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Analyticity of the density of electronic wavefunctions

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Abstract. We prove that the electronic densities of atomic and molecular eigenfunctions are real analytic in $\mathbf{R}^3$ away from the nuclei.

1. Introduction and statement of the results

We consider an N-electron molecule with L fixed nuclei. The non-relativistic Hamiltonian of the molecule is given by

$$\begin{aligned} H &= H_{N,L}(\mathbf{R},\mathbf{Z}) \\ &= \sum_{j=1}^{N}\left(-\Delta_j - \sum_{l=1}^{L}\frac{Z_l}{|x_j-R_l|}\right) + \sum_{1\leq i<j\leq N}\frac{1}{|x_i-x_j|} + \sum_{1\leq l<k\leq L}\frac{Z_l Z_k}{|R_l-R_k|}, \end{aligned} \tag{1.1}$$

where $\mathbf{R}=(R_1,R_2,\dots,R_L)\in\mathbf{R}^{3L}$, $R_l\neq R_k$ for $k\neq l$, denote the positions of the L nuclei whose positive charges are given by $\mathbf{Z}=(Z_1,Z_2,\dots,Z_L)$. The positions of the N electrons are denoted by $\mathbf{x}=(x_1,x_2,\dots,x_N)\in\mathbf{R}^{3N}$, where x_j denotes the position of the jth electron in $\mathbf{R}^3$. For shortness, we will sometimes write

$$H = -\Delta + V(\mathbf{x}), \tag{1.2}$$

where $\Delta=\sum_{j=1}^{N}\Delta_j$ is the $3N$-dimensional Laplacian, and V is the Coulomb potential. It is a standard fact that H with domain $W^{2,2}(\mathbf{R}^{3N})$ is selfadjoint.

We consider eigenfunctions ψ of H, i.e., solutions $\psi\in L^2(\mathbf{R}^{3N})$ to the equation

$$H\psi = E\psi, \tag{1.3}$$

with $E\in\mathbf{R}$. Since we describe electronic wave functions, and the electrons are Fermions, ψ has to transform according to certain irreducible representations of the symmetric group $\mathfrak{S}^N$. However, our results are independent of this condition and we do not impose it.

Analyzing the spectrum of H and calculating (usually by some approximation scheme) the eigenvalues E and the corresponding eigenfunction(s) ψ is the central theme of most of the investigations done by quantum chemists and physicists. For the interpretation of these investigations the eigenfunction ψ is much too complex being a function of $3N$ variables and hence the *one-electron density* $\hat{\varrho}(x)$ plays a prominent role. It is defined by

$$\hat{\varrho}(x) = \sum_{j=1}^{N} \int_{\mathbf{R}^{3N-3}} |\psi(\hat{\mathbf{x}}_j)|^2 \, d\hat{\mathbf{x}}_j, \tag{1.4}$$

where $\hat{\mathbf{x}}_j = (x_1, \dots, x_{j-1}, x, x_{j+1}, \dots, x_N)$ and $d\hat{\mathbf{x}}_j = dx_1 \dots dx_{j-1} dx_{j+1} \dots dx_N$.

The mathematical analysis of H has mainly centered around the operator theoretical point of view, see for instance [7], [9] and references therein. The fact that (1.3) is an elliptic partial differential equation has not been exploited in such depth; so many questions which are natural from a partial differential equations point of view are not really understood. In particular, regularity questions concerning ψ and $\hat{\varrho}$ are natural and interesting. Note first that V is singular in

$$\Sigma = \left\{ \mathbf{x} \in \mathbf{R}^{3N} \,\middle|\, \left(\prod_{i=1}^{N} \prod_{l=1}^{L} |x_i - R_l| \right) \left(\prod_{1 \le i < j \le N} |x_j - x_i| \right) = 0 \right\} \tag{1.5}$$

and real analytic in $\mathbf{R}^{3N} \setminus \Sigma$. Hence by standard methods of elliptic partial differential equations, see for instance [5], ψ is real analytic in $\mathbf{R}^{3N} \setminus \Sigma$. The first results concerning the regularity of ψ on all of $\mathbf{R}^{3N}$ are due to Kato [6]. He showed that ψ is Lipschitz continuous and first formulated the well-known cusp conditions, which describe the behaviour of an eigenfunction near the points where two particles are close to each other [6, Theorems II and IIb]. See also the important paper by Simon [10] in which the Coulombic many-particle potential V is identified as a special member of the so called Kato class and some results concerning the regularity of solutions of Schrödinger equations (equations of type (1.3) with general V) are given.

Regularity results concerning the Coulombic case extending Kato's result have been obtained more recently in [4] and [3]; see also the more complete references therein to other results concerning regularity.

There are now two related problems:

(i) Describe in more detail how the specific structure of the singularities in Σ turn up in the non-analyticity of ψ. Partial results can be found in the references cited above.

(ii) Analyse the regularity properties of the one-electron density, defined in (1.4), an object which has an immediate physical interpretation (see any textbook on quantum mechanics, for instance [8]) and enters all approximation schemes in a crucial way (Hartree–Fock, Thomas–Fermi, density functional theories etc.).

For the regularity questions concerning $\hat{\varrho}$ defined in (1.4) it suffices to consider the (non-symmetrized) density ϱ defined by

$$\varrho(x) = \int_{\mathbf{R}^{3N-3}} |\psi(x, x_2, \dots, x_N)|^2 \, dx_2 \dots dx_N. \tag{1.6}$$

It is not clear a priori that ϱ is real analytic away from the nuclei since in (1.6) one integrates over subsets of Σ where ψ is not analytic. In two recent papers ([1] and [2]) the present authors have shown that ϱ is smooth away from the positions of the nuclei (or in the case of an atom, away from the origin). The natural question is now whether ϱ is real analytic away from the nuclei. This will be answered affirmatively in this paper. Of course in the proof of this result new difficulties arise, in particular all the estimates have to be much more explicit.

Theorem 1.1. *Let $\psi \in L^2(\mathbf{R}^{3N})$ satisfy the equation*

$$H\psi = E\psi,$$

with $E \in \mathbf{R}$ and H given by (1.1). *Let the density ϱ be defined as in* (1.6). *Then ϱ is a real analytic function in $\mathbf{R}^3 \setminus \{R_1, \dots, R_L\}$.*

Remark 1.2. (Atoms versus molecules) In order to keep notation simple, we will only give the proof of Theorem 1.1 in the case of an atom. In this case we only have one nucleus, which we place at the origin, so the potential V is given by

$$V = -\sum_{i=1}^{N} \frac{Z}{|x_i|} + \sum_{1 \le i < j \le N} \frac{1}{|x_j - x_i|}. \tag{1.7}$$

The necessary modifications for the molecular case were indicated in the proof of the smoothness results in [1]. In the present proof of analyticity one has to make similar changes when working with molecules.

