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THE ELECTRON DENSITIES OF PSEUDORELATIVISTIC EIGENFUNCTIONS ARE SMOOTH AWAY FROM THE NUCLEI

SØREN FOURNAIS AND THOMAS ØSTERGAARD SØRENSEN

ABSTRACT. We consider a pseudorelativistic model of atoms and molecules, where the kinetic energy of the electrons is given by $\sqrt{p^2 + m^2} - m$. In this model the eigenfunctions are generally not even bounded, however, we prove that the corresponding one-electron densities are smooth away from the nuclei.

1. INTRODUCTION AND RESULTS

It was proved recently [3, 4] that the one-electron densities of atomic and molecular eigenstates are smooth away from the nuclei (actually, real analyticity was proved in [5]). The model studied was the non-relativistic Schrödinger operator with fixed nuclei. The proofs in [3, 4] depend heavily on special properties of the non-relativistic kinetic energy operator $-\Delta$. However, the strategy of large parts of the proof is very robust. In the present paper we generalise the result to the case of so-called pseudorelativistic molecules.

We consider an N-electron molecule with L fixed nuclei. The pseudo-relativistic Hamiltonian is (in units where $\hbar = c = 1$) given by

$$\mathbf{H}_{N,L}(\mathbf{R}, \mathbf{Z}) = \sum_{j=1}^{N} \left\{ T(p_j) - \sum_{\ell=1}^{L} \frac{Z_\ell \alpha}{|x_j - R_\ell|} \right\} + \sum_{1 \leq i < j \leq N} \frac{\alpha}{|x_i - x_j|},$$

$$(1.1)$$

where the kinetic energy $T(p_j)$ of the j'th electron is given by the operator

$$T(p) = \sqrt{p^2 + m^2} - m = \sqrt{-\Delta + m^2} - m,$$

with $m \in [0, \infty)$ being the mass of the electron; α is the fine structure constant (in these units, $\alpha = e^2$, with e the unit charge). In (1.1), $\mathbf{R} = (R_1, R_2, \ldots, R_L) \in \mathbb{R}^{3L}$, $R_\ell \neq R_k$ for $k \neq \ell$, denote the positions of the L nuclei whose positive charges are given by $\mathbf{Z} = (Z_1, Z_2, \ldots, Z_L)$.

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The positions of the N electrons are denoted by $\mathbf{x} = (x_1, x_2, \ldots, x_N) \in \mathbb{R}^{3N}$ where x_j denotes the position of the j'th electron in $\mathbb{R}^3$; Δ_j is the Laplacian with respect to x_j. We write $\nabla = (\nabla_1, \ldots, \nabla_N)$ for the gradient operator in $\mathbb{R}^{3N}$. In (1.1) we have omitted the nucleus-nucleus interaction, $\sum_{\ell < k} \frac{Z_\ell Z_k \alpha}{|R_\ell - R_k|}$, since this is just an additive constant.

The natural space for studying the operator $\mathbf{H}_{N,L}(\mathbf{R}, \mathbf{Z})$ is, in view of the Pauli Exclusion Principle, the antisymmetric spinor space, $\wedge_{j=1}^N L^2(\mathbb{R}^3; \mathbb{C}^2)$, however, our results will not depend on spin and we do therefore not impose this antisymmetry condition. Instead we work on the space $L^2(\mathbb{R}^{3N})$.

We will assume that $0 < Z_\ell \alpha < 2/\pi$ for all $\ell \in \{1, \ldots, L\}$.[1] In this case we get from [2, Proposition 2.2] (see also [6] and [11] for the case of Hydrogen) that the negative Coulomb potentials constitute a *small form perturbation* of the (total) kinetic energy (i.e., it is relatively form bounded with relative bound less than one). The electron-electron interactions being positive, and relative form bounded too, we get that the quadratic form

$$\mathfrak{q}(u, v) := \left\langle u, \sum_{j=1}^N T(p_j)\, v \right\rangle - \left\langle u, \sum_{j=1}^N \sum_{\ell=1}^L \frac{Z_\ell \alpha}{|x_j - R_\ell|}\, v \right\rangle \qquad (1.2)$$
$$+ \left\langle u, \sum_{1 \le i < j \le N} \frac{\alpha}{|x_i - x_j|}\, v \right\rangle, \quad u, v \in H^{1/2}(\mathbb{R}^{3N}),$$

is closed and semi-bounded. Here, $\langle \cdot, \cdot \rangle$ is the scalar product in $L^2(\mathbb{R}^{3N})$. Hence, we can define the operator $\mathbf{H} \equiv \mathbf{H}_{N,L}(\mathbf{R}, \mathbf{Z})$ as the corresponding (unique) self-adjoint operator. It satisfies

$$H^1(\mathbb{R}^{3N}) \subset \mathcal{D}(\mathbf{H}) \subset H^{1/2}(\mathbb{R}^{3N}),$$

and

$$\mathfrak{q}(u, v) = \langle u, \mathbf{H}v \rangle, \quad v \in \mathcal{D}(\mathbf{H}), \quad u \in H^{1/2}(\mathbb{R}^{3N}). \qquad (1.3)$$

Here, $\mathcal{D}(\mathbf{H})$ denotes the operator domain of $\mathbf{H}$; we denote its form domain by $\mathcal{Q}(\mathbf{H})$. All this follows from (the statements and proofs of) [9, Theorem X.17] and [10, Theorem VIII.15]. See [8] for further references on $\mathbf{H}_{N,L}(\mathbf{R}, \mathbf{Z})$.

Suppose $\psi \in L^2(\mathbb{R}^{3N})$ is an eigenfunction of $\mathbf{H}$, i.e., there exists $E \in \mathbb{R}$ such that

$$\mathbf{H}\psi = E\psi.$$

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[1] The experimental value of the fine structure constant is $\alpha \approx 1/137$. For this value of α, $2/(\pi\alpha) \approx 87$

We define the *one-electron density* $\rho \in L^1(\mathbb{R}^3)$ (associated to ψ) by

$$\rho(x) = \sum_{j=1}^{N} \rho_j(x)$$

$$= \sum_{j=1}^{N} \int_{\mathbb{R}^{3N}} |\psi(x_1, \ldots, x_N)|^2 \, \delta(x - x_j) \, dx_1 \cdots dx_N \,. \qquad (1.4)$$

The main result of this paper is the following.

