ESTIMATES ON DERIVATIVES OF COULOMBIC
WAVE FUNCTIONS AND THEIR ELECTRON
DENSITIES

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Abstract. We prove a priori bounds for all derivatives of non-
relativistic Coulombic eigenfunctions $\psi$, involving negative powers
of the distance to the singularities of the many-body potential. We
use these to derive bounds for all derivatives of the corresponding
one-electron densities $\rho$, involving negative powers of the distance
from the nuclei. The results are both natural and optimal, as seen
from the ground state of Hydrogen.

1. Introduction and results

In a series of papers [15, 19, 16, 18], the present authors (together
with M. and T. Hoffmann-Ostenhof) have studied the regularity prop-
erties of molecular Coulombic eigenfunctions $\psi$ and their electron den-
sities $\rho$ at the singularities of the many-body Coulomb potential. For
a recent review, see [39, pp. 170–178]. Some relevant previous wor-
ks not mentioned in that review are [24, 26, 28].

In this paper we take a different approach. Away from these sin-
gularities (where eigenfunctions are real analytic) we prove local $L^p$
estimates on all pointwise derivatives of such eigenfunctions $\psi$, with the
optimal behaviour in the distance to the singularities. The estimates
are a priori, so, if $\psi$ decays exponentially—as is typically the case
for atomic and molecular eigenfunctions—we get exponential decay of
these estimates. As a corollary we get that all pointwise derivatives of $\psi$
belong to certain weighted Sobolev-spaces. This formulation is inspired
by the results in [3], which we improve and clarify (see Remarks 1.6(iv)
and 1.7 below for more details).

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the European Research Council, ERC grant agreement 202859.
We then apply this to obtain estimates on pointwise derivatives of the corresponding electron density \( \rho \) away from the nuclei, with the optimal behaviour in the distance to the positions of the nuclei.

Both types of results are of mathematical interest in themselves, but also of importance for numerical calculations in Quantum Chemistry.

We now formulate the problem. For simplicity of the presentation (and only therefore), we restrict our attention to the case of atoms (i.e., one nucleus). Let \( H \) be the non-relativistic Schrödinger operator of an \( N \)-electron atom with nuclear charge \( Z \) in the fixed nucleus approximation,

\[
H = \sum_{j=1}^{N} \left( -\Delta_j - \frac{Z}{|x_j|} \right) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} = -\Delta + V. \tag{1.1}
\]

Here the \( x_j = (x_{j,1}, x_{j,2}, x_{j,3}) \in \mathbb{R}^3, j = 1, \ldots, N \), denote the positions of the electrons, and the \( \Delta_j \) are the associated Laplacians so that \( \Delta = \sum_{j=1}^{N} \Delta_j \) is the \( 3N \)-dimensional Laplacian. Let \( x = (x_1, x_2, \ldots, x_N) \in \mathbb{R}^{3N} \) and let \( \nabla = (\nabla_1, \ldots, \nabla_N) \) denote the \( 3N \)-dimensional gradient operator. By abuse of notation, we use \( | \cdot | \) for the Euclidean norm in both \( \mathbb{R}^3 \) and \( \mathbb{R}^{3N} \). The operator \( H \) is selfadjoint with operator domain \( \mathcal{D}(H) = W^{2,2}(\mathbb{R}^{3N}) \) and form domain \( \mathcal{Q}(H) = W^{1,2}(\mathbb{R}^{3N}) \) [33]. We are interested in the behaviour of (pointwise) derivatives away from the singularities of the potential \( V \) in (1.1) of \( L^2 \)-eigenfunctions \( \psi \) of the operator \( H \),

\[
H \psi = E \psi, \quad \text{with } \psi \in W^{2,2}(\mathbb{R}^{3N}), \ E \in \mathbb{R}. \tag{1.2}
\]

More precisely, let \( \Sigma \) denote the set of coalescence points (i.e., singularities of \( V \)),

\[
\Sigma := \{ x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \mid \prod_{j=1}^{N} |x_j| \prod_{1 \leq i < j \leq N} |x_i - x_j| = 0 \}. \tag{1.3}
\]

Note that \( V \) is real analytic in the open set \( \mathbb{R}^{3N} \setminus \Sigma \). Hence if, for some open \( \Omega \subset \mathbb{R}^{3N} \), \( \psi \) is a weak solution to (1.2) in \( \Omega \), then [30, Section 7.5, pp. 177–180] \( \psi \) is real analytic away from \( \Sigma \), that is, \( \psi \in C^\omega(\Omega \setminus \Sigma) \). In particular, any eigenfunction \( \psi \in W^{2,2}(\mathbb{R}^{3N}) \) of the operator \( H \) is real analytic in \( \mathbb{R}^{3N} \setminus \Sigma \). Moreover it is known that \( \psi \in C_{loc}^{0,1}(\mathbb{R}^{3N}) \) [27, Proposition 1.5], an improvement of Kato’s famous Cusp Condition [34]; see also [29].