Remark 1.3. (Density matrices) We get analogous results for the one-electron density matrix $\gamma_1(x, x')$ and the two-electron density $\varrho_2(x, x')$, which we will define next. Let $(x, x') \in \mathbf{R}^6$. Let $\hat{\mathbf{x}}_j$ and $d\hat{\mathbf{x}}_j$ be as defined after (1.4), and define

$$\begin{aligned}
\hat{\mathbf{x}}'_j &= (x_1, \dots, x_{j-1}, x', x_{j+1}, \dots, x_N), \\
\hat{\mathbf{x}}_{j,k} &= (x_1, \dots, x_{j-1}, x, x_{j+1}, \dots, x_{k-1}, x', x_{k+1}, \dots, x_N), \\
d\hat{\mathbf{x}}_{j,k} &= dx_1 \dots dx_{j-1} \, dx_{j+1} \dots dx_{k-1} dx_{k+1} \dots dx_N.
\end{aligned}$$

Then γ_1 and ϱ_2 are defined by

(1.8)
$$\gamma_1(x,x') = \sum_{j=1}^{N} \int_{\mathbf{R}^{3N-3}} \psi(\hat{\mathbf{x}}_j)\overline{\psi(\hat{\mathbf{x}}'_j)}\, d\hat{\mathbf{x}}_j,$$

(1.9)
$$\varrho_2(x,x') = \sum_{\substack{j,k=1\\ j\neq k}}^{N} \int_{\mathbf{R}^{3N-6}} |\psi(\hat{\mathbf{x}}_{j,k})|^2\, d\hat{\mathbf{x}}_{j,k}.$$

In order to describe the regularity of γ_1 and ϱ_2 we introduce $D=\{(x,x)\in\mathbf{R}^6\}$ and

$$S = (\{R_1,\dots,R_L\}\times\mathbf{R}^3)\cup(\mathbf{R}^3\times\{R_1,\dots,R_L\})\subset\mathbf{R}^6.$$

Our method implies that γ_1 is real analytic on $\mathbf{R}^6\setminus S$ and that ϱ_2 is real analytic on $\mathbf{R}^6\setminus(D\cup S)$.

Remark 1.4. In the case of an atom, consider the density ϱ in polar coordinates ($x=r\omega$, $r=|x|$, $\omega=x/|x|\in\mathbf{S}^2$), and define $\tilde{\varrho}(r)=\int_{\mathbf{S}^2}\varrho(r\omega)\,d\omega$. An important question is for which $k\in\mathbf{N}$,

(1.10)
$$\left(\frac{d^k\tilde{\varrho}}{dr^k}\right)(0)$$

exists. An even more demanding question is whether $\tilde{\varrho}(r)$ is real analytic for $r\geq 0$, i.e., whether $\tilde{\varrho}$ can be continued analytically beyond 0. The analysis of such questions show the intimate relation between the problems (i) and (ii). In [3] it was shown that the derivatives in (1.10) exist for $k\leq 2$. But the general problem remains open.

Remark 1.5. (Generalisations) As will be seen from the proof, Theorem 1.1 can easily be generalised to many other potentials. We do not use any of the special properties of Coulomb potentials, such as symmetry, homogeneity, etc. To be precise, let

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

satisfy the following conditions:

(1) There exists $C>0$ such that for all $u\in W^{1,2}(\mathbf{R}^{3N})$,

$$\|Vu\|_{L^2(\mathbf{R}^{3N})}\leq C\|u\|_{W^{1,2}(\mathbf{R}^{3N})}. \tag{1.11}$$

(2) There exists a constant $L>0$ (depending on ε) such that for all $\alpha\in\mathbf{N}^3$, we have

$$\sum_{j=1}^{N}\|\partial^\alpha V_j\|+\sum_{\substack{j,k=1\\ j\neq k}}^{N}\|\partial^\alpha W_{j,k}\|\leq L^{|\alpha|+1}|\alpha|!, \tag{1.12}$$

where the norms in (1.12) are in $L^\infty(\{x\in\mathbf{R}^3\,|\,|x|>\varepsilon\})$.
The first condition, (1.11), is a kind of relative boundedness assumption. The second condition, (1.12), means that V is real analytic away from Σ (with a uniformity at infinity). Theorem 1.1 remains true for any V satisfying these two assumptions. For instance, replacing one or more of the Coulomb potentials in V by the Yukawa potential $e^{-\alpha|x|}/|x|$ (with $\alpha>0$), we still get Theorem 1.1. But here we concentrate on the physically important case of Coulomb potentials and do not strive for generality.

Organisation of the paper. In Section 3 we present in Lemma 3.1 a result concerning 'partial analyticity' of an eigenfunction ψ of H in the following sense: Upper bounds to the L^2-norms of certain directional derivatives of ψ of arbitrary order $|\alpha|$ are given. They show the right behaviour in $|\alpha|$ needed later on for the proof of the analyticity of ϱ away from the origin. (The proof of Lemma 3.1 is given in Appendix A.) We note that this kind of directional derivatives correspond, roughly speaking, to 'taking derivatives along singularities of the potential', see Lemma A.3 and its proof, and compare also with [1] and [2]. Corollary 3.2 is an immediate consequence of Lemma 3.1 and essential for the further steps in the proof of Theorem 1.1.

In Section 4 we state and prove Proposition 4.1 which gives us the necessary control on $|(\partial^\alpha\varrho)(x)|$ for $|x|\geq\varepsilon>0$ and arbitrary α. Therefrom the analyticity of ϱ follows immediately. The key point of the proof of Proposition 4.1 is Lemma 4.3. For its proof we use a suitable partition of unity of $\mathbf{R}^{3N}$ and then proceed by a similar construction as in [1] which together with Corollary 3.2 implies Lemma 4.3, in particular (4.10). Once Lemma 4.3 is proved, Proposition 4.1 follows by easy arguments.

2. Basic facts and notation

Remember that for multiindices $\alpha=(a_1,\dots,a_{3M})\in\mathbf{N}^{3M}$,

$$|\alpha|=\sum_{j=1}^{3M}a_j.$$

Furthermore, we have the usual ordering on multiindices: For $\alpha=(a_1,\dots,a_{3M})$, $\beta=(b_1,\dots,b_{3M})$ we write $\alpha\le\beta$ if and only if $a_j\le b_j$ for all j.

We will need one simple and standard combinatorical fact. We recall it here for the reader's convenience.

Proposition 2.1. *Let $\alpha\in\mathbf{N}^{3M}$ be a multiindex. Then*

$$\sum_{\substack{\beta\le\alpha\\|\beta|=b}}\binom{\alpha}{\beta}=\binom{|\alpha|}{b}.$$

Proposition 2.1 will be used as follows. Use Leibniz' rule to calculate

$$\partial^\alpha(fg)=\sum_{\beta\le\alpha}\binom{\alpha}{\beta}(\partial^\beta f)(\partial^{\alpha-\beta}g).$$

Then the number of terms where exactly b differentiations fall on f is given by $\binom{|\alpha|}{b}$.