Theorem 1.1. *Let $\psi \in L^2(\mathbb{R}^{3N})$ be an eigenfunction of $\mathbf{H}$. Let the associated density ρ be as defined in (1.4).*
  Then

$$\rho \in C^\infty\big(\mathbb{R}^3 \setminus \{R_1, \ldots, R_L\}\big) \,. \qquad (1.5)$$

Remark 1.2.

   (i) Theorem 1.1 will follow from the more general abstract Theorem 2.2 below.
  (ii) We state Theorem 1.1 for Coulomb interactions, but it holds for more general potentials. For instance, one can use the Yukawa potential $\frac{e^{-c|x|}}{|x|}$, with $c > 0$, in one or all of the two-particle interactions. See Theorem 2.2 below for a more general statement of the result.
 (iii) Since we are only interested in regularity properties of ρ, we can study each of the (finitely many) terms in (1.4) separately. We will restrict ourselves to proving the statement in (1.5) for

$$\rho_1(x) := \int_{\mathbb{R}^{3N-3}} |\psi(x, x_2, \ldots, x_N)|^2 \, dx_2 \cdots dx_N \,, \qquad (1.6)$$

the proof for the other terms being analogous. Furthermore, to simplify the presentation, we limit ourselves to the atomic case ($L = 1, R_1 = 0, Z_1 = Z, 0 < Z\alpha < 2/\pi$).

Notation. We denote by $\mathcal{B}^\infty(U)$ the smooth functions with bounded derivatives on the open set U, i.e.,

$$\mathcal{B}^\infty(U) = \big\{ u \in C^\infty(U) \,\big|\, \partial^\alpha u \in L^\infty(U) \text{ for all } \alpha \big\} \,.$$

2. THE ABSTRACT THEOREM

Our main interest in this paper is the regularity of one-electron densities of pseudorelativistic atoms and molecules with Coulomb interactions, as stated in Theorem 1.1. However, our result holds in a more general case, which we will state here.

It is known that, in the case of relativistic atoms, the potential energy is not a small *operator* perturbation of the kinetic energy, if the values of α, N, and Z become too large. (This is also the case in other relativistic models than the one studied here.) In this case, as discussed in the introduction, the Hamiltonian is only defined as the (unique) self-adjoint operator associated to a semi-bounded closed quadratic form. On the other hand, the pseudorelativistic kinetic energy has an extra, important property: It is the generator of a positivity preserving semigroup.

Our abstract conditions below are thus based on the kinetic energy $\mathbf{T}$ below being the generator of a positivity preserving semigroup. This fact follows from the explicit formula for the integral kernel of the semigroup generated by $T(p)$; see e.g. [7, 7.11(11)].

The Hamiltonians considered will be of the form

$$\mathbf{H} = \mathbf{T} + \mathbf{V}, \tag{2.1}$$

where (with $\mathbf{p} = (p_1, \ldots, p_N) \in \mathbb{R}^{3N}$)

$$\mathbf{T} = \mathbf{T}(\mathbf{p}) = \sum_{j=1}^{N} T(p_j) = \sum_{j=1}^{N} \sqrt{-\Delta_j + m^2} - m, \tag{2.2}$$

$$\mathbf{V} = \mathbf{V}(\mathbf{x}) = \sum_{j=1}^{N} V_j(x_j) + \sum_{1 \leq j < k \leq N} W_{j,k}(x_j - x_k). \tag{2.3}$$

The following are the assumptions on the potential $\mathbf{V}$.

Assumption 2.1.   (i)   – For all $j \in \{1, \ldots, N\}$,

$$V_j \in C^{\infty}\big(\mathbb{R}^3 \setminus \{0\}\big) \cap \mathcal{B}^{\infty}\big(\mathbb{R}^3 \setminus B(0,1)\big).$$

 – For all $Q \subset \{1, \ldots, N\}$, the quadratic form on $\otimes_{j \in Q} L^2(\mathbb{R}^3)$ given by the multiplication operator $\mathbf{V}_Q := \sum_{j \in Q} V_j(x_j)$ is a small form perturbation of $\mathbf{T}_Q := \sum_{j \in Q} |p_j|$.

(ii) For all $j, k \in \{1, \ldots, N\}$ with $j \neq k$,
  – $W_{j,k} \geq 0$ pointwise and $W_{j,k}(x) = W_{k,j}(-x)$.
  – $W_{j,k} \in C^{\infty}\big(\mathbb{R}^3 \setminus \{0\}\big) \cap \mathcal{B}^{\infty}\big(\mathbb{R}^3 \setminus B(0,1)\big).$
  – Multiplication by $W_{j,k}$ defines a bounded operator from $H^1(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3)$ (by interpolation boundedness from $H^{1/2}(\mathbb{R}^3)$ to $H^{-1/2}(\mathbb{R}^3)$ therefore follows).

Under the above assumptions it is clear that $\mathbf{H} = \mathbf{T} + \mathbf{V}$ is well defined as the (unique) self-adjoint operator of the the corresponding closed and semi-bounded quadratic form (see the introduction for details).

The main abstract result of this paper is the following.

Theorem 2.2. *Let $m \geq 0$ and let $\mathbf{T}$ be the (total) pseudorelativistic kinetic energy operator*

$$\mathbf{T} = \sum_{j=1}^{N} \sqrt{-\Delta_j + m^2} - m. \qquad (2.4)$$

Let functions

$$V_j : \mathbb{R}^3 \to \mathbb{R}, \quad j \in \{1, \ldots, N\},$$
$$W_{j,k} : \mathbb{R}^3 \to \mathbb{R}, \quad j, k \in \{1, \ldots, N\}, j \neq k,$$

be given such that Assumption 2.1 is satisfied, and let

$$\mathbf{V}(\mathbf{x}) = \sum_{j=1}^{N} V_j(x_j) + \sum_{1 \leq j < k \leq N} W_{j,k}(x_j - x_k).$$

Let $\mathbf{H} = \mathbf{T} + \mathbf{V}$ be the self-adjoint operator associated to the corresponding quadratic form (closed on $H^{1/2}(\mathbb{R}^{3N})$). Let finally $\psi \in L^2(\mathbb{R}^{3N})$ be an eigenfunction of $\mathbf{H}$ and let ρ be the associated density as defined in (1.4).
   Then

$$\rho \in C^{\infty}\big(\mathbb{R}^3 \setminus \{0\}\big). \qquad (2.5)$$

Remark 2.3. As pointed out in Remark 1.2 (i), Theorem 1.1 follows from Theorem 2.2.

