a sequence which belongs to $\tilde{\mathfrak{S}}_S(\mathbb{R}^{3N})$. For a small $\epsilon > 0$ choose normalized $\phi \in L^2(\mathbb{R}_{p'}^{3(|C_1|-1)}) \otimes L^2(\mathbb{R}_{p''}^{3(|C_2|-1)})$ such that $\phi$ satisfies

$$\|(H_{\mathfrak{P}_1}^{C_1} \otimes 1 + 1 \otimes H_{\mathfrak{P}_2}^{C_2} - \lambda)\phi\| < \epsilon.$$

First consider the case in which $C_1$ and $C_2$ are not identical, *i.e.*, there is a different number of electrons and nuclei corresponding to $C_1$ and $C_2$. (Of course, in general the number of electrons and nuclei corresponding to each $C_1$ and $C_2$ may be equal but $C_1$ and $C_2$ are not said to be identical unless each corresponding mass is equal as well. In the simplified case that we study here that is an assumption.) Here we choose $f$ as in §2 and choose

$$\psi_n := U^{-1}\Pi_S[(\Pi_{S_{\mathbf{a}}}\phi) \cdot f(P_1 - P_2)].$$

The case in which $C_1$ and $C_2$ are identical requires special attention (Zislin [19]). In this case let $\sigma^0 = (\sigma_1^0, \sigma_2^0) \in S$ be the unique permutation that exchanges electrons and nuclei corresponding to $C_1$ and $C_2$ while observing the order dictated by $C_1$ and $C_2$, that is, the *first* electron from $C_1$ is exchanged with the *first* electron from $C_2$, etc. For $f$ chosen as in §2 let $f^{\pm}$ be the even and odd parts of $f$, *i.e.*, $f^{\pm}(x) := (f(x) \pm f(-x))/2$. The even and the odd parts of the function $\phi$ with respect to $\sigma^0$ is defined by

$$(\Pi_{S_{\mathbf{a}}}\phi)^{\pm} := \frac{1}{2}[(\Pi_{S_{\mathbf{a}}}\phi) \pm \sigma^0(\Pi_{S_{\mathbf{a}}}\phi)].$$

Note that $\epsilon(\sigma^0) = \pm 1$ according to whether the number of electrons in the cluster corresponding to $C_1$ (or to $C_2$) is an even or an odd number, respectively. If $\epsilon(\sigma^0) = 1$ we take

$$\psi_n := U^{-1}\Pi_S[(\Pi_{S_{\mathbf{a}}}\phi)^+ \cdot f^+(P_1 - P_2) + (\Pi_{S_{\mathbf{a}}}\phi)^- \cdot f^-(P_1 - P_2)].$$

and if $\epsilon(\sigma^0) = -1$ we take

$$\psi_n := U^{-1}\Pi_{\mathcal{S}}[(\Pi_{\mathcal{S}_a}\phi)^+ \cdot f^-(P_1 - P_2) + (\Pi_{\mathcal{S}_a}\phi)^- \cdot f^+(P_1 - P_2)].$$

Note that in either case $U\psi_n \in \tilde{\mathfrak{S}}_{\mathcal{S}}(\mathbb{R}^{3N})$ as required. Now we are able to proceed as in §2.

THEOREM 2. – *Let $V_-$ be relatively $T_{\mathfrak{P}}$-form-bounded with bound strictly less than* 1, *assume that $V$ fulfills condition* (21), *and take $\Sigma_{\mathfrak{P}}$ as in* (27). *Then* $\inf \sigma_{\text{ess}}(H_{\mathfrak{P}}) = \Sigma_{\mathfrak{P}}$.

In the following $\alpha = e^2$ is the Sommerfeld fine structure constant in which $-e$ is the charge of the electron. Let $V_c$ be the Coulomb interaction potential of $N_n$ nuclei with charges $Z_1, ..., Z_{N_n}$ and $N_e$ electrons:

$$V_c(\mathbf{r}_1, \ldots, \mathbf{r}_{N_e}; \mathbf{R}_1, \ldots, \mathbf{R}_{N_n}) := -\sum_{\nu=1}^{N_e}\sum_{\kappa=1}^{N_n} \frac{\alpha Z_\kappa}{|\mathbf{r}_\nu - \mathbf{R}_\kappa|} + \sum_{1\le\mu<\nu\le N_e} \frac{\alpha}{|\mathbf{r}_\mu - \mathbf{r}_\nu|} + \sum_{0\le\kappa<\lambda\le N_n} \frac{\alpha Z_\kappa Z_\lambda}{|\mathbf{R}_\kappa - \mathbf{R}_\lambda|}$$

where $r = (\mathbf{r}_1, \ldots, \mathbf{r}_{N_e}; \mathbf{R}_1, \ldots, \mathbf{R}_{N_n})$.