In the following we shall work with certain directional derivatives. Let e_s for $s\in\{1,2,3\}$ denote the standard basis for $\mathbf{R}^3$. Let P be a (non-empty) subset of $\{1,\dots,N\}$. We define the coordinate x_P by

$$x_P=\frac{1}{\sqrt{|P|}}\sum_{j\in P}x_j.$$

We will now define $\partial_{x_P}^{e_s}f$ for a function $f\in C^1(\mathbf{R}^{3N})$. For the given P and s let $\mathbf{v}=(v_1,\dots,v_N)\in\mathbf{R}^{3N}$ with $v_j=0$ for $j\notin P$, and $v_j=e_s/\sqrt{|P|}$ for $j\in P$. Then we define

$$\partial_{x_P}^{e_s}f(x)=\nabla f\cdot\mathbf{v}.$$

The definition of $\partial_{x_P}^{\alpha}$ then follows by iteration for any $\alpha\in\mathbf{N}^3$ (that is, for $\alpha=(\alpha_1,\alpha_2,\alpha_3)$, $\partial_{x_P}^{\alpha}=(\partial_{x_P}^{e_1})^{\alpha_1}(\partial_{x_P}^{e_2})^{\alpha_2}(\partial_{x_P}^{e_3})^{\alpha_3}$). One can clearly reformulate this definition in terms of Fourier transforms (multiplication by $\xi_P^{e_s}$ for suitably defined ξ_P in Fourier space). In the previous paper [1] we used a coordinate transformation to describe these derivatives.

3. Partial analyticity of atomic eigenfunctions

We will need a result on partial analyticity of the eigenfunctions of H.

Lemma 3.1. *Let $\psi \in L^2(\mathbf{R}^{3N})$ be an eigenfunction of H. Let the index sets $P_1, \dots, P_M \subset \{1, \dots, N\}$ satisfy $P_s \neq \emptyset$ for all $s \in \{1, \dots, M\}$. Define for each s, $Q_s = \{1, \dots, N\} \setminus P_s$. Define also, for $\varepsilon > 0$,*

$$U_{P_s}(\varepsilon) = \{\mathbf{x} \in \mathbf{R}^{3N} \mid |x_j| > \varepsilon \text{ and } |x_j - x_k| > \varepsilon \text{ for } j \in P_s, \text{ and } k \in Q_s\}. \tag{3.1}$$

Let

$$U_{P_1, \dots, P_M}(\varepsilon) = \bigcap_{s=1}^{M} U_{P_s}(\varepsilon). \tag{3.2}$$

Then there exist C and L (depending on ε) such that for all multiindices, $\alpha = (\alpha_1, \dots, \alpha_M) \in \mathbf{N}^{3M}$, we have

$$\|\partial_{x_{P_1}}^{\alpha_1} \dots \partial_{x_{P_M}}^{\alpha_M} \psi\|_{L^2(U_{P_1, \dots, P_M}(\varepsilon))} \leq C L^{|\alpha|} (|\alpha| + 1)^{|\alpha|}.$$

The proof of Lemma 3.1 is similar to the standard proof that solutions to elliptic equations with analytic coefficients are analytic (see [5, Section 7.5, pp. 177–180]) and will be given in Appendix A.

Let us introduce the following practical notation. For a multiindex $\alpha = (\alpha_1, \dots, \alpha_M) \in \mathbf{N}^{3M}$ and given $P_1, \dots, P_M$ as in Lemma 3.1, we define $\partial_{x_\mathbf{P}}^{\alpha}$ and $U_\mathbf{P}(\varepsilon)$ by

$$\partial_{x_\mathbf{P}}^{\alpha} = \partial_{x_{P_1}}^{\alpha_1} \dots \partial_{x_{P_M}}^{\alpha_M} \quad \text{and} \quad U_\mathbf{P}(\varepsilon) = U_{P_1, \dots, P_M}(\varepsilon). \tag{3.3}$$

We will need the result of Lemma 3.1 in a slightly different form for the proof of Theorem 1.1. For later convenience, we state and prove this reformulation here.

Corollary 3.2. *Let the notation and assumptions be as in Lemma 3.1 (using (3.3)). Then there exist constants C_1 and L_1 such that*

$$\int_{U_\mathbf{P}(\varepsilon)} \left|\partial_{x_\mathbf{P}}^{\alpha} |\psi|^2(\mathbf{x})\right| d\mathbf{x} \leq C_1 L_1^{|\alpha|} (|\alpha| + 1)^{|\alpha|}.$$

Proof. By Leibniz' rule, we have

$$\partial^{\alpha}_{x_{\mathbf{P}}}|\psi|^2=\sum_{\beta\leq\alpha}\binom{\alpha}{\beta}\overline{\partial^{\beta}_{x_{\mathbf{P}}}\psi}\,\partial^{\alpha-\beta}_{x_{\mathbf{P}}}\psi. \tag{3.4}$$

Applying Cauchy–Schwarz's inequality and Lemma 3.1 to both $\overline{\partial^{\beta}_{x_{\mathbf{P}}}\psi}$ and $\partial^{\alpha-\beta}_{x_{\mathbf{P}}}\psi$ in (3.4), we find, using Proposition 2.1 for the equality below,

$$\begin{aligned}\int_{U_{\mathbf{P}}(\varepsilon)}\left|\partial^{\alpha}_{x_{\mathbf{P}}}|\psi|^2(\mathbf{x})\right|d\mathbf{x} &\leq C^2L^{|\alpha|}\sum_{\beta\leq\alpha}\binom{\alpha}{\beta}(|\beta|+1)^{|\beta|}(|\alpha|-|\beta|+1)^{|\alpha|-|\beta|}\\ &=C^2L^{|\alpha|}\sum_{b=0}^{|\alpha|}\binom{|\alpha|}{b}(b+1)^b(|\alpha|-b+1)^{|\alpha|-b}\\ &\leq C^2(2L)^{|\alpha|}(|\alpha|+1)^{|\alpha|}.\end{aligned}$$

Thus, Corollary 3.2 holds with $C_1=C^2$ and $L_1=2L$. □

4. Differentiating the density

Fix an arbitrary $\varepsilon>0$. We will always study $\varrho(x_1)$ in the region $\{x_1\,|\,|x_1|>\varepsilon\}$. We will prove the following estimate.

Proposition 4.1. *Let $\varepsilon>0$ be given. Then there exist constants $C, L>0$, such that for all $|x|>\varepsilon$ and all $\alpha\in\mathbf{N}^3$, ϱ satisfies*

$$|\partial^{\alpha}\varrho(x)|\leq CL^{|\alpha|}(|\alpha|+1)^{|\alpha|}. \tag{4.1}$$

Remark 4.2. It is clear that Proposition 4.1 implies Theorem 1.1.