Proof of Theorem 2.2.
The smoothness of ρ is a direct consequence of Propostion 3.1 below. The argument is exactly the same as the one given in [4, Section 3] in the proof of [4, Theorem 1.1]. We therefore omit the details.   □

   All that remains is to (state and) prove Proposition 3.1 below.

3. The parallel differentiation

   The fact that one is allowed to differentiate the eigenfunction ψ parallel to the singularities of the (total) potential V is the key ingredient in proving the smoothness of the density ρ. This approach was carried out for the non-relativistic Schrödinger operator—that is, with $T(p_j) = -\Delta_j$ in (1.1)—in [3, Proposition 1] (see also [4]). We sketch the main ideas before giving the exact statement of the result (Proposition 3.1 below) and its proof.
   Let $u \in L^2(\mathbb{R}^d)$ and $\mathcal{V} \in L^{\infty}(\mathbb{R}^d)$, and assume that

$$\Delta u = \mathcal{V} u. \qquad (3.1)$$

Then (3.1) implies that $u \in H^2(\mathbb{R}^d)$, in particular, $\partial u \in L^2(\mathbb{R}^d)$ for any derivative ∂. Assume furthermore that, for some specific directional derivative $\partial_a = \sum_j a_j \partial_j$, $a_j \in \mathbb{R}$, we have $\partial_a \mathcal{V} \in L^\infty(\mathbb{R}^d)$. As just argued, $\partial_a u \in L^2(\mathbb{R}^d)$. Then, by differentiation of (3.1), we find that

$$\Delta(\partial_a u) = \mathcal{V}\partial_a u + (\partial_a \mathcal{V})u \,, \tag{3.2}$$

from which it follows that, in fact, $\partial_a u \in H^2(\mathbb{R}^d)$. Moreover, the above argument is easily localised: If $\partial_a \mathcal{V} \in L^\infty(U)$ for some open set $U \subset \mathbb{R}^d$, then we can conclude that $\partial_a u \in H^2(U)$.

Using this idea (and an induction argument) on the eigenvalue equation one finds that eigenfunctions of the non-relativistic molecular Hamiltonian are smooth in certain directions and on certain open sets (see Proposition 3.1 for a precision of the geometry, which is the same as in the non-relativistic case). In the molecular case the (Coulomb) potential is not a bounded function, but one easily sees that the argument carries over to the case of potentials $\mathcal{V}$ which are a small *operator* perturbation of the kinetic energy.

For the pseudorelativistic operator in (1.1) this procedure does not work immediately, since we cannot separate the kinetic and potential energies: Since the potential $\mathbf{V}$ is only a small quadratic form perturbation of the kinetic energy $\mathbf{T}$, the operator $\mathbf{H} = \mathbf{T} + \mathbf{V}$ is only given as a form sum.

The idea is then to move the term $\mathcal{V}u$ to the left hand side in (3.1) to find the following substitute for the argument above. Let the operator $\mathfrak{H}$ be self-adjoint with operator domain (contained in) $H^s(\mathbb{R}^d)$, for some $s \geq 1$. Suppose $u \in L^2(\mathbb{R}^d)$ satisfies (in the weak sense) the equation

$$\mathfrak{H}u = v \in L^2(\mathbb{R}^d) \,. \tag{3.3}$$

It follows that $u \in \mathcal{D}(\mathfrak{H}) \subset H^s(\mathbb{R}^d)$. If furthermore $v \in H^1(\mathbb{R}^d)$ one can then take a derivative in (3.3) and use arguments as above to conclude that $\partial u \in \mathcal{D}(\mathfrak{H}) \subset H^s(\mathbb{R}^d)$.

However, in our case it is not easy to identify the operator domain of $\mathbf{H}$. By the definition as a form sum, we only get that $H^1(\mathbb{R}^{3N}) \subset \mathcal{D}(\mathbf{H}) \subset H^{1/2}(\mathbb{R}^{3N})$. That is, we cannot take one derivative on something in $\mathcal{D}(\mathbf{H})$ as explained above and still be sure to obtain a function in $L^2(\mathbb{R}^{3N})$. Furthermore, the relativistic kinetic energy is not *local*, so introduction of cut-off functions in the induction argument becomes somewhat more complicated.

Nevertheless, the above idea of a proof and therefore the main technical step in [4]—Proposition 3.1 below—can still be justified. That is, the strategy of repeatedly differentiating an equation of the form (3.3) in 'good' directions remains: We partially identify the operator domain

$\mathcal{D}(\mathbf{H})$ in order to be able to take one *parallel* derivative (∂_{x_P} below) on functions therein.

Proposition 3.1. *Let P, Q be a partition of $\{1, \ldots, N\}$ satisfying*

$$P \neq \emptyset, \qquad P \cap Q = \emptyset, \qquad P \cup Q = \{1, \ldots, N\} \,.$$

Define, for P, Q as above and $\epsilon > 0$,

$$U_P(\epsilon) = \big\{ (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \,\big|\, |x_j| > \epsilon \text{ for } j \in P,$$
$$|x_j - x_k| > \epsilon \text{ for } j \in P, k \in Q \big\} \,. \quad (3.4)$$

Define also

$$x_P = \frac{1}{\sqrt{|P|}} \sum_{j \in P} x_j \quad (\in \mathbb{R}^3) \,. \tag{3.5}$$

Let furthermore $\mathbf{H}$ be as in Theorem 2.2, and let $\psi \in L^2(\mathbb{R}^{3N})$ be an eigenfunction of $\mathbf{H}$, i.e., there exists $E \in \mathbb{R}$ such that

$$\mathbf{H}\psi = E\psi \,.$$

Then

$$\partial_{x_P}^\gamma \psi \in L^2(U_P(\epsilon)) \text{ for all } \gamma \in \mathbb{N}^3 \,.$$

Proof. Since the proof is somewhat technical we split it in a number of steps in order to make the structure more transparent. We first prove a lemma on localization.

Lemma 3.2. *Let $\varphi \in \mathcal{B}^\infty(\mathbb{R}^{3N})$ and $u \in \mathcal{D}(\mathbf{H})$. Then $\varphi u \in \mathcal{D}(\mathbf{H})$ and*

$$\mathbf{H}(\varphi u) = \varphi(\mathbf{H}u) + Bu \,, \tag{3.6}$$

where $B \in \mathcal{B}(L^2(\mathbb{R}^{3N}))$ is the commutator $[\mathbf{T}, \varphi]$.