COROLLARY 2. – *Let $H_{\mathfrak{P}}$ be the Hamiltonian with the Coulomb interaction potential $V_c$ and let $Z \ge Z_1, ..., Z_{N_n} \ge 0$. If either $Z\alpha < 2/\pi$ and $\alpha < 1/47$ hold or $(\pi/2)Z + 2.2159Z^{2/3} + 1.0307 \le 1/\alpha$, then* $\inf \sigma_{\text{ess}}(H_{\mathfrak{P}}) = \Sigma_{\mathfrak{P}}$.

*Proof.* – We only need to verify the relative boundedness. This, however, follows from Lieb and Yau [9] and Lieb *et al.* [8] under the hypothesis given above. These references investigate the operator where the position of the nuclei are just parameters and not dynamical variables. Their result shows that our hypothesis is verified, since our kinetic energy operator plus $N_e m$ is only bigger because of the inclusion of the kinetic energy of the nuclei. □

Note that the hypotheses of the corollary cover different ranges of $\alpha$ and $Z$. Whereas the first condition (Lieb and Yau [9]) gives the best critical charges, the second condition (Lieb *et al.* [8]) gives the best (close to optimal) value for $\alpha$ for small $Z$.

## APPENDIX A

### Change of Variables

For a molecule with $N+1$ particles at positions $r_\nu \in \mathbb{R}^3$, $\nu = 0, \ldots, N$, mass $m_\nu$, momenta $k_\nu$, and total mass $M := \sum_{\nu=0}^{N} m_\nu$, the position $x_0$ of the center-of-mass of the system is identified using a nonsingular matrix $A$ (typically associated with either Jacobi coordinates or atomic coordinates as in (1)) with constant real-valued entries to change to position variables $x_0, x_1, \ldots, x_N$:

$$x = Ar, \qquad x_0 = \frac{1}{M} \sum_{\nu=0}^{N} m_\nu r_\nu, \tag{28}$$

which will result in a change in momenta from $k$ to $p$

$$k = A^t p.$$

To see this change in momenta consider the following: Denote the Fourier transform by $U : \varphi \mapsto \hat{\varphi}$, which is unitary. We may assume that $\det(A) = 1$. For $F(k) : \mathbb{R}^{3(N+1)} \to \mathbb{R}$, all $\varphi, \vartheta \in C_0^\infty(\mathbb{R}^{3(N+1)})$ and $\phi = \hat{\varphi}, \theta = \hat{\vartheta}$,

$$\begin{aligned}(\vartheta, U^{-1} F(k) U \varphi) &= \frac{1}{(2\pi\hbar)^{3(N+1)/2}} \int_{\mathbb{R}^{3(N+1)}} dr \overline{\vartheta(r)} \\ &\quad \times \int_{\mathbb{R}^{3(N+1)}} dk e^{\frac{i}{\hbar} k \cdot r} F(k) \phi(k) \\ &= \frac{1}{(2\pi\hbar)^{3(N+1)/2}} \int_{\mathbb{R}^{3(N+1)}} dx \overline{\vartheta(A^{-1}x)} \\ &\quad \times \int_{\mathbb{R}^{3(N+1)}} dp e^{\frac{i}{\hbar} p \cdot x} F(A^t p) \phi(A^t p) \\ &= (\vartheta(A^{-1}x), U^{-1} F(A^t p) U \varphi(A^{-1}x)) \\ &= (\vartheta(r), U^{-1} F(A^t p) U \varphi(r))\end{aligned}$$

for $A^t p := k$ showing that $U^{-1} F(k) U = U^{-1} F(A^t p) U$. Then, $T = \sum_{\nu=0}^{N} \sqrt{c^2 |k_\nu|^2 + m_\nu^2 c^4} - m_\nu c^2$, in the $p$-variable is given by