Proof. Choose $\chi_1,\chi_2\in C^{\infty}(\mathbf{R}^3)$, satisfying

$$\chi_1+\chi_2=1,\quad \chi_1\equiv 1 \text{ on } B(0,\varepsilon/4N)\quad\text{and}\quad \operatorname{supp}\chi_1\subset B(0,\varepsilon/2N),$$

and let further χ_1 and χ_2 be radially symmetric functions. Using this partition of unity and letting

$$\mathcal{M}=\{(j,k)\in\{1,\dots,N\}^2\,|\,j<k\},$$

we can write

$$\varrho(x_1)=\int_{\mathbf{R}^{3N-3}}|\psi(\mathbf{x})|^2\prod_{1\le j<k\le N}(\chi_1(x_j-x_k)+\chi_2(x_j-x_k))\,dx_2\dots\,dx_N$$

$$=\sum_{I\subset\mathcal{M}}\int_{\mathbf{R}^{3N-3}}|\psi|^2(\mathbf{x})\phi_I(\mathbf{x})\,dx_2\dots\,dx_N\equiv\sum_{I\subset\mathcal{M}}\varrho_I(x_1). \tag{4.2}$$

Equation (4.2) defines ϕ_I as

$$\phi_I=\Bigg(\prod_{(j,k)\in I}\chi_1(x_j-x_k)\Bigg)\Bigg(\prod_{(j,k)\in\mathcal{M}\setminus I}\chi_2(x_j-x_k)\Bigg). \tag{4.3}$$

We will prove that $\varrho_I(x_1)$ satisfies an estimate like (4.1) on $\{x_1\,|\,|x_1|>\varepsilon\}$ for all $I\subset\mathcal{M}$, namely

$$|\partial^\alpha\varrho_I|\le CL^{|\alpha|}(|\alpha|+1)^{|\alpha|}. \tag{4.4}$$

The estimate (4.1) follows from (4.4) (with a different C) since the sum in (4.2) is finite.

The estimate (4.4) is a consequence of (4.10) (with $\phi=\phi_I$) in Lemma 4.3 below, using a Sobolev imbedding theorem. Since we have not found an ideal reference we include the following easy argument:

Let $v\in C^\infty(\mathbf{R}^3)$ with $v(x)=1$ for $|x|\ge\varepsilon$ and $v(x)=0$ for $|x|\le\frac{1}{2}\varepsilon$. Let furthermore $\mathcal{F}$ denote the Fourier transform. We get for $\alpha\in\mathbf{N}^3$ and $|x|\ge\varepsilon$,

$$\partial^\alpha\varrho(x)=(v\partial^\alpha\varrho)(x)=c\int_{\mathbf{R}^3}\frac{e^{ix\cdot p}}{(1+|p|^2)^2}\mathcal{F}((1-\Delta)^2(v\partial^\alpha\varrho))\,dp.$$

Therefore,

$$|\partial^\alpha\varrho(x)|\le c\left\|\frac{1}{(1+|p|^2)^2}\right\|_{L^1(\mathbf{R}^3)}\|(1-\Delta)^2(v\partial^\alpha\varrho)\|_{L^1(\mathbf{R}^3)}. \tag{4.5}$$

We can estimate $\|(1-\Delta)^2(v\partial^\alpha\varrho)\|_{L^1(\mathbf{R}^3)}$ using (4.10) by,

$$\|(1-\Delta)^2(v\partial^\alpha\varrho)\|_{L^1(\mathbf{R}^3)}\le c_1L_1^{|\alpha|+4}(|\alpha|+4+1)^{|\alpha|+4}\le c_2L_2^{|\alpha|}(|\alpha|+1)^{|\alpha|}, \tag{4.6}$$

for some constants c_1, L_1, c_2 and L_2. Combining (4.5) and (4.6) yields (4.4). Proving Lemma 4.3 therefore finishes the proof of Proposition 4.1. $\square$

Lemma 4.3. *Let $\varepsilon>0$ be given and let*

$$\phi=\prod_{1\le j<k\le N} f_{j,k}(x_j-x_k), \tag{4.7}$$

where each $f_{j,k}$ is one of the functions χ_1, χ_2 and $\partial^{e_s}\chi_2$, with $e_s\in\mathbf{N}^3$, $|e_s|=1$.

(i) *Let $P_1,\dots,P_M$ be subsets of $\{1,\dots,N\}$ satisfying that $1\in P_j$ for $j=1,\dots,M$ and*

$$(\operatorname{supp}\phi)\cap\{\mathbf{x}\mid |x_1|>\varepsilon\}\subset\bigcap_{j=1}^{M} U_{P_j}\Big(\frac{\varepsilon}{4N}\Big). \tag{4.8}$$

Then there exist constants $C,L>0$ (depending on ε) such that for all multiindices $\alpha=(\alpha_0,\alpha_1,\dots,\alpha_M)\in\mathbf{N}^{3M+3}$, we have

$$\begin{aligned}\bigg\|\partial_{x_1}^{\alpha_0}\int_{\mathbf{R}^{3N-3}}(\partial_{x_{P_1}}^{\alpha_1}\dots\partial_{x_{P_M}}^{\alpha_M}|\psi|^2)(\mathbf{x})\phi(\mathbf{x})\,dx_2\dots dx_N\bigg\|_{L^1(\{x_1\,|\,|x_1|>\varepsilon\})}&\\ \le CL^{|\alpha|}(|\alpha|+1)^{|\alpha|}.&\end{aligned} \tag{4.9}$$

(ii) *There exist constants $C,L>0$ (depending on ε) such that for all $\alpha\in\mathbf{N}^3$ we have*

$$\bigg\|\partial_{x_1}^{\alpha}\int_{\mathbf{R}^{3N-3}}|\psi|^2(\mathbf{x})\phi(\mathbf{x})\,dx_2\dots dx_N\bigg\|_{L^1(\{x_1\,|\,|x_1|>\varepsilon\})}\le CL^{|\alpha|}(|\alpha|+1)^{|\alpha|}. \tag{4.10}$$

Proof. To a function ϕ as given in (4.7) we will associate $P=P(\phi)\subset\{1,\dots,N\}$ satisfying $1\in P$ and such that

$$(\operatorname{supp}\phi)\cap\{\mathbf{x}\mid |x_1|>\varepsilon\}\subset U_{P(\phi)}\Big(\frac{\varepsilon}{4N}\Big). \tag{4.11}$$

We will now describe the map $\phi\mapsto P(\phi)$. We note that the following construction is similar to the one from [1]. Define $I=I(\phi)\subset\mathcal{M}$ by

$$(j,k)\in I(\phi)\quad\text{if and only if}\quad f_{j,k}\in\{\chi_1,\partial^{e_1}\chi_2,\partial^{e_2}\chi_2,\partial^{e_3}\chi_2\}.$$

In other words, $(j,k)\in I(\phi)$ means precisely that $f_{j,k}\neq\chi_2$. The set $I(\phi)$ generates an equivalence relation on $\{1,\dots,N\}$ and we define $P(\phi)$ to be the equivalence class of 1. Less abstractly, this means that

(1) $1 \in P(\phi)$;

(2) for $j \geq 2$ we have $j \in P(\phi)$ if and only if there exists $\{j_1, \dots, j_s\} \subseteq \{1, \dots, N\}$, $s \leq N$, satisfying

(a) $(1, j_1) \in I(\phi)$;

(b) $(j_t, j_{t+1}) \in I(\phi)$ or $(j_{t+1}, j_t) \in I(\phi)$ for $1 \leq t < s$;

(c) $(j_s, j) \in I(\phi)$ or $(j, j_s) \in I(\phi)$.