Proof. Notice first that $\varphi u \in \mathcal{Q}(\mathbf{H})$ since $u \in \mathcal{D}(\mathbf{H}) \subset \mathcal{Q}(\mathbf{H}) = H^{1/2}(\mathbb{R}^{3N})$ and multiplication by φ maps $H^s(\mathbb{R}^{3N})$ into itself for all $s \in \mathbb{R}$. Let $v \in \mathcal{D}(\mathbf{H}) \subset \mathcal{Q}(\mathbf{H})$, then also $\overline{\varphi}v \in \mathcal{Q}(H)$, and, since $u \in \mathcal{D}(\mathbf{H})$ and $\mathfrak{q}$ is symmetric (see (1.2)),

$$\mathfrak{q}(\varphi u, v) = \langle \varphi u, \mathbf{H}v \rangle \,, \quad \mathfrak{q}(u, \overline{\varphi}v) = \langle \mathbf{H}u, \overline{\varphi}v \rangle \,. \tag{3.7}$$

Now, we can calculate on a form core ($C_0^\infty(\mathbb{R}^{3N})$) to obtain

$$\mathfrak{q}(\varphi u, v) = \mathfrak{q}(u, \overline{\varphi}v) + \langle Bu, v \rangle \,, \tag{3.8}$$

where B is the operator $[\mathbf{T}, \varphi]$, which is bounded on $L^2(\mathbb{R}^{3N})$ since $\varphi \in \mathcal{B}^\infty(\mathbb{R}^{3N})$ (see Lemma A.2 below). It follows from (3.7) and (3.8) that

$$\langle \varphi u, \mathbf{H}v \rangle = \langle \varphi \mathbf{H}u + Bu, v \rangle \text{ for all } v \in \mathcal{D}(\mathbf{H}) \,. \tag{3.9}$$

Since $\varphi \mathbf{H}u + Bu \in L^2(\mathbb{R}^{3N})$ and $\mathcal{D}(\mathbf{H})$ is dense in $L^2(\mathbb{R}^{3N})$ we deduce from (3.9) that $\varphi u \in \mathcal{D}(\mathbf{H}^*) = \mathcal{D}(\mathbf{H})$ and that (3.6) holds. This proves the lemma. $\square$

An auxiliary operator. We introduce the following two operators:

$$\mathbf{H}_Q = \sum_{j \in Q} \big(T(p_j) + V_j(x_j) \big) + \sum_{j,k \in Q, j < k} W_{j,k}(x_j - x_k)\,, \qquad (3.10)$$

on $\otimes_{j \in Q} L^2(\mathbb{R}^3)$, and

$$\mathbf{H}_P = \sum_{j \in P} T(p_j) + \sum_{j,k \in P, j < k} W_{j,k}(x_j - x_k)\,, \qquad (3.11)$$

on $\otimes_{j \in P} L^2(\mathbb{R}^3)$.

By Assumption 2.1 (notice that the $W_{j,k}$ are non-negative, and that $T(p_j) - |p_j|$ is a bounded operator on $L^2(\mathbb{R}^3)$) the quadratic form defined by $\mathbf{H}_Q$ is closed and bounded from below on $H^{1/2}(\mathbb{R}^{3|Q|})$. The operator $\mathbf{H}_Q$ is then defined as the (unique) self-adjoint operator associated to this form; see [10, Theorem VIII.15].

It follows from Lemma A.1 in Appendix A that $\mathbf{H}_P$ is self-adjoint with domain $H^1(\mathbb{R}^{3|P|})$. We here used Assumption 2.1 (ii) and that $T(p)$ (and therefore, $\sum_{j \in P} T(p_j)$), as mentioned earlier in this section, is the generator of a positivity preserving semigroup.

Define furthermore

$$\widehat{\mathbf{H}} = \mathbf{H}_Q \otimes 1 + 1 \otimes \mathbf{H}_P$$

on

$$L^2(\mathbb{R}^{3N}) \simeq \big(\otimes_{j \in Q} L^2(\mathbb{R}^3) \big) \otimes \big(\otimes_{j \in P} L^2(\mathbb{R}^3) \big)\,.$$

Since $\mathbf{H}_Q$ and $\mathbf{H}_P$ are bounded below, it follows from results on tensor products [1, p. 86] that $\widehat{\mathbf{H}}$ is self-adjoint with domain

$$\mathcal{D}(\widehat{\mathbf{H}}) = \big[\mathcal{D}(\mathbf{H}_Q) \otimes L^2(\mathbb{R}^{3|P|}) \big] \cap \big[L^2(\mathbb{R}^{3|Q|}) \otimes \mathcal{D}(\mathbf{H}_P) \big]$$

$$\subseteq L^2(\mathbb{R}^{3|Q|}) \otimes \mathcal{D}(\mathbf{H}_P) = L^2(\mathbb{R}^{3|Q|}) \otimes H^1(\mathbb{R}^{3|P|})\,. \qquad (3.12)$$

Choose $\widehat{V}_j \in \mathcal{B}^\infty(\mathbb{R}^3)$ for $j \in P$ and $\widehat{W}_{j,k} \in \mathcal{B}^\infty(\mathbb{R}^3)$ for $j \in P, k \in Q$ (and $k \in P, j \in Q$) satisfying

$$\widehat{V}_j = V_j \text{ on } \mathbb{R}^3 \setminus B(0, \epsilon/2) \quad \text{and} \quad \widehat{W}_{j,k} = W_{j,k} \text{ on } \mathbb{R}^3 \setminus B(0, \epsilon/2)\,.$$

This is possible by Assumption 2.1. Define finally

$$\widetilde{\mathbf{H}} = \widehat{\mathbf{H}} + I_P\,, \qquad (3.13)$$

$$I_P(\mathbf{x}) = \sum_{j \in P} \widehat{V}_j(x_j) + \sum_{(j \in P, k \in Q) \cup (j \in Q, k \in P)} \widehat{W}_{j,k}(x_j - x_k)\,.$$