Define the distance from a point \( x \in \mathbb{R}^{3N} \) to a subset \( K \subset \mathbb{R}^{3N} \) by

\[
d(x, K) = \inf \left\{ |x - y| \mid y \in K \right\}. \tag{1.4}
\]
Note that
\[ d(x, \Sigma) = \min \left\{ |x_i|, \frac{1}{\sqrt{2}} |x_j - x_k| \mid i, j, k \in \{1, \ldots, N\}, j \neq k \right\}. \]  
(1.5)
More generally, for \( k \in \{1, \ldots, N\} \), let \( \Sigma^k \subseteq \Sigma \) (the singularities of \( V \) involving \( x_k \)) be defined by
\[ \Sigma^k := \{ x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \mid |x_k| \prod_{j=1, j \neq k}^{N} |x_j - x_k| = 0 \}; \]  
(1.6)
then \( \Sigma = \bigcup_{k=1}^{N} \Sigma^k \), and we note that, for \( k \in \{1, \ldots, N\} \),
\[ d(x, \Sigma^k) = \min \left\{ |x_k|, \frac{1}{\sqrt{2}} |x_k - x_j| \mid j \in \{1, \ldots, N\}, j \neq k \right\} \geq d(x, \Sigma). \]  
(1.7)
For \( Q \subseteq \{1, \ldots, N\} \), let \( \Sigma^Q := \bigcup_{k \in Q} \Sigma^k \subseteq \Sigma \) (the singularities of \( V \) involving some \( x_k \) with \( k \in Q \)). This way, \( d(x, \Sigma^Q) \leq d(x, \Sigma^k) \) for all \( k \in Q \), and
\[ d(x, \Sigma^Q) = \min \left\{ |x_k|, \frac{1}{\sqrt{2}} |x_k - x_j| \mid k \in Q, j \in \{1, \ldots, N\}, j \neq k \right\} \geq d(x, \Sigma). \]  
(1.8)
For \( \alpha = (\alpha_1, \ldots, \alpha_N) \in (\mathbb{N}^3_0)^N = \mathbb{N}^{3N}_0 \), let
\[ Q_\alpha := \{ k \in \{1, \ldots, N\} \mid \alpha_k \neq 0 \in \mathbb{N}^3_0 \} \subseteq \{1, \ldots, N\}, \]
\[ \Sigma^\alpha := \Sigma^{Q_\alpha} \subseteq \Sigma, \quad d_\alpha(x, \Sigma) := d(x, \Sigma^\alpha). \]  
(1.9)
That is, for \( \alpha \in \mathbb{N}^{3N}_0 \) fixed, \( \Sigma^\alpha \) is the set of singularities of \( V \) involving the \( x_k \)'s for which \( \alpha_k \neq 0 \). Hence,
\[ d_\alpha(x, \Sigma) = \min \left\{ |x_k|, \frac{1}{\sqrt{2}} |x_k - x_j| \mid k \in Q_\alpha, j \in \{1, \ldots, N\}, j \neq k \right\}, \]
\[ |x| \geq d_\alpha(x, \Sigma) \geq d(x, \Sigma). \]  
(1.10)
Note that \( \Sigma^\alpha = \Sigma \) (and therefore, \( d_\alpha(x, \Sigma) = d(x, \Sigma) \)) for all \( \alpha = (\alpha_1, \ldots, \alpha_N) \in \mathbb{N}^{3N}_0 \) for which \( \alpha_k \neq 0 \) for all \( k \in \{1, \ldots, N\} \).

Let \( B_n(x, r) \subseteq \mathbb{R}^n \) denote the open ball of centre \( x \in \mathbb{R}^n \) and radius \( r > 0 \). We recall that for \( \alpha = (\alpha_1, \ldots, \alpha_N) \in (\mathbb{N}^3_0)^N = \mathbb{N}^{3N}_0 \), \( \alpha_k = (\alpha_{k,1}, \alpha_{k,2}, \alpha_{k,3}) \in \mathbb{N}^3_0 \), we let \( |\alpha| = \sum_{k=1}^{N} \sum_{j=1}^{3} \alpha_{k,j} \).

The first main result of this paper is the following. Our main interest are the cases \( p = 2 \) and \( p = \infty \) (for the proof, see Section 2 below).

**Theorem 1.1.** Let \( H \) be the non-relativistic Hamiltonian given by (1.1). Let the singular set \( \Sigma \subseteq \mathbb{R}^{3N} \) be defined by (1.3), and let the distance \( d(x, \Sigma) \) from \( x \in \mathbb{R}^{3N} \) to \( \Sigma \) be given by (1.5). Furthermore, for every \( \alpha \in \mathbb{N}^{3N}_0 \), \( |\alpha| \geq 1 \), let the corresponding singular set \( \Sigma^\alpha \subseteq \mathbb{R}^{3N} \) be defined by (1.9), and the distance \( d_\alpha(x, \Sigma) \) from \( x \in \mathbb{R}^{3N} \) to \( \Sigma^\alpha \) be given by (1.10).
Then:

(i) For all $p \in (1, \infty]$, all $\alpha \in \mathbb{N}_0^3 N$, $|\alpha| \geq 1$, all $0 < r < R < 1$, and all $E \in \mathbb{C}$, there exists a constant $C = C(p, \alpha, r, R, E)$ (depending also on $N, Z$) such that, for all $\psi \in W_{loc}^{2,2}(\mathbb{R}^3 \mathbb{N})$ satisfying

\[
H \psi = E \psi,
\]

and for all $x \in \mathbb{R}^3 \mathbb{N} \setminus \Sigma^\alpha$, the following inequality holds:

\[
\|\partial^\alpha \psi\|_{L^p(B_{3N}(x, R\lambda_\alpha(x)))} \leq C \lambda_\alpha(x)^{1-|\alpha|} (\|\psi\|_{L^p(B_{3N}(x, R\lambda_\alpha(x)))} + \|\nabla \psi\|_{L^p(B_{3N}(x, R\lambda_\alpha(x)))}),
\]

where $\lambda_\alpha(x) := \min \{1, d_\alpha(x, \Sigma)\}$.