$$T := \sum_{\nu=0}^{N} \sqrt{c^2 |(A^t p)_\nu|^2 + m_\nu^2 c^4} - m_\nu c^2.$$

If $A$ is chosen to correspond to (1) in which $\det(A) = 1$ then we show below that the momentum $P$ for the center of mass

$$P := p_0 = \sum_{\nu=0}^{N} k_\nu \tag{29}$$

and

$$T = \sqrt{c^2 \left| \frac{m_0}{M} P - \sum_{\nu=1}^{N} p_\nu \right|^2 + m_0^2 c^4} - m_0 c^2$$

$$+ \sum_{\nu=1}^{N} \sqrt{c^2 \left| \frac{m_\nu}{M_T} P + p_\nu \right|^2 + m_\nu^2 c^4} - m_\nu c^2.$$

To show that (29) holds in the general case described by (28) we may (without loss of generality) define $\tilde{X}$ to be $\mathbb{R}^{3(N+1)}$ with the inner product

$$(r, s)_{\tilde{X}} := \sum_{\nu=0}^{N} m_\nu r_\nu \cdot s_\nu, \qquad r, s \in \tilde{X}.$$

Then we restrict the operator to the $3N$-dimensional subspace

$$X := \left\{ r \in \mathbb{R}^{3(N+1)} : \sum_{\nu=0}^{N} m_\nu r_\nu = 0 \right\}.$$

Note that each element of $X^\perp$ in $\tilde{X}$ is a vector of the form $r^\perp = (\alpha, \alpha, \ldots, \alpha)$ for some non-zero $\alpha \in \mathbb{R}^3$. If we make a change of variable with a nonsingular matrix $A$

$$\begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_N \end{pmatrix} = A \begin{pmatrix} r_0 \\ r_1 \\ \vdots \\ r_N \end{pmatrix}$$

in order that

$$x_0 = \frac{1}{M} \sum_{\nu=0}^{N} m_\nu r_\nu$$

and $Ar \in X$ for $r \in X$, then we may require that $\sum_{\nu=1}^{N} a_{\mu\nu} = 0$ for each row $\mu = 1, \ldots, N$. (This is the case with the classical transformations: Jacobi coordinates and atomic coordinates (1) in which $\det(A) = 1$.) Hence, the sum of each column of $A^t$, except for the first, is 0. Since $k = A^t p$, then this implies that

$$P = \sum_{\nu=0}^{N} k_\nu.$$

## APPENDIX B

### Direct Integrals

We adapt to our purposes the concept of a *constant fiber direct integral* $\mathcal{H} := L^2(M, d\mu; \mathcal{H}')$, which is a generalization of the direct sum of Hilbert spaces, discussed in Reed and Simon [12], §XIII.16. Here the $\sigma$-finite measure space $< M, \mu >$ is $\mathbb{R}^3$ with Lebesgue measure $\mu$ and

$$\mathcal{H} = \int_M^{\oplus} \mathcal{H}' d\mu \qquad (= L^2(M, d\mu; \mathcal{H}')).$$

The Hilbert space $\mathcal{H}'$ is given in terms of Fourier variables by

$$\mathcal{H}_{\mathfrak{P}} := L^2\left(\mathbb{R}^{3(N+1)}; \delta\left(\mathfrak{P} - \sum_{\nu=0}^{N} k_\nu\right) dk_0 dk_1 \cdots dk_N\right).$$

A measurable function

$$A :< \mathbb{R}^3, \mu > \longrightarrow \{\text{self-adjoint operators on } \mathcal{H}_{\mathfrak{P}}\}$$

is defined by $A : \mathfrak{P} \mapsto H_{\mathfrak{P}}$ (see the complete Definition on p. 283 of [12]). Here $A(\mathfrak{P}) = H_{\mathfrak{P}}$ is called a *fiber of* $A$ and

$$H_{\mathfrak{P}} = \sum_{\nu=0}^{N} \sqrt{c^2 k_\nu^2 + m_\nu^2 c^4} - m_\nu c^2 + U^{-1} V U \qquad \text{on} \quad \mathcal{H}_{\mathfrak{P}}$$

in which $U$ is the Fourier transform in $k_0, \ldots, k_N$. Then in terms of this scheme

$$H = \int_{\mathbb{R}^3}^{\oplus} H_{\mathfrak{P}} d\mathfrak{P}.$$

We refer the reader to [12] for a more complete discussion.

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