The operator $\widetilde{\mathbf{H}}$ is self-adjoint, with $\mathcal{D}(\widetilde{\mathbf{H}}) = \mathcal{D}(\widehat{\mathbf{H}})$, since $\widehat{V}_j, \widehat{W}_{j,k} \in L^\infty(\mathbb{R}^3)$. We have (in the form sense)

$$\widetilde{\mathbf{H}} = \mathbf{T} + \widetilde{\mathbf{V}} \tag{3.14}$$

with

$$\widetilde{\mathbf{V}}(\mathbf{x}) = I_P(\mathbf{x}) + \sum_{j \in Q} V_j(x_j) + \sum_{(j,k \in P, j < k) \cup (j,k \in Q, j < k)} W_{j,k}(x_j - x_k) \,. \tag{3.15}$$

Let $\widetilde{\mathfrak{q}}$ be the quadratic form associated with $\widetilde{\mathbf{H}}$. An approximation argument, using that $C_0^\infty(\mathbb{R}^{3N})$ is a form core for both $\mathfrak{q}$ and $\widetilde{\mathfrak{q}}$, gives that for $u, v \in H^{1/2}(\mathbb{R}^{3N})$ with $\operatorname{supp} u \subset U_P(\epsilon/2)$,

$$\mathfrak{q}(u, v) = \widetilde{\mathfrak{q}}(u, v) \,. \tag{3.16}$$

The parallel differentiation. Let $f_1, f_2 \in C^\infty(\mathbb{R})$ be a partition of unity on $\mathbb{R}$ satisfying that f_1 is non-increasing and $f_1(t) = 1$ for $t \le 5/4$, $f_1(t) = 0$ for $t \ge 2$, $f_1 + f_2 = 1$.

For $\epsilon > 0$ and $P \subset \{1, \dots, N\}$, $P \ne \emptyset$ define

$$\varphi_{P,\epsilon}(\mathbf{x}) := \prod_{j \in P} f_2(2|x_j|/\epsilon) \prod_{j \in P, k \in Q} f_2(2|x_j - x_k|/\epsilon) \,. \tag{3.17}$$

Then $\varphi_{P,\epsilon} \in \mathcal{B}^\infty(\mathbb{R}^{3N})$ and $\operatorname{supp} \varphi_{P,\epsilon} \subset U_P(\epsilon/2)$.

We will prove the following lemma, by induction in $k \in \mathbb{N} \cup \{0\}$. Notice that part (1) in the lemma implies that $\partial_{x_P}^\gamma \psi \in L^2(U_P(\epsilon))$. Therefore, Proposition 3.1 clearly follows once we have proved Lemma 3.3.

Lemma 3.3. *For all $k \in \mathbb{N} \cup \{0\}$ the following holds:*
For all $\epsilon > 0$, all $P \subset \{1, \dots, N\}$ with $P \ne \emptyset$, and all $\gamma \in \mathbb{N}^3$ with $|\gamma| \le k$:

    (1) $\partial_{x_P}^\gamma(\varphi_{P,\epsilon}\psi) \in \mathcal{D}(\mathbf{H}) \cap \mathcal{D}(\widetilde{\mathbf{H}})$.
    (2) *If $\gamma = \gamma_1 + \dots + \gamma_k$, with $|\gamma_j| = 1$ for all j, then*

$$\mathbf{H}(\partial_{x_P}^\gamma(\varphi_{P,\epsilon}\psi)) = E\partial_{x_P}^\gamma(\varphi_{P,\epsilon}\psi) + \partial_{x_P}^\gamma[\mathbf{T}, \varphi_{P,\epsilon}]\psi \tag{3.18}$$

$$- \sum_{j=1}^k \partial_{x_P}^{\gamma_1 + \dots + \gamma_{j-1}} \big\{ (\partial_{x_P}^{\gamma_j} I_P) \partial_{x_P}^{\gamma_{j+1} + \dots + \gamma_k}(\varphi_{P,\epsilon}\psi) \big\} \,.$$

Proof: We proceed by induction.

It follows from Lemma 3.2 that the statement is correct for $k = 0$ (in which case (3.18) reduces to (3.6), when using that $\mathbf{H}\psi = E\psi$).

Suppose that the statement is true for some $k \ge 0$. Let $\gamma \in \mathbb{N}^3$ with $|\gamma| = k$, and write $u_\gamma = \partial_{x_P}^\gamma(\varphi_{P,\epsilon}\psi)$.

Let $\mathbf{e}_P$ be any of the three unit vectors in $\mathbb{R}^{3N}$ which define the directions of x_P. More precisely, introduce the canonical basis for $\mathbb{R}^{3N}$, $\{\mathbf{e}_j^k\}$ with $j \in \{1, \ldots, N\}$, $k \in \{1, 2, 3\}$. Then the vector $\mathbf{e}_P$ is one of the three possibilities

$$\mathbf{e}_P^k := \frac{1}{\sqrt{|P|}} \sum_{j \in P} \mathbf{e}_j^k , \ k \in \{1, 2, 3\} . \tag{3.19}$$

Let $\partial_{\mathbf{e}_P} = \mathbf{e}_P \cdot \nabla$ be the directional derivative in the direction $\mathbf{e}_P$, and define the self-adjoint operator $\mathbf{e}_P \cdot \mathbf{p} = -i\mathbf{e}_P \cdot \nabla$ with domain

$$\mathcal{D}(\mathbf{e}_P \cdot \mathbf{p}) = \{f \in L^2(\mathbb{R}^{3N}) \,\big|\, \partial_{\mathbf{e}_P} f \in L^2(\mathbb{R}^{3N})\} .$$

Let furthermore, for $t \in \mathbb{R}$, $\tau_{t\mathbf{e}_P}$ be the translation operator $(\tau_{t\mathbf{e}_P} f)(\mathbf{x}) = f(\mathbf{x} + t\mathbf{e}_P)$. Clearly $t \mapsto \tau_{t\mathbf{e}_P}$ defines a strongly continuous semigroup with generator $\mathbf{e}_P \cdot \mathbf{p}$.

Notice that for t sufficiently small, $\operatorname{supp} \tau_{t\mathbf{e}_P} u_\gamma \subset U_P(\epsilon/2)$. Since $u_\gamma \in \mathcal{D}(\widetilde{\mathbf{H}}) \subset L^2(\mathbb{R}^{3|Q|}) \otimes H^1(\mathbb{R}^{3|P|})$ by the induction hypothesis, we know that

$$\partial_{\mathbf{e}_P} u_\gamma \in L^2(\mathbb{R}^{3N}) ,$$

so $u_\gamma \in \mathcal{D}(\mathbf{e}_P \cdot \mathbf{p})$ and

$$\lim_{t \to 0} \frac{1}{t} (\tau_{t\mathbf{e}_P} u_\gamma - u_\gamma) = \partial_{\mathbf{e}_P} u_\gamma , \tag{3.20}$$

in $L^2(\mathbb{R}^{3N})$.