(ii) For all $p \in (1, \infty]$, all $\alpha \in \mathbb{N}_0^3 N$, $|\alpha| \geq 1$, all $0 < r < R < 1$, and all $E \in \mathbb{C}$, there exists a constant $C = C(p, \alpha, r, R, E)$ (depending also on $N, Z$) such that, for all $\psi \in W_{loc}^{2,2}(\mathbb{R}^3 \mathbb{N})$ satisfying (1.11), and for all $x \in \mathbb{R}^3 \mathbb{N} \setminus \Sigma$, the following inequality holds:

\[
\|\partial^\alpha \psi\|_{L^p(B_{3N}(x, r\lambda_\alpha(x)))} \leq C \lambda(x)^{1-|\alpha|} (\|\psi\|_{L^p(B_{3N}(x, R\lambda_\alpha(x)))} + \|\nabla \psi\|_{L^p(B_{3N}(x, R\lambda_\alpha(x)))}),
\]

where $\lambda(x) := \min \{1, d(x, \Sigma)\}$.

As a corollary of the case $p = \infty$ we have the following pointwise estimates, one of our main motivations for the study of these problems (for the proof, see Section 3 below):

**Corollary 1.2.** Let the notation and assumptions be as in Theorem 1.1 above and let $\alpha \in \mathbb{N}_0^3 N$, $|\alpha| \geq 1$, and $R > 0$. Then:

(i) There exists a constant $C = C(\alpha, R, E)$ (depending also on $N, Z$) such that for all $x \in \mathbb{R}^3 \mathbb{N} \setminus \Sigma^\alpha$,

\[
|\partial^\alpha \psi(x)| \leq C \lambda_\alpha(x)^{1-|\alpha|} \|\psi\|_{L^\infty(B_{3N}(x, R))},
\]

where $\lambda_\alpha(x) = \min \{1, d_\alpha(x, \Sigma)\}$.

(ii) There exists a constant $C = C(\alpha, R, E)$ (depending also on $N, Z$) such that for all $x \in \mathbb{R}^3 \mathbb{N} \setminus \Sigma$,

\[
|\partial^\alpha \psi(x)| \leq C \lambda(x)^{1-|\alpha|} \|\psi\|_{L^\infty(B_{3N}(x, R))},
\]

where $\lambda(x) = \min \{1, d(x, \Sigma)\}$.

If $\psi$ is an eigenfunction of $H$ (that is, $\psi \in W^{2,2}(\mathbb{R}^3 \mathbb{N})$ and $\psi$ satisfies (1.11) for some $E \in \mathbb{R}$), and $\psi$ also decays exponentially, then we have the following corollary to Theorem 1.1 (for the proof, see Section 3 below).
Corollary 1.3. With the notation and assumptions as in Theorem 1.1, assume \( \psi \) is an eigenfunction of \( H \) (that is, \( \psi \in W^{2,2}(\mathbb{R}^{3N}) \) and \( \psi \) satisfies (1.2) for some \( E \in \mathbb{R} \)). Assume furthermore that \( E \) and \( \psi \) are such that there exist constants \( C_0, c_0 > 0 \) such that

\[
|\psi(x)| \leq C_0 e^{-c_0|x|} \text{ for all } x \in \mathbb{R}^{3N}.
\]  

(1.16)

Then for all multiindices \( \alpha \in \mathbb{N}_0^{3N} \) with \( |\alpha| \geq 1 \):

(i) There exist constants \( C_\alpha, c_\alpha > 0 \) such that, for all \( x \in \mathbb{R}^{3N} \setminus \Sigma^\alpha \),

\[
|\partial^\alpha \psi(x)| \leq C_\alpha d_\alpha(x, \Sigma)^{1-|\alpha|} e^{-c_\alpha|x|}.
\]  

(1.17)

(ii) There exist constants \( C_\alpha, c_\alpha > 0 \) such that, for all \( x \in \mathbb{R}^{3N} \setminus \Sigma \),

\[
|\partial^\alpha \psi(x)| \leq C_\alpha d(x, \Sigma)^{1-|\alpha|} e^{-c_\alpha|x|}.
\]  

(1.18)

(iii)

\[
d_\alpha(\cdot, \Sigma)|^{\alpha|-a}\partial^\alpha \psi \in L^2(\mathbb{R}^{3N} \setminus \Sigma^\alpha) \text{ for all } a < \frac{\alpha}{2}.
\]  

(1.19)

(iv)

\[
d(\cdot, \Sigma)^{|\alpha|-a}\partial^\alpha \psi \in L^2(\mathbb{R}^{3N} \setminus \Sigma) \text{ for all } a < \frac{\alpha}{2}.
\]  

(1.20)

Remark 1.4. Of course, \( \Sigma^\alpha, \Sigma \subset \mathbb{R}^{3N} \) are of Lebesgue measure zero, so \( L^2(\mathbb{R}^{3N} \setminus \Sigma^\alpha) = L^2(\mathbb{R}^{3N} \setminus \Sigma) = L^2(\mathbb{R}^{3N}) \). However, in (1.19)–(1.20) we want to emphasize that the derivatives \( \partial^\alpha \psi \) are the pointwise (classical) derivatives in \( \mathbb{R}^{3N} \setminus \Sigma \) and \( \mathbb{R}^{3N} \setminus \Sigma^\alpha \) (which exist), and not weak derivatives in \( \mathbb{R}^{3N} \) (on which we have no statements). The same remark holds for (1.21)–(1.22) below.