Notice that, since $\chi_1 + \chi_2 = 1$, $\operatorname{supp} \partial^{e_j} \chi_2 \subset \operatorname{supp} \chi_1$, $j = 1, 2, 3$. Therefore we get (4.11) by the same elementary geometrical considerations (the triangle inequality) as in [1].

In the proof we shall use $P = P(\phi)$ in order to replace the derivative $\partial_{x_1}^{\alpha_0}$ outside the integral in the left-hand side of (4.9) by the derivative $\partial_{x_P}^{\alpha_0}$ inside the integral. That will enable us to apply Corollary 3.2.

Let $P = P(\phi)$ according to our construction. We will prove the lemma recursively in $|P|$. In the proof below we will freely interchange the order of differentiation (in the distributional sense) and integration. This is permitted, due to Corollary 3.2, which ensures that the derivatives of the functions in question belong to $L^1(\{x_1 \,|\, |x_1| > \varepsilon\} \times \mathbf{R}^{3N-3})$. We will only prove part (i) of Lemma 4.3. The changes necessary for the case (ii) are obvious and therefore omitted.

Step 1. *The case* $|P| = N$. In the case when $P = \{1, \dots, N\}$ we make the change of variables $y_j = x_j - x_1$ for $j = 2, \dots, N$. Then we get $x_j - x_k = y_j - y_k$ for $j, k \neq 1$. The point is that ϕ only depends on the differences $x_j - x_k$, and therefore, after the change of variables, the only dependence on x_1 will be in $|\psi|^2$, where we can apply Corollary 3.2. Let us carry this out.

Denote $\mathbf{y} = (y_2, \dots, y_N)$. Then we see that after the change of variables we have

$$\phi(\mathbf{x}) = \tilde{\phi}(\mathbf{y})$$

for some function $\tilde{\phi}$. Explicitly, we see from (4.7) that

$$\tilde{\phi}(y_2, \dots, y_N) = \prod_{1 < j < k \leq N} f_{j,k}(y_j - y_k) \prod_{s=2}^{N} f_{1,s}(-y_s).$$

Therefore,

$$\begin{aligned} &\int_{\mathbf{R}^{3N-3}} (\partial_{x_{P_1}}^{\alpha_1} \cdots \partial_{x_{P_M}}^{\alpha_M} |\psi|^2)(\mathbf{x}) \phi(\mathbf{x}) \, dx_2 \dots dx_N \\ &\qquad = \int_{\mathbf{R}^{3N-3}} (\partial_{x_{P_1}}^{\alpha_1} \cdots \partial_{x_{P_M}}^{\alpha_M} |\psi|^2)(x_1, x_1 + y_2, \dots, x_1 + y_N) \tilde{\phi}(\mathbf{y}) \, d\mathbf{y}. \end{aligned} \tag{4.12}$$

From (4.12) we get by differentiation under the integral sign and change of coordinates back to $\mathbf{x}$:

$$
\begin{aligned}
&\partial_{x_1}^{\alpha_0} \int_{\mathbf{R}^{3N-3}} (\partial_{x_{P_1}}^{\alpha_1} \dots \partial_{x_{P_M}}^{\alpha_M} |\psi|^2)(\mathbf{x})\phi(\mathbf{x})\, dx_2 \dots dx_N \\
(4.13) \qquad &= \int_{\mathbf{R}^{3N-3}} (\partial_{x_P}^{\alpha_0} \partial_{x_{P_1}}^{\alpha_1} \dots \partial_{x_{P_M}}^{\alpha_M} |\psi|^2)(x_1, x_1+y_2, \dots, x_1+y_N)\tilde{\phi}(\mathbf{y})\, d\mathbf{y} \\
&= \int_{\mathbf{R}^{3N-3}} (\partial_{x_P}^{\alpha_0} \partial_{x_{P_1}}^{\alpha_1} \dots \partial_{x_{P_M}}^{\alpha_M} |\psi|^2)(\mathbf{x})\phi(\mathbf{x})\, dx_2 \dots dx_N.
\end{aligned}
$$

Notice the support conditions (4.11) and (4.8). We can now apply Corollary 3.2 to get (4.9) in the case $|P|=N$.

Step 2. The case $|P|<N$. Suppose that Lemma 4.3 holds under the additional assumption $|P|>K$ for some $0\le K<N$. We will prove the statement for $|P|=K$.

Define $Q=\{1,\dots,N\}\setminus P$. Since $|P|<N$, $Q\neq\emptyset$. Note that if $j\in P$ and $k\in Q$ then, by the definition of $I(\phi)$ and $P=P(\phi)$, we have $(j,k)\notin I(\phi)$ and $(k,j)\notin I(\phi)$. Therefore, if $j<k$ we have $f_{j,k}=\chi_2$ and if $k<j$ we have $f_{k,j}=\chi_2$. So ϕ contains the factor (remember that χ_2 is rotationally symmetric, and in particular even)

$$\phi_{P,Q}=\prod_{\substack{j\in P\\ k\in Q}} \chi_2(x_j-x_k),$$

and can be written as

$$\phi=\phi_P\phi_Q\phi_{P,Q},$$

where

$$\phi_P=\prod_{\substack{j,k\in P\\ j<k}} f_{j,k}(x_j-x_k) \quad \text{and} \quad \phi_Q=\prod_{\substack{j,k\in Q\\ j<k}} f_{j,k}(x_j-x_k).$$

We do the following change of variables for $j\ge2$:

$$y_j=\begin{cases} x_j-x_1 & \text{for } j\in P\setminus\{1\},\\ x_j & \text{for } j\in Q.\end{cases}$$

For convenience of notation we define $y_1=0$. We clearly get for $j,k\in P$ or $j,k\in Q$, that $x_j-x_k=y_j-y_k$ (also when either $j=1$ or $k=1$—remember that $1\in P$). Thus, as in the case $|P|=N$, we can write $\phi_P(\mathbf{x})=\tilde{\phi}_P(\mathbf{y})$ and $\phi_Q(\mathbf{x})=\tilde{\phi}_Q(\mathbf{y})$.