Let $v \in \mathcal{D}(\mathbf{H})$ and consider $\langle \mathbf{H}v, \partial_{\mathbf{e}_P} u_\gamma \rangle$. Using (3.20) and (3.16), we get

$$\langle \mathbf{H}v, \partial_{\mathbf{e}_P} u_\gamma \rangle = \lim_{t \to 0} t^{-1} \langle \mathbf{H}v, \tau_{t\mathbf{e}_P} u_\gamma - u_\gamma \rangle = \lim_{t \to 0} t^{-1} \mathfrak{q}(v, \tau_{t\mathbf{e}_P} u_\gamma - u_\gamma)$$
$$= \lim_{t \to 0} t^{-1} \widetilde{\mathfrak{q}}(v, \tau_{t\mathbf{e}_P} u_\gamma - u_\gamma) . \tag{3.21}$$

Since the translation $\tau_{t\mathbf{e}_P}$ commutes with $\widehat{\mathbf{H}} = \mathbf{H}_P + \mathbf{H}_Q$ (see (3.10) and (3.11)), we get that, with I_P from (3.13),

$$\widetilde{\mathbf{H}} \tau_{t\mathbf{e}_P} = \tau_{t\mathbf{e}_P} \widetilde{\mathbf{H}} + [I_P, \tau_{t\mathbf{e}_P}] .$$

Thus, using (3.16)

$$\langle \mathbf{H}v, \partial_{\mathbf{e}_P} u_\gamma \rangle = \lim_{t \to 0} t^{-1} \widetilde{\mathfrak{q}}(v, \tau_{t\mathbf{e}_P} u_\gamma - u_\gamma)$$
$$= \lim_{t \to 0} t^{-1} \langle v, \tau_{t\mathbf{e}_P}(\widetilde{\mathbf{H}} u_\gamma) - \widetilde{\mathbf{H}} u_\gamma \rangle - \langle v, (\partial_{\mathbf{e}_P} I_P) u_\gamma \rangle . \tag{3.22}$$

To prove that $\partial_{\mathbf{e}_P} u_\gamma \in \mathcal{D}(\mathbf{H}^*) = \mathcal{D}(\mathbf{H})$ from this, it remains to show that when applying $\partial_{\mathbf{e}_P}$ to $\widetilde{\mathbf{H}} u_\gamma$ we obtain a function belonging to $L^2(\mathbb{R}^{3N})$. Then, from (3.22), also

$$\mathbf{H}(\partial_{\mathbf{e}_P} u_\gamma) = \mathbf{H}^*(\partial_{\mathbf{e}_P} u_\gamma) = \partial_{\mathbf{e}_P}(\widetilde{\mathbf{H}} u_\gamma) - (\partial_{\mathbf{e}_P} I_P) u_\gamma .$$

By (3.18), localization and (1) from the induction hypothesis, we find

$$\widetilde{\mathbf{H}}u_\gamma = \mathbf{H}u_\gamma = E\partial_{x_P}^\gamma(\varphi_{P,\epsilon}\psi) + \partial_{x_P}^\gamma[\mathbf{T}, \varphi_{P,\epsilon}]\psi \qquad (3.23)$$
$$- \sum_{j=1}^k \partial_{x_P}^{\gamma_1+\cdots+\gamma_{j-1}}\left\{(\partial_{x_P}^{\gamma_j}I_P)\partial_{x_P}^{\gamma_{j+1}+\cdots+\gamma_k}(\varphi_{P,\epsilon}\psi)\right\}.$$

We will show that when applying $\partial_{\mathbf{e}_P}$ to each term on the right side of (3.23) we obtain a function belonging to $L^2(\mathbb{R}^{3N})$.

For the first term, since $\partial_{x_P}^\gamma(\varphi_{P,\epsilon}\psi) \in \mathcal{D}(\widetilde{\mathbf{H}}) \subset L^2(\mathbb{R}^{3|Q|}) \otimes H^1(\mathbb{R}^{3|P|})$ by (3.12) and the induction hypothesis, we know that

$$\partial_{\mathbf{e}_P}\partial_{x_P}^\gamma(\varphi_{P,\epsilon}\psi) \in L^2(\mathbb{R}^{3N}). \qquad (3.24)$$

For the third term, the function I_P from (3.13) satisfies $I_P \in \mathcal{B}^\infty(\mathbb{R}^{3N})$, and, as just shown, $\partial_{x_P}^\alpha(\varphi_{P,\epsilon}\psi) \in L^2(\mathbb{R}^{3N})$ for all $|\alpha| \leq k+1$, so, by Leibniz' rule,

$$\partial_{\mathbf{e}_P}\left(\sum_{j=1}^k \partial_{x_P}^{\gamma_1+\cdots+\gamma_{j-1}}\left\{(\partial_{x_P}^{\gamma_j}I_P)\partial_{x_P}^{\gamma_{j+1}+\cdots+\gamma_k}(\varphi_{P,\epsilon}\psi)\right\}\right) \in L^2(\mathbb{R}^{3N}). \quad (3.25)$$

Finally, we consider the commutator term $\partial_{x_P}^\gamma[\mathbf{T}, \varphi_{P,\epsilon}]\psi$ in (3.23). Define $\varphi_1 = \varphi_{P,\epsilon/4}$, $\varphi_2 = 1 - \varphi_1$. Notice that, by the definition of f_1, f_2,

$$f_1(8t/\epsilon)f_2(2t/\epsilon) = 0. \qquad (3.26)$$

By using that $f_1 + f_2 = 1$ we find

$$\varphi_2 = \sum_{(\{s_j\},\{s_{j,k}\})} \prod_{j\in P} f_{s_j}(8|x_j|/\epsilon) \prod_{j\in P, k\in Q} f_{s_{j,k}}(8|x_j - x_k|/\epsilon), \qquad (3.27)$$

where the sum is over all tuples $(\{s_j\}, \{s_{j,k}\}) \in \{1,2\}^{|P|+|P|\cdot|Q|}$ with at least one entry different from 2. Write the commutator term $\partial_{x_P}^\gamma[\mathbf{T}, \varphi_{P,\epsilon}]\psi$ as

$$\partial_{x_P}^\gamma[\mathbf{T}, \varphi_{P,\epsilon}]\psi = \partial_{x_P}^\gamma[\mathbf{T}, \varphi_{P,\epsilon}](\varphi_1\psi) + \partial_{x_P}^\gamma[\mathbf{T}, \varphi_{P,\epsilon}](\varphi_2\psi), \qquad (3.28)$$