Using Theorem 1.1 with \( p = 2 \), we can prove the following variant of Corollary 1.3 (iii)–(iv), which does not assume any decay of \( \psi \) (apart from \( \psi \in W^{2,2}(\mathbb{R}^{3N}) \); for the proof, see Section 4 below):

Theorem 1.5. Let the notation and assumptions be as in Theorem 1.1, and assume furthermore that \( \psi \in W^{2,2}(\mathbb{R}^{3N}) \). Then, for all multiindices \( \alpha \in \mathbb{N}_0^{3N} \) with \( |\alpha| \geq 1 \) we have

\[
\lambda_\alpha^{|\alpha|-a}\partial^\alpha \psi \in L^2(\mathbb{R}^{3N} \setminus \Sigma^\alpha) \text{ for all } a < \frac{\alpha}{2},
\]  

(1.21)

and

\[
\lambda^{|\alpha|-a}\partial^\alpha \psi \in L^2(\mathbb{R}^{3N} \setminus \Sigma) \text{ for all } a < \frac{\alpha}{2},
\]  

(1.22)

where \( \lambda_\alpha(x) = \min \{1, d_\alpha(x, \Sigma)\} \) and \( \lambda(x) = \min \{1, d(x, \Sigma)\} \).

In fact, for all \( \alpha \in \mathbb{N}_0^{3N} \) with \( |\alpha| \geq 1 \) there exists \( C_\alpha > 0 \) such that

\[
\|\lambda_\alpha^{|\alpha|-a}\partial^\alpha \psi\|_{L^2(\mathbb{R}^{3N} \setminus \Sigma^\alpha)} \leq C_\alpha \|\psi\|_{W^{2,2}(\mathbb{R}^{3N})},
\]  

(1.23)

\[
\|\lambda^{|\alpha|-a}\partial^\alpha \psi\|_{L^2(\mathbb{R}^{3N} \setminus \Sigma)} \leq C_\alpha \|\psi\|_{W^{2,2}(\mathbb{R}^{3N})}.
\]  

(1.24)
We now give some remarks on the results stated above.

**Remark 1.6.**

(i) For $\alpha \in \mathbb{N}_0^3$ with $|\alpha| = 1$, (1.17)–(1.18) was proved in [27, Theorem 1.2; Remark 1.9].

(ii) The ground state function of Hydrogen (that is, of the operator $-\Delta - \frac{1}{|x|}$, $x \in \mathbb{R}^3$, $N = 1$) is $\phi_0(x) = c_0e^{-|x|/2}$. In this case $\Sigma = \{0\} \subset \mathbb{R}^3$ and $d(x, \Sigma) = |x|$. This example shows that the results in Theorem 1.1, Corollary 1.2, Corollary 1.3, and Theorem 1.5 are both natural and optimal.

(iii) As will be clear from the proofs, Theorem 1.1, Corollary 1.2, Corollary 1.3, and Theorem 1.5 generalize to the case of molecules (i.e., $K$ nuclei with positive charges $Z_1, \ldots, Z_K > 0$, fixed at positions $R_1, \ldots, R_K$ in $\mathbb{R}^3$) in the obvious way. In this case (compare with (1.1)),

$$V(x) = \sum_{j=1}^{N} \sum_{k=1}^{K} \left( -\frac{Z_k}{x_j - R_k} \right) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|}. \quad (1.25)$$

(iv) The local version (i.e., without the exponential decay) of (1.18) for $N = 1$ was already known: It follows immediately from [16, Theorem 1.1] (also in the case of several nuclei). In fact, more generally, for any $N$ the local version of (1.17) for points $x$ in a small neighbourhood of so-called ‘two-particle coalescence points’ follows from [16, Theorem 1.4].

(v) For references on the exponential decay of eigenfunctions (i.e., (1.16)), see e.g. Froese and Herbst [20] and Simon [38, 37]. Exponential decay is known to hold for any eigenfunction $\psi$ associated to an eigenvalue $E$ which is not a so-called ‘threshold energy’. This includes (but is not restricted to) any eigenvalue below the essential spectrum in any symmetry subspace, for instance, the fermionic ground state energy.

**Remark 1.7.** As seen from the example in Remark 1.6(ii), the natural critical value for $a$ in (1.19)–(1.22) is $5/2$, as long as $|\alpha| \geq 1$. Hence, the result is optimal. However, for $\alpha = 0$, one has (1.19)–(1.22) only for all $a < 3/2$; this follows from (A.25) in Proposition A.3 below. The example in Remark 1.6(ii) again shows that this is optimal.