Write $\mathbf{z}=(z_1,z_2,\dots,z_N)\in\mathbf{R}^{3N}$ with

$$z_j=\begin{cases} x_1, & j=1,\\ x_1+y_j, & j\in P\setminus\{1\},\\ x_j, & j\in Q.\end{cases}$$

Then

$$\begin{aligned}(4.14)\qquad &\int_{\mathbf{R}^{3N-3}} (\partial^{\alpha_1}_{x_{P_1}} \dots \partial^{\alpha_M}_{x_{P_M}} |\psi|^2)(\mathbf{x})\phi(\mathbf{x})\,dx_2 \dots dx_N \\ &= \int_{\mathbf{R}^{3N-3}} (\partial^{\alpha_1}_{x_{P_1}} \dots \partial^{\alpha_M}_{x_{P_M}} |\psi|^2)(\mathbf{z})\tilde{\phi}_P(\mathbf{y}) \Bigg(\prod_{\substack{j\in P\\ k\in Q}} \chi_2(x_1+y_j-y_k) \Bigg) \tilde{\phi}_Q(\mathbf{y})\,d\mathbf{y}.\end{aligned}$$

Differentiation under the integral sign yields

$$\begin{aligned}&\nabla_{x_1} \int_{\mathbf{R}^{3N-3}} (\partial^{\alpha_1}_{x_{P_1}} \dots \partial^{\alpha_M}_{x_{P_M}} |\psi|^2)(\mathbf{x})\phi(\mathbf{x})\,dx_2 \dots dx_N \\ &= \int_{\mathbf{R}^{3N-3}} (\nabla_{x_P}\partial^{\alpha_1}_{x_{P_1}} \dots \partial^{\alpha_M}_{x_{P_M}} |\psi|^2)(\mathbf{z})\tilde{\phi}_P(\mathbf{y}) \Bigg(\prod_{\substack{j\in P\\ k\in Q}} \chi_2(x_1+y_j-y_k) \Bigg) \tilde{\phi}_Q(\mathbf{y})\,d\mathbf{y} \\ (4.15)\qquad &+ \sum_{\substack{j\in P\\ k\in Q}} \int_{\mathbf{R}^{3N-3}} (\partial^{\alpha_1}_{x_{P_1}} \dots \partial^{\alpha_M}_{x_{P_M}} |\psi|^2)(\mathbf{z})\tilde{\phi}_P(\mathbf{y})\tilde{\phi}_Q(\mathbf{y}) \\ &\times \Bigg(\prod_{\substack{j'\in P\\ k'\in Q\\ (j',k')\neq(j,k)}} \chi_2(x_1+y_{j'}-y_{k'}) \Bigg) (\nabla\chi_2)(x_1+y_j-y_k)\,d\mathbf{y}.\end{aligned}$$

Let us explain roughly how we will proceed for higher derivatives with respect to x_1. For each consecutive differentiation we will get terms as in (4.15). The term where all differentiations fall on ψ can be differentiated again in a manner similar to (4.15). If one differentiation falls on χ_2 we stop differentiating that term under the integral sign—leaving the rest of the differentiations outside the integral. The result of this procedure is (4.16), the notation of which we will define below. The important point is that when all derivatives fall on ψ, we can apply Corollary 3.2 to obtain our conclusion. On the other hand a differentiation of χ_2 will lead to a situation with a larger $|P|$—so these terms can be handled by the induction hypothesis.

Let $\eta_s \in \mathbf{N}^3$, $|\eta_s|=1$, $s=1,2,\dots,S$. Define for $t\in\{1,\dots,S\}$

$$A_0=0, \quad A_t=\sum_{s=1}^{t}\eta_s, \quad B_t=\sum_{s=t+1}^{S}\eta_s \quad \text{and} \quad B_S=0.$$

Notice that the definition of B_t depends on S, i.e., $B_t=B_t(S)$. We get the following formula (4.16) from (4.15), using the procedure described above, by induction with respect to S:

$$
\begin{aligned}
&\partial_{x_1}^{A_S}\left(\int_{\mathbf{R}^{3N-3}}(\partial_{x_{P_1}}^{\alpha_1}\dots\partial_{x_{P_M}}^{\alpha_M}|\psi|^2)(\mathbf{x})\phi(\mathbf{x})\,dx_2\dots dx_N\right)\\
&\quad=\int_{\mathbf{R}^{3N-3}}(\partial_{x_P}^{A_S}\partial_{x_{P_1}}^{\alpha_1}\dots\partial_{x_{P_M}}^{\alpha_M}|\psi|^2)(\mathbf{x})\phi(\mathbf{x})\,dx_2\dots dx_N\\
&\quad+\sum_{t=1}^{S}\partial_{x_1}^{B_t}\left(\sum_{\substack{j\in P\\k\in Q}}\int_{\mathbf{R}^{3N-3}}(\partial_{x_P}^{A_{t-1}}\partial_{x_{P_1}}^{\alpha_1}\dots\partial_{x_{P_M}}^{\alpha_M}|\psi|^2)(\mathbf{z})\tilde{\phi}_P(\mathbf{y})\tilde{\phi}_Q(\mathbf{y})\right.\\
&\quad\times\left.\left(\prod_{\substack{j'\in P\\k'\in Q\\(j',k')\neq(j,k)}}\chi_2(x_1+y_{j'}-y_{k'})\right)(\partial^{\eta_t}\chi_2)(x_1+y_j-y_k)\,dy_2\dots dy_N\right).
\end{aligned}
\tag{4.16}
$$

For $S=1$ the equation (4.16) reduces to (4.15). We will use (4.16) with $S=|\alpha_0|$ and $A_S=\alpha_0$. Consider the function

$$
\phi_{j,k}=\phi_P\phi_Q(\partial^{\eta_t}\chi_2)(x_j-x_k)\prod_{\substack{j'\in P\\k'\in Q\\(j',k')\neq(j,k)}}\chi_2(x_{j'}-x_{k'}).
$$

By construction we have $|P(\phi_{j,k})|>|P(\phi)|$. Therefore, we get by the induction hypothesis on $|P|$ that

$$
\left\|\partial_{x_1}^{B_t}\int_{\mathbf{R}^{3N-3}}(\partial_{x_P}^{A_{t-1}}\partial_{x_{P_1}}^{\alpha_1}\dots\partial_{x_{P_M}}^{\alpha_M}|\psi|^2)(\mathbf{x})\phi_{j,k}(\mathbf{x})\,dx_2\dots dx_N\right\|_{L^1(\{x_1||x_1|>\varepsilon\})}\leq CL^p(p+1)^p,
$$

where $p=|B_t|+|A_{t-1}|+|\alpha_1|+\dots+|\alpha_M|=|\alpha|-1$. Furthermore, using Corollary 3.2 on the first term in the right-hand side of (4.16), we obtain

$$
\left\|\int_{\mathbf{R}^{3N-3}}(\partial_{x_P}^{A_S}\partial_{x_{P_1}}^{\alpha_1}\dots\partial_{x_{P_M}}^{\alpha_M}|\psi|^2)(\mathbf{x})\phi(\mathbf{x})\,dx_2\dots dx_N\right\|_{L^1(\{x_1||x_1|>\varepsilon\})}\leq CL^p(p+1)^p,
$$

with $p=|A_S|+|\alpha_1|+\dots+|\alpha_M|=|\alpha|$.

Thus the desired estimate holds for the individual terms on the right-hand side in (4.16). Since the number of terms is bounded by $c|\alpha|$ this finishes the proof of (4.9). $\square$

Appendix A. Proof of Lemma 3.1

In this appendix we will prove Lemma 3.1. For convenience define $H_E = H - E$, with E being the eigenvalue corresponding to the eigenfunction ψ, i.e. ψ satisfies $H_E\psi = 0$. Recall the notation given in (3.3).

Let us start the proof by stating a well-known result explicitly. Since the domain of H_E is known to be $W^{2,2}(\mathbf{R}^{3N})$, we get the following result.