The term with φ_1 we write, using Leibniz' rule, as

$$\partial_{x_P}^\gamma[\mathbf{T}, \varphi_{P,\epsilon}](\varphi_1\psi) = \sum_{\beta\leq\gamma}\binom{\gamma}{\beta}[\mathbf{T}, \partial_{x_P}^\beta\varphi_{P,\epsilon}]\partial_{x_P}^{\gamma-\beta}(\varphi_1\psi),$$

so,

$$\partial_{\mathbf{e}_P}\partial_{x_P}^{\gamma}[\mathbf{T}, \varphi_{P,\epsilon}](\varphi_1\psi) = \sum_{\beta \leq \gamma}\binom{\gamma}{\beta}[\mathbf{T}, \partial_{\mathbf{e}_P}\partial_{x_P}^{\beta}\varphi_{P,\epsilon}]\partial_{x_P}^{\gamma-\beta}(\varphi_1\psi)$$

$$+ \sum_{\beta \leq \gamma}\binom{\gamma}{\beta}[\mathbf{T}, \partial_{x_P}^{\beta}\varphi_{P,\epsilon}]\partial_{\mathbf{e}_P}\partial_{x_P}^{\gamma-\beta}(\varphi_1\psi).$$

By Lemma A.2 and the induction hypothesis, we therefore see that

$$\partial_{\mathbf{e}_P}\partial_{x_P}^{\gamma}[\mathbf{T}, \varphi_{P,\epsilon}](\varphi_1\psi) \in L^2(\mathbb{R}^{3N}). \qquad (3.29)$$

Now we consider the term with φ_2 in (3.28). We will prove that also

$$\partial_{\mathbf{e}_P}\partial_{x_P}^{\gamma}[\mathbf{T}, \varphi_{P,\epsilon}](\varphi_2\psi) \in L^2(\mathbb{R}^{3N}). \qquad (3.30)$$

Since $\mathbf{T}$ is a finite sum and $\varphi_{P,\epsilon}\varphi_2 = 0$ it suffices, up to renumbering of the terms, to prove that

$$-\partial_{\mathbf{e}_P}\partial_{x_P}^{\gamma}\big[\sqrt{p_1^2 + m}, \varphi_{P,\epsilon}\big](\varphi_2\psi)$$

$$= \partial_{\mathbf{e}_P}\partial_{x_P}^{\gamma}\varphi_{P,\epsilon}\sqrt{p_1^2 + m}\,(\varphi_2\psi) \in L^2(\mathbb{R}^{3N}). \qquad (3.31)$$

Proof of (3.31).
Case 1. $1 \in P$.
The case $P = \{1\}$ being immediate by Lemma A.2, we will assume that $P_1 \neq \emptyset$, where $P_1 := P \setminus \{1\}$.

Since $\sqrt{p_1^2 + m}$ commutes with multiplication operators in other variables, and using the support condition (3.26), we find

$$\varphi_{P,\epsilon}\sqrt{p_1^2 + m}\,\varphi_2 = \prod_{j \in P_1}f_2(2|x_j|/\epsilon)\prod_{j \in P_1, k \in Q}f_2(2|x_j - x_k|/\epsilon)$$

$$\times \left\{ f_2(2|x_1|/\epsilon)\prod_{k \in Q}f_2(2|x_1 - x_k|/\epsilon)\sqrt{p_1^2 + m}\,f \right\},$$

with

$$f := \sum_{\sigma}f_{\sigma_1}(8|x_1|/\epsilon)\prod_{k \in Q}f_{\sigma_k}(8|x_1 - x_k|/\epsilon), \qquad (3.32)$$

where the sum is over all $\sigma \in \{1,2\}^{1+|Q|}$ with $\sigma \neq (2, \ldots, 2)$. Since at least one factor for each summand has to be f_1 we find

$$\operatorname{supp} f \subset \big\{\mathbf{x}\,\big|\, \min\big(|x_1|, \min_{k \in Q}|x_1 - x_k|\big) \leq \epsilon/4\big\}.$$

Thus, by the triangle inequality

$$\operatorname{supp}\Big(\prod_{j \in P_1}f_2(2|x_j|/\epsilon)\prod_{j \in P_1, k \in Q}f_2(2|x_j - x_k|/\epsilon)f\Big) \subset U_{P_1}(\epsilon/4).$$

Since $\varphi_{P_1,\epsilon/4} = 1$ on $U_{P_1}(\epsilon/4)$ we get the identity

$$\varphi_{P,\epsilon}\sqrt{p_1^2 + m}\,\varphi_2 = \left(\varphi_{P,\epsilon}\sqrt{p_1^2 + m}\,\varphi_2\right)\varphi_{P_1,\epsilon/4}\,. \qquad (3.33)$$

By the induction hypothesis

$$\partial_{x_P}^{\gamma'}\left(\varphi_{P_1,\epsilon/4}\psi\right) \in L^2(\mathbb{R}^{3N})\,, \qquad (3.34)$$

for all $|\gamma'| \le n$. Furthermore, since $\operatorname{supp}\varphi_{P,\epsilon} \cap \operatorname{supp}\varphi_2 = \emptyset$, Lemma A.2 yields that

$$(\partial_{x_P}^{\alpha}\varphi_{P,\epsilon})\sqrt{p_1^2 + m}\,(\partial_{x_P}^{\beta}\varphi_2)(1 + p_1^2)^M$$

is a bounded operator on $L^2(\mathbb{R}^{3N})$ for all α, β, M.