The statements in (1.19)–(1.22) can be re-formulated in terms of certain weighted Sobolev-spaces: Define the following spaces (called
'Babuška-Kondratiev' spaces in [3]; recall that $\lambda(x) = \min\{1, d(x, \Sigma)\}$:

$$K_m^a(\mathbb{R}^{3N} \setminus \Sigma, \lambda) = \{ u : \mathbb{R}^{3N} \to \mathbb{C} \mid \lambda^{|\alpha|-a} \partial^\alpha u \in L^2(\mathbb{R}^{3N} \setminus \Sigma), |\alpha| \leq m \}. \quad (1.26)$$

Then it follows from Theorem 1.5, and the remark above, that any eigenfunction $\psi \in W^{2,2}(\mathbb{R}^{3N})$ of the operator $H$ in (1.1) belongs to $K_m^a(\mathbb{R}^{3N} \setminus \Sigma, \lambda)$ for any $m \in \mathbb{N}$ and any $a < 3/2$. However, Theorem 1.5 gives much more, since the restriction on $a$ is only due to the case $\alpha = 0$: It also follows that, for any $|\alpha| = 1$, also $\partial^\alpha \psi$ belongs to $K_m^a(\mathbb{R}^{3N} \setminus \Sigma, \lambda)$ for any $m \in \mathbb{N}$ and any $a < 3/2$. The example in Remark 1.6(ii) again gives optimality.

In the case of exponentially decaying eigenfunctions, Corollary 1.3 gives the same statements, but with $K_m^a(\mathbb{R}^{3N} \setminus \Sigma, d(\cdot, \Sigma))$ replaced by $K_m^a(\mathbb{R}^{3N} \setminus \Sigma, d(\cdot, \Sigma))$. It is natural that without any additional decay assumptions on $\psi$, one can only expect to get this type of result with a 'regularised distance function' like $\lambda(x) = \min\{1, d(x, \Sigma)\}$. This vastly improves and clarifies the results proved and the conjectures stated in [3] (which were also for a regularised distance function). (See also Remark 1.6(iv) above.)

Note that the results in [3] are stated for slightly more general potentials $V$ than the one in (1.1): Let

$$W(x) = \sum_{j=1}^{N} b_j \frac{x_j}{|x_j|} \left( \sum_{1 \leq i < j \leq N} \frac{c_{ij}(x_i - x_j)}{|x_i - x_j|} \right), \quad (1.27)$$

with $b_j, c_{ij} \in C^\infty(S^2)$ (with $S^2$ the unit sphere in $\mathbb{R}^3$). Then all our results hold with the operator $H$ in (1.1) replaced with $-\Delta + W$. For simplicity of the presentation, we have chosen to stick to the physically most relevant case of atoms and molecules, as in (1.1).

For another approach, via a singular pseudo-differential operator calculus, giving a parametrix for the resolvent of $H$ in (1.1) in the case of Hydrogen ($N = 1$) [9] and Helium ($N = 2$) [10] with the correct asymptotic behaviour at two-particle coalescence points, see [8].

An important quantity derived from any eigenfunction $\psi$ of the operator $H$ in (1.1) is its associated one-electron density $\rho$ defined by

$$\rho(x) \equiv \rho_\psi(x) = \sum_{j=1}^{N} \rho_j(x) = \sum_{j=1}^{N} \int_{\mathbb{R}^{3N-3}} |\psi(x, \hat{x}_j)|^2 d\hat{x}_j, \quad (1.28)$$

where we have introduced the notation

$$\hat{x}_j = (x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_N) \quad (1.29)$$
and

\[ d\hat{x}_j = dx_1 \ldots dx_{j-1} dx_{j+1} \ldots dx_N. \]  

(1.30)

By abuse of notation, we identify \((x_1, \ldots, x_{j-1}, x, x_{j+1}, \ldots, x_N)\) and \((x, \hat{x}_j)\).

The regularity properties of \(\rho\) at the origin (or, more generally, at the positions of the nuclei, when studying a molecule, see Remark 1.6(iii) above) have been studied recently in [19, 18] (see also [4, 27, 40]). In [14] it was proved that \(\rho\) is real analytic away from the position of the nucleus (i.e., \(\rho \in C^\omega(\mathbb{R}^3 \setminus \{0\})\); for another recent proof of this, see [32] (see also [12, 13])). (This result is known as the Holographic Electron Density Theorem (HEDT) in Quantum Chemistry; see [36].)

Our main result on \(\rho\) in this paper is the following.

**Theorem 1.8.** Let \(H\) be the non-relativistic Hamiltonian given by (1.1), and assume that \(\psi \in W^{2,2}((\mathbb{R}^3)^N)\) satisfies, for some \(E \in \mathbb{R}\),

\[ H\psi = E\psi. \]  

(1.31)

Define the associated one-electron density \(\rho\) as in (1.28).

Then, for all multiindices \(\alpha \in \mathbb{N}_0^3\) with \(|\alpha| \geq 1:\)

(i) For all \(R > 0\) there exists a constant \(C_\alpha(R) > 0\) such that

\[ |\partial^\alpha \rho(x)| \leq C_\alpha(R) r(x)^{1-|\alpha|} \int_{B_3(x,R)} \rho(y) dy \quad \text{for all} \quad x \in \mathbb{R}^3 \setminus \{0\}, \]  

(1.32)

where \(r(x) := \min\{1, |x|\}, \ x \in \mathbb{R}^3\).

In particular, \(r^{1-|\alpha|} \partial^\alpha \rho \in L^\infty(\mathbb{R}^3 \setminus \{0\})\) for all \(a \in [0,1]\), with

\[ \|r^{1-|\alpha|} \partial^\alpha \rho\|_{L^\infty(\mathbb{R}^3 \setminus \{0\})} \leq C_\alpha \|\rho\|_{L^1(\mathbb{R}^3)} = C_\alpha \|\psi\|_{L^2((\mathbb{R}^3)^N)}^2. \]  

(1.33)

(ii) Furthermore, for all \(p \in [0,\infty)\) and all \(a \in [0, \frac{p+3}{p}]\), there exists a constant \(C_\alpha(a,p) > 0\) such that

\[ \|r^{1-|\alpha|} \partial^\alpha \rho\|_{L^p((\mathbb{R}^3)^N \setminus \{0\})} \leq C_\alpha(a,p) \|\rho\|_{L^1(\mathbb{R}^3)}. \]  

(1.34)

In particular, \(r^{1-|\alpha|} \partial^\alpha \rho \in L^p(\mathbb{R}^3 \setminus \{0\})\) for all \(p \in [1,\infty)\) and all \(a \in [0, \frac{p+3}{p}]\).