Lemma A.1. *Let $v \in W^{1,2}(\mathbf{R}^{3N})$. Then $v \in W^{2,2}(\mathbf{R}^{3N})$ if and only if $H_E v \in L^2(\mathbf{R}^{3N})$. Furthermore, there exists a constant $K_0 > 0$ such that for all $v \in W^{2,2}(\mathbf{R}^{3N})$,*

$$\|v\|_{W^{2,2}(\mathbf{R}^{3N})} \le K_0\big(\|H_E v\|_{L^2(\mathbf{R}^{3N})} + \|v\|_{L^2(\mathbf{R}^{3N})}\big).$$

This follows from the fact that V is infinitesimally small (in the operator sense) with respect to $-\Delta$.

We now state and prove the estimate.

Lemma A.2. *Let $P_1, \ldots, P_M$ be defined as in Lemma 3.1 and $U_{\mathbf{P}}$ as in (3.3). Then there exists a constant C_0 such that for all $\eta, \eta_1 \in (0,1)$, all $\alpha_0 \in \mathbf{N}^{3N}$, $\alpha' \in \mathbf{N}^{3M}$ with $|\alpha_0| + |\alpha'| \le 2$ and all $v \in W^{2,2}\big(U_{\mathbf{P}}\big(\tfrac{1}{2}\varepsilon + \eta_1\big)\big)$ we have the estimate*

$$\eta^{|\alpha_0|+|\alpha'|}\|\partial^{\alpha_0}\partial^{\alpha'}_{x_{\mathbf{P}}} v\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+\eta+\eta_1))} \le C_0\Bigg(\eta^2\|H_E v\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+\eta_1))} + \sum_{\substack{\beta\in\mathbf{N}^{3N}\\ |\beta|<2}} \eta^{|\beta|}\|\partial^\beta v\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+\eta_1))}\Bigg). \tag{A.1}$$

Furthermore, if the right-hand side of (A.1) *is finite for all $\eta, \eta_1 > 0$ then*

$$v \in W^{2,2}\Big(U_{\mathbf{P}}\Big(\frac{1}{2}\varepsilon + \eta_1\Big)\Big) \quad \textit{for all } \eta_1 > 0.$$

Proof. Since

$$U_{\mathbf{P}}\Big(\frac{1}{2}\varepsilon + \eta + \eta_1\Big) \subset U_{\mathbf{P}}\Big(\frac{1}{2}\varepsilon + \eta_1\Big),$$

the estimate is obviously true for $|\alpha_0| + |\alpha'| < 2$. Let $\alpha_0 \in \mathbf{N}^{3N}$ and $\alpha' \in \mathbf{N}^{3M}$ with $|\alpha_0| + |\alpha'| = 2$. Choose $\phi \in C^\infty(\mathbf{R}^{3N})$, $0 \le \phi \le 1$, with $\phi \equiv 1$ on $U_{\mathbf{P}}\big(\tfrac{1}{2}\varepsilon + \eta + \eta_1\big)$ and $\operatorname{supp}\phi \subset U_{\mathbf{P}}\big(\tfrac{1}{2}\varepsilon + \eta_1\big)$, satisfying $\|\partial^\gamma\phi\|_\infty \le C_\gamma \eta^{-|\gamma|}$, with C_γ independent of η and η_1.

We can now estimate, using Lemma A.1 in the third inequality below

$$\begin{aligned}
\|\partial^{\alpha_0}\partial^{\alpha'}_{x_{\mathbf{P}}} v\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+\eta+\eta_1))} &\le \|\partial^{\alpha_0}\partial^{\alpha'}_{x_{\mathbf{P}}}(\phi v)\|_{L^2(\mathbf{R}^{3N})} \\
&\le c\|\phi v\|_{W^{2,2}(\mathbf{R}^{3N})} \\
&\le C(\|H_E(\phi v)\|_{L^2(\mathbf{R}^{3N})} + \|\phi v\|_{L^2(\mathbf{R}^{3N})}) \\
&\le C(\|\phi H_E v\|_{L^2(\mathbf{R}^{3N})} + \|(\Delta\phi)v\|_{L^2(\mathbf{R}^{3N})} \\
&\quad + 2\|(\nabla\phi)\nabla v\|_{L^2(\mathbf{R}^{3N})} + \|\phi v\|_{L^2(\mathbf{R}^{3N})}) \\
&\le C\Bigg(\|H_E v\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+\eta_1))} + \frac{c_1}{\eta}\|\nabla v\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+\eta_1))} \\
&\quad + \frac{c_2}{\eta^2}\|v\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+\eta_1))}\Bigg)
\end{aligned}$$

for some constants c, C, c_1 and c_2. Inequality (A.1) follows by multiplying with η^2.

The last statement of the lemma follows easily from Lemma A.1. □

Finally, we state and prove the properties of V that we need in the proof of Lemma 3.1.

Lemma A.3. *Let V be the Coulomb potential defined in* (1.7).

(1) *There exists $C_V > 0$ such that for all $v \in W^{1,2}(\mathbf{R}^{3N})$ we have*

$$\|(V-E)v\|_{L^2(\mathbf{R}^{3N})} \le C_V\|v\|_{W^{1,2}(\mathbf{R}^{3N})}. \tag{A.2}$$

(2) *There exists a constant $L_V > 0$ (depending on ε) such that for all $\alpha \in \mathbf{N}^{3M}$ with $|\alpha| \ge 1$, we have*

$$\|\partial^{\alpha}_{x_{\mathbf{P}}} V\|_{L^\infty(U_{\mathbf{P}}(\varepsilon/2))} \le L_V^{|\alpha|+1}|\alpha|!. \tag{A.3}$$

Remark A.4. These are the only properties of V that we need (together with Lemmas A.1 and A.2). They are easily seen to hold (see the arguments in the proof below) for potentials satisfying the general conditions in Remark 1.5.

Proof. The first property (A.2) is a consequence of Hardy's inequality (see for instance [9, Vol. II, p. 169]). To prove the second property (A.3) let P_s be one of the index sets defined in Lemma 3.1. Notice that

$$\partial^{\alpha}_{x_{P_s}} \frac{1}{|x_j|} = \begin{cases} 0 & \text{for } j \notin P_s, \\ |P_s|^{-|\alpha|/2}\, \partial^{\alpha}_{x}|x|^{-1}\,\big|_{x=x_j} & \text{for } j \in P_s. \end{cases}$$

and

$$\partial^{\alpha}_{x_{P_s}} \frac{1}{|x_j - x_k|} = \begin{cases} 0 & \text{for } j,k \notin P_s \text{ or } j,k \in P_s, \\ |P_s|^{-|\alpha|/2}\partial^{\alpha}_{x}|x|^{-1}\,\big|_{x=x_j-x_k} & \text{for } j \in P_s,\ k \notin P_s. \end{cases}$$

Therefore, (A.3) follows from the structure of V, the real analyticity of $x\mapsto|x|^{-1}$ away from 0 and the definitions of $U_{\mathbf{P}}\left(\frac{1}{2}\varepsilon\right)$ and $\partial^{\alpha}_{x_{\mathbf{P}}}$. $\square$