By Leibniz rule and (3.33),

$$\partial_{x_P}^{\gamma'}\left(\varphi_{P,\epsilon}\sqrt{p_1^2 + m}\,\varphi_2\right)$$
$$= \sum_{\alpha_1 + \alpha_2 + \alpha_3 = \gamma'} c_{\alpha_1,\alpha_2,\alpha_3}\left\{\partial_{x_P}^{\alpha_1}\varphi_{P,\epsilon})\sqrt{p_1^2 + m}\,(\partial_{x_P}^{\alpha_2}\varphi_2)(1 + p_1^2)^M\right\}$$
$$\times \left\{(1 + p_1^2)^{-M}\partial_{x_P}^{\alpha_3}\left(\varphi_{P_1,\epsilon/4}\psi\right)\right\}, \qquad (3.35)$$

for some constants $c_{\alpha_1,\alpha_2,\alpha_3}$.

By definition, $\partial_{x_P}^{\alpha} = \sum_{\beta \le \alpha} c_{\alpha,\beta}\partial_1^{\beta}\partial_{x_{P_1}}^{\alpha-\beta}$ for some constants $c_{\alpha,\beta}$. So using (3.34) and choosing $\partial_{x_P}^{\gamma'} = \partial_{\mathbf{e}_P}\partial_{x_P}^{\gamma}$ and $M \ge |\gamma| + 1$ in (3.35), we see that

$$\partial_{\mathbf{e}_P}\partial_{x_P}^{\gamma}\left(\varphi_{P,\epsilon}\sqrt{p_1^2 + m}\,\varphi_2\right) \in L^2(\mathbb{R}^{3N})\,.$$

This finishes the proof of (3.31) in the case $1 \in P$.

Case 2. $1 \notin P$.

This case is similar but simpler than Case 1. In this case we define $P_1 = P$. Arguing as previously we realize that the identity (3.33) remains valid. Also (3.34) follows from the induction hypothesis. Since $P = P_1$, we can in this case choose $M = 0$ in (3.35) and get the desired result. This finishes the proof of (3.31) in the case $1 \notin P$ and combining with Case 1, we get the general result. $\qquad\square$

Combining (3.24), (3.25), (3.30), and (3.29), we get that

$$\partial_{\mathbf{e}_P}(\widetilde{\mathbf{H}}u_{\gamma}) \in L^2(\mathbb{R}^{3N})\,. \qquad (3.36)$$

So we see from (3.22) that for all $v \in \mathcal{D}(\mathbf{H})$,

$$\langle \mathbf{H}v, \partial_{\mathbf{e}_P}u_{\gamma}\rangle = \langle v, \partial_{\mathbf{e}_P}(\widetilde{\mathbf{H}}u_{\gamma}) - (\partial_{\mathbf{e}_P}I_P)u_{\gamma}\rangle\,. \qquad (3.37)$$

From (3.36), (3.37), and (3.16) we conclude that

$$\partial_{\mathbf{e}_P}u_{\gamma} \in \mathcal{D}(\mathbf{H}^*) \cap \mathcal{D}(\widetilde{\mathbf{H}}^*) = \mathcal{D}(\mathbf{H}) \cap \mathcal{D}(\widetilde{\mathbf{H}})\,, \qquad (3.38)$$

and

$$\mathbf{H}(\partial_{\mathbf{e}_P} u_\gamma) = \partial_{\mathbf{e}_P}(\mathbf{H}u_\gamma) - (\partial_{\mathbf{e}_P} I_P)u_\gamma. \qquad (3.39)$$

The equations (3.38) and (3.39) combine to give the statement in Lemma 3.3 for $k + 1$.

This finishes the induction step, and by induction the statement in Lemma 3.3 therefore holds for all $k \in \mathbb{N} \cup \{0\}$. $\qquad \square$

As mentioned above, this finishes the proof of Proposition 3.1. $\qquad \square$

Appendix A. Auxiliary results from operator theory

In the proof of Lemma 3.1 we need the following consequence of the Davies-Faris Theorem ([9, Theorem X.31]).

Lemma A.1. *Suppose $T \geq 0$ is self-adjoint with domain $\mathcal{D}(T)$, and that T is the generator of a positivity preserving semigroup. Let V be a positive multiplication operator, which is bounded relative to T. Then $\mathbf{H} = T + V$ is self-adjoint on $\mathcal{D}(T)$.*

Proof. Choose $g > 0$ such that gV is relatively bounded with respect to T with bound $a < 1$. We will prove by induction that $K_n = T + ngV$ is self-adjoint on $\mathcal{D}(T)$ for all $n \in \mathbb{N}$. In order to do so, let us consider the following statement $S(n)$:

(1) $K_n = T + ngV$ is self-adjoint on $\mathcal{D}(T)$.
(2) $\|gV\varphi\| \leq a\|(K_n + 1)\varphi\|$ for all $\varphi \in \mathcal{D}(T)$.
(3) K_n is the generator of a positivity preserving semigroup.

Note first that $S(0)$ is true by assumption.

Suppose now $S(n)$ holds true for some $n \geq 0$. By $S(n)$ point (2), gV is a small operator perturbation of K_n, so $K_{n+1} = K_n + gV$ is (by the Kato-Rellich Theorem [9, Theorem X.12]) self-adjoint on $\mathcal{D}(K_n) = \mathcal{D}(T)$. Furthermore, using the Trotter product formula [9, Theorem X.51] and the induction hypothesis, it is easy to see that $e^{-tK_{n+1}}$ is positivity preserving (for $t > 0$). Then, by the Davies-Faris Theorem [9, Theorem X.31], it follows that gV satisfies the bound

$$\|gV\varphi\| \leq a\|(K_{n+1} + 1)\varphi\| \text{ for all } \varphi \in \mathcal{D}(T).$$

Therefore $S(n + 1)$ holds. This finishes the proof that $S(n)$ implies $S(n + 1)$ for any $n \geq 0$.

The proof of Lemma A.1 now follows by induction. $\qquad \square$

We also state the following lemma which is used repeatedly in Section 3. The proof is standard and is omitted.

Lemma A.2. *Let* $\chi, \phi \in \mathcal{B}^\infty(\mathbb{R}^{3N})$ *have disjoint support and let* $m \geq 0$. *Then* $[\sqrt{p_j^2 + m}, \varphi]$ *defines a bounded operator on* $H^s(\mathbb{R}^{3N})$ *for all* $s \in \mathbb{R}$ *and* $(1 + p_j^2)^M \chi[\sqrt{p_j^2 + m}, \varphi](1 + p_j^2)^M$ *is a bounded operator on* $L^2(\mathbb{R}^{3N})$ *for all* M.

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