(iii) Under the decay assumption (1.16), \(r(x)\) can be replaced with \(|x|\) above: \(|x|^{1-|\alpha|} \partial^\alpha \rho \in L^p(\mathbb{R}^3 \setminus \{0\})\) for all \(p \in [1,\infty)\) and all \(a \in [0, \frac{p+3}{p}]\), and all \(a \in [0,1]\) for \(p = \infty\). In fact, if we assume exponential decay of \(\psi\) (i.e., there exist constants \(C_0, c_0 > 0\) such that (1.16) holds), then for all multiindices \(\alpha \in \mathbb{N}_0^3\) with \(|\alpha| \geq 1\) there exist constants \(C_\alpha, c_\alpha > 0\) such that

\[ |\partial^\alpha \rho(x)| \leq C_\alpha |x|^{1-|\alpha|} e^{-c_\alpha|x|} \]  

(1.35)
for all $x \in \mathbb{R}^3 \setminus \{0\}$.

Remark 1.9.

(i) Again, the example in Remark 1.6(ii) above (for which $\rho(x) = c_0^2 e^{-|x|}$) shows that the results in Theorem 1.8 are both natural and optimal.

(ii) As will be clear from the proof, also this result generalizes to the case of molecules (see Remark 1.6(iii) above) in the obvious way.

(iii) The corresponding local version of (1.35) near $x = 0$ for the case of the one-electron density of Hartree-Fock states (i.e., Slater-determinants of solutions to the Hartree-Fock equations) follows from [17, Corollary 1.5]. It says that in this case there exist $\varepsilon > 0$ and real analytic functions $\rho_1, \rho_2 : B_3(0, \varepsilon) \to \mathbb{R}$ (i.e., $\rho_1, \rho_2 \in C^\omega(B_3(0, \varepsilon))$), such that

$$\rho(x) = \rho_1(x) + |x| \rho_2(x) \text{ for all } x \in B_3(0, \varepsilon).$$

(1.36)

See also [7, 11] for related work. It would be interesting to determine whether the same result holds in the (present) Schrödinger case (recall that then $\rho \in C^\omega(\mathbb{R}^3 \setminus \{0\})$). Note that, as for Hartree-Fock, (1.35) (near $x = 0$) would follow from such a result.

(iv) The statements in (1.33)–(1.34) can again be re-formulated in terms of weighted Sobolev-spaces (see also Remark 1.7 above): Define the following spaces (recall that $r(x) = \min\{1, |x|\}$):

$$K_m^m, p(\mathbb{R}^3 \setminus \{0\}, r) = \{f : \mathbb{R}^3 \to \mathbb{C} | r^{\alpha - a} \partial^\alpha f \in L^p(\mathbb{R}^3 \setminus \{0\}), |\alpha| \leq m\}. \tag{1.37}$$

Then it follows from Theorem 1.8 that for the electron density $\rho$ (given by (1.28)) of any eigenfunction $\psi \in W^{2,2}(\mathbb{R}^{3N})$ of the operator $H$ in (1.1), and any $|\alpha| = 1, \partial^\alpha \rho$ belongs to $K_m^m, p(\mathbb{R}^3 \setminus \{0\}, r)$ for every $m \in \mathbb{N}$, for any $a \in [0, 1]$ if $p = \infty$, and any $a \in [0, \frac{p+3}{p}]$ if $p \in [1, \infty)$.

(v) For precise information on the behaviour at infinity of $\rho$ itself (f.ex., similar to (1.35), but for $\alpha = 0$), see [2, 23, 25].

An important ingredient in the proof of Theorem 1.8 is an estimate on derivatives of $\psi$ along certain singularities of $V$ (‘parallel derivatives’; see also [12, Proposition 2], [13, Lemma 2.2], [14, Lemma 3.1]). Since this estimate is interesting in itself, we formulate it here.
First we need some additional notation. For \( Q \subset \{1, \ldots, N \} \), \( Q \neq \emptyset \), define the (‘centre of mass’) coordinate \( x_Q \in \mathbb{R}^3 \) by

\[
x_Q := \frac{1}{\sqrt{|Q|}} \sum_{j \in Q} x_j.
\] (1.38)

We now define \( \partial^s_{x_Q} f \), \( s = 1, 2, 3 \), for a function \( f \in C^1(\mathbb{R}^{3N}) \) and \( e_s \) the canonical unit vectors in \( \mathbb{R}^3 \). For the given \( Q \) and \( s \), let \( \mathbf{v} = (v_1, \ldots, v_N) \in \mathbb{R}^{3N} \) with \( v_j = 0 \) for \( j \notin Q \), and \( v_j = e_s/\sqrt{|Q|} \) for \( j \in Q \). Then we define

\[
\partial^s_{x_Q} f(\mathbf{x}) := \nabla f(\mathbf{x}) \cdot \mathbf{v} = \frac{1}{\sqrt{|Q|}} \sum_{j \in Q} \frac{\partial f}{\partial x_j} (\mathbf{x}) = \left( \frac{1}{\sqrt{|Q|}} \sum_{j \in Q} \partial_{x_j,s} f \right)(\mathbf{x}).
\] (1.39)