Proof of Lemma 3.1. Notice that (A.3) trivially implies that for $j,\eta>0$, $j\eta<1$ and $|\alpha|\geq 1$ we have

$$\eta^{|\alpha|}\|\partial^{\alpha}_{x_{\mathbf{P}}}V\|_{L^{\infty}(U_{\mathbf{P}}(\varepsilon/2+j\eta))}\leq L_V^{|\alpha|+1}|\alpha|!j^{-|\alpha|}. \tag{A.4}$$

We will prove that there exists $L_{\psi}>0$, such that for all $\eta\in(0,1)$ and all $j\in\mathbf{N}$ with $j\eta<1$ we have, for all $\alpha\in\mathbf{N}^{3M}$, $\alpha_0\in\mathbf{N}^{3N}$, $|\alpha_0|\leq 2$ and $|\alpha|+|\alpha_0|<2+j$,

$$\eta^{|\alpha|+|\alpha_0|}\|\partial^{\alpha_0}\partial^{\alpha}_{x_{\mathbf{P}}}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+j\eta))}\leq L_{\psi}^{|\alpha|+|\alpha_0|+1}. \tag{A.5}$$

Before proving (A.5), let us note that Lemma 3.1 follows easily from it. In fact, let $\alpha\in\mathbf{N}^{3M}$, $|\alpha|\geq 1$, and choose $|\alpha_0|=0$, $\eta=\varepsilon/(2|\alpha|)$ and $j=|\alpha|$. Then (A.5) becomes

$$\|\partial^{\alpha}_{x_{\mathbf{P}}}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon))}\leq L_{\psi}^{|\alpha|+1}\left(\frac{2}{\varepsilon}\right)^{|\alpha|}|\alpha|^{|\alpha|},$$

which is the statement of Lemma 3.1.

We now prove (A.5) by induction in j. For $j=0,1$, there is nothing to prove since we know that $\psi\in W^{2,2}(\mathbf{R}^{3N})$. Let L_{ψ} be sufficiently large for (A.5) to be true for $j=0,1$ and satisfying furthermore,

$$L_{\psi}\geq\max\left\{2L_V,C_0\left(1+\sum_{|\beta|<2}1\right)\right\}. \tag{A.6}$$

Here the sum is over all $\beta\in\mathbf{N}^{3N}$ with $|\beta|<2$, C_0 is the constant from Lemma A.2, and L_V is the constant from (A.3).

Suppose that we have proved (A.5) for all $j\leq j_0$ and all $\eta\in(0,1)$ with $j\eta<1$. We will prove that (A.5) holds for $j=j_0+1$ and all $\eta\in(0,1)$ with $(j_0+1)\eta<1$.

Let $|\alpha|+|\alpha_0|<2+j_0$. Then clearly $U_{\mathbf{P}}\left(\frac{1}{2}\varepsilon+(j_0+1)\eta\right)\subset U_{\mathbf{P}}\left(\frac{1}{2}\varepsilon+j_0\eta\right)$. Therefore,

$$\eta^{|\alpha|+|\alpha_0|}\|\partial^{\alpha_0}\partial^{\alpha}_{x_{\mathbf{P}}}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+(j_0+1)\eta))}\leq\eta^{|\alpha|+|\alpha_0|}\|\partial^{\alpha_0}\partial^{\alpha}_{x_{\mathbf{P}}}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+j_0\eta))},$$

and the result holds by the induction hypothesis. So we only have to consider the case $|\alpha|+|\alpha_0|=2+j_0$. Choose a decomposition $\alpha=\alpha'+\alpha''$, with $|\alpha'|=2-|\alpha_0|$, i.e., with $|\alpha''|=j_0$. Using Lemma A.2 with $\eta_1=j_0\eta$ and $v=\partial^{\alpha''}_{x_{\mathbf{P}}}\psi$ we find

$$\begin{aligned}\eta^{2+j_0}\|\partial^{\alpha_0}\partial^{\alpha}_{x_{\mathbf{P}}}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+(j_0+1)\eta))}\leq C_0\Bigg(&\eta^{2+j_0}\|H_E\partial^{\alpha''}_{x_{\mathbf{P}}}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+j_0\eta))}\\ &+\sum_{|\beta|<2}\eta^{|\beta|+j_0}\|\partial^{\beta}\partial^{\alpha''}_{x_{\mathbf{P}}}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+j_0\eta))}\Bigg).\end{aligned} \tag{A.7}$$

Since $H_E\psi=0$, we get

$$\begin{aligned}
&\eta^{2+j_0}\|H_E\partial_{x_{\mathbf{P}}}^{\alpha''}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+j_0\eta))} \\
&\quad=\eta^{2+j_0}\Bigg\|\sum_{\substack{\gamma<\alpha''\\ \beta+\gamma=\alpha''}}\binom{\alpha''}{\gamma}(\partial_{x_{\mathbf{P}}}^{\beta}(V-E))\partial_{x_{\mathbf{P}}}^{\gamma}\psi\Bigg\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+j_0\eta))}.
\end{aligned}\tag{A.8}$$

We now use (A.4), the combinatorical result from Proposition 2.1 together with the induction hypothesis, to estimate (A.8) as

$$\begin{aligned}
\eta^{2+j_0}\|H_E\partial_{x_{\mathbf{P}}}^{\alpha''}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+j_0\eta))} &\leq \sum_{k=1}^{|\alpha''|}\binom{|\alpha''|}{k}L_V^{k+1}k!j_0^{-k}L_\psi^{|\alpha''|-k+1} \\
&\leq \sum_{k=1}^{|\alpha''|}L_V^{k+1}L_\psi^{|\alpha''|-k+1} \\
&\leq L_\psi^{|\alpha''|+2}\sum_{k=1}^{|\alpha''|}\left(\frac{L_V}{L_\psi}\right)^{k+1} \\
&\leq L_\psi^{|\alpha''|+2}.
\end{aligned}\tag{A.9}$$

Here we used the assumption $L_\psi \geq 2L_V$ from (A.6) in the last estimate.

Due to the induction hypothesis we can also estimate the other term in (A.7),

$$\sum_{|\beta|<2}\eta^{|\beta|+j_0}\|\partial^\beta\partial_{x_{\mathbf{P}}}^{\alpha''}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+j_0\eta))} \leq \sum_{|\beta|<2}L_\psi^{|\alpha''|+|\beta|+1}.\tag{A.10}$$

So using (A.9) and (A.10), we can estimate (A.7) as

$$\eta^{2+j_0}\|\partial^{\alpha_0}\partial_{x_{\mathbf{P}}}^{\alpha}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon/2+(j_0+1)\eta))} \leq L_\psi^{|\alpha|+|\alpha_0|+1}\left(\frac{C_0(1+\sum_{|\beta|<2}1)}{L_\psi}\right).$$

The last factor is ≤ 1, by the choice of L_ψ (see (A.6)). This finishes the proof of (A.5) and therefore of Lemma 3.1. □

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