The definition of \( \partial^\alpha_{x_Q} \) then follows by iteration for any \( \alpha = (\alpha_1, \alpha_2, \alpha_2) \in \mathbb{N}_0^3 \):

\[
\partial^\alpha_{x_Q} f = \left[ \prod_{s=1}^3 \left( \frac{1}{\sqrt{|Q|}} \sum_{j \in Q} \partial_{x_j,s} \right)^{\alpha_s} \right] f.
\] (1.40)

In particular, if \( Q = \{j, k\}, \ j, k \in \{1, \ldots, N\}, \ j \neq k \), then

\[
\partial_{x_j+x_k}^\alpha f := \partial^\alpha_{x_Q} f = \left[ \prod_{s=1}^3 \left( \frac{1}{\sqrt{2}} (\partial_{x_j,s} + \partial_{x_k,s}) \right)^{\alpha_s} \right] f.
\] (1.41)

It follows that if \( Q \subseteq \{1, \ldots, N\}, \ Q \neq \emptyset \), and \( f(\mathbf{x}) = g(x_j - x_k) \) for some \( j, k \in Q \) and \( g : \mathbb{R}^3 \to \mathbb{R} \), then

\[
\partial^\alpha_{x_Q} f = \partial^\alpha_{x_j+x_k} f = \partial^\alpha_{x_j+x_k} g = 0.
\] (1.42)

One can clearly reformulate these definition in terms of Fourier transforms (multiplication by \( \xi_Q^s \) for suitably defined \( \xi_Q \) in Fourier space). In a previous paper [12] we used a coordinate transformation to describe these derivatives.

Furthermore, we define (notice that generally \( \Sigma_Q \) is different from the previously defined \( \Sigma^Q \))

\[
\Sigma_Q := \{ \mathbf{x} = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \mid \prod_{j \in Q} |x_j| \prod_{j \in Q, k \notin Q} |x_j - x_k| = 0 \},
\] (1.43)

so that

\[
d_Q(\mathbf{x}, \Sigma) := d(\mathbf{x}, \Sigma_Q) = \min \left\{ |x_j|, \frac{1}{\sqrt{2}} |x_j - x_k| \mid j \in Q, \ k \notin Q \right\}. \] (1.44)

We then have the following estimate, concerning derivatives \( \partial^\alpha_{x_Q} \) of local solutions \( \psi \) along/parallel to the singularity \( \Sigma_Q \):
Proposition 1.10. Let $H$ be the non-relativistic Hamiltonian given by (1.1). For any $Q \subset \{1, \ldots, N\}$, $Q \neq \emptyset$, let the singular set $\Sigma_Q \subset \mathbb{R}^{3N}$ be defined by (1.43), and let the distance $d_Q(x, \Sigma)$ from $x \in \mathbb{R}^{3N}$ to $\Sigma_Q$ be given by (1.44). Furthermore, for $\alpha \in \mathbb{N}^3$, $|\alpha| \geq 1$, let $\partial^\alpha_{x_Q}$ be defined by (1.40).

Then: For all $p \in (1, \infty]$, all $Q \subset \{1, \ldots, N\}$, $Q \neq \emptyset$, all $\alpha \in \mathbb{N}^3$, $|\alpha| \geq 1$, all $0 < r < R < 1$, and all $E \in \mathbb{C}$, there exists a constant $C = C(p, Q, \alpha, r, R, E)$ (depending also on $N, Z$) such that for all $\psi \in W^{2,2}_\text{loc}(\mathbb{R}^{3N})$ satisfying

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

and for all $x \in \mathbb{R}^{3N} \setminus \Sigma_Q$, the following inequality holds:

$$\left\| \partial^\alpha_{x_Q} \overline{\psi} \right\|_{L^p(B_{3N}(x,r\lambda_Q(x)))} \leq C \lambda_Q(x)^{1-|\alpha|} \left( \left\| \psi \right\|_{L^p(B_{3N}(x,R\lambda_Q(x)))} + \left\| \nabla \psi \right\|_{L^p(B_{3N}(x,R\lambda_Q(x)))} \right),$$

where $\lambda_Q(x) = \min\{1, d_Q(x, \Sigma)\}$.

1.1. Organisation of the paper and strategy of the proofs.

The first main idea of the proofs of Theorem 1.1 (in Section 2 below) and Proposition 1.10 (in Section 5 below) (see also Proposition A.2 in Appendix A below) is an 'Ansatz', $\psi = e^F \psi_F$, for the solution of $H\psi = E\psi$, for various suitable (see below), slightly different, choices of $F$ (see (2.2), (5.2), and (A.3) below). The function $e^F$ is often called a 'Jastrow factor' in the Chemistry literature [31]. In the mathematical study of Coulombic eigenfunctions, it was introduced in [35] (with $F = \tilde{F}$ in (A.3) below). It was applied (with the same $F$) to study unique continuation in [28, Corollary 4.1; (4.7)] and regularity from [27] onwards. Using that $H\psi = E\psi$, the function $\psi_F$ solves the equation

$$-\Delta \psi_F - 2\nabla F \cdot \nabla \psi_F + (V - \Delta F - |\nabla F|^2 - E)\psi_F = 0.$$  \hspace{1cm}(1.47)

The second main idea is to re-scale the resulting equation (1.47), from a ball around a (fixed) $x \in \mathbb{R}^{3N}$ (away from the relevant singularity of $V$) of the size of the distance $d$ from $x$ to the relevant part of the singular set $\Sigma$ (i.e., $d_a(x, \Sigma)$ or $d_Q(x, \Sigma)$), to a ball of size one around $x$. The $F$ above has been chosen such that, by the homogeneity of the potential $V$ (see (1.1)), this re-scaled equation has coefficients whose (relevant) derivatives are either zero (see (2.17) and (5.14)), or are uniformly bounded on compact subsets of the unit ball (see (2.21) and (5.15)). For this to work, one needs to work with $\lambda = \min\{1, d\}$, not $d$. 

\hspace{1cm}
Successive differentiation of this re-scaled equation (with respect to the relevant variable), and application of standard elliptic regularity theory ($C^{1,\theta}$ and $W^{2,p}$; see Appendix C below) to the resulting equations, produces a priori estimates (on balls of size slightly less than one, hence the $r$ and $R$ in the theorems) with constants independent of $x$. This fact is the essential part of the argument.

Scaling back these a priori estimates for $\alpha$ derivatives delivers the explicit dependence (in $\alpha$) on the distance $d$ to the relevant part of the singular set $\Sigma$ (or rather, on the corresponding $\lambda$) of the a priori bounds of $\partial^\alpha \psi_F$ on balls of the size of this distance around $x$ (see (1.12)–(1.13) and (1.46) above). An extra argument/iteration is needed to get the optimal behavior in the number of derivatives. This is assured by an a priori estimate on first derivatives, see Proposition A.2 in Appendix A. The estimates for $\partial^\alpha \psi$ follow by the properties of $F$.

The (short) proofs of Corollaries 1.2 and 1.3 can be found in Section 3 below.

The proof of Theorem 1.5 (in Section 4 below) consists in carefully integrating up the (local) a priori estimates from Theorem 1.1 (for $p = 2$), and applying the aforementioned a priori estimate in Proposition A.2 in Appendix A.

To prove Theorem 1.8 (in Section 6 below), on $\alpha$ derivatives (with respect to $x_1 \in \mathbb{R}^3$) of the electron density $\rho$, we introduce (see (B.4)–(B.2) in Appendix B below) a particular partition of unity, $1 = \sum I \chi_I$, in the integration variable $\hat{x}_1$ (here, $x = (x_1, \hat{x}_1) \in \mathbb{R}^{3N}$) in the integral defining $\rho$ (see (1.28) above). This partition has the property that, on $\text{supp} \chi_I$, the derivative $\partial_{x_1}$ can be changed into a $\partial_{x_Q}$ for a certain $Q \subset \{1, \ldots, N\}$ (i.e., a 'derivative parallel to a singularity $\Sigma_Q$'; see (1.38)–(1.44) above). Furthermore (again, on $\text{supp} \chi_I$), $\lambda_Q := \min \{1, d_Q\}$ is comparable to $r(x_1) \big(= \min \{1, |x_1|\}; \text{see Lemma B.2 and Lemma B.4 below}\big)$. Applying Proposition 1.10 to each $\chi_I$, and summing, then leads to (1.32).

2. Proof of Theorem 1.1

We give the proof of (i) and indicate the necessary changes for the (much simpler) case of (ii).

We first derive an associated model-equation ((2.25) below).

Fix $\alpha = (\alpha_1, \ldots, \alpha_N) \in \mathbb{N}_0^N$, $\alpha_i \in \mathbb{N}_0^3$ with $|\alpha| \geq 1$, and recall that $\Sigma^\alpha = \Sigma^{Q_\alpha} = \bigcup_{k \in Q_\alpha} \Sigma^k$ (see (1.6) for $\Sigma^k$), with $Q_\alpha = \{k \in \{1, \ldots, N\} \mid \alpha_k \neq 0\}$. For $x^0 = (x^0_1, \ldots, x^0_N) \in \mathbb{R}^3 \setminus \Sigma^\alpha$, let

$$\lambda_\alpha := \min \{1, d_\alpha(x^0, \Sigma)\} = \min \{1, d(x^0, \Sigma^\alpha)\} > 0 . \quad (2.1)$$
Define, for \( x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \),
\[
F_\alpha(x) = \sum_{j \not\in Q_\alpha} \left( -\frac{\zeta}{2} |x_j| + \frac{\zeta}{2} \sqrt{|x_j|^2 + 1} \right) + \sum_{j,k \not\in Q_\alpha, j < k} \left( \frac{1}{4}|x_j - x_k| - \frac{1}{4} \sqrt{|x_j - x_k|^2 + 1} \right). \tag{2.2}
\]

Note that there exists \( C = C(N, Z) > 0 \) such that
\[
|F_\alpha(x)|, |\nabla_x F_\alpha(x)| \leq C \quad \text{for all } x \in \mathbb{R}^{3N} \setminus \Sigma,
\tag{2.3}
\]
and that \( \partial^3_x F_\alpha \equiv 0 \) for all \( \beta \in \mathbb{N}_0^{3N} \) satisfying \( 0 < \beta \leq \alpha \). This follows from the definition of \( Q_\alpha \), since for such \( \beta = (\beta_1, \ldots, \beta_N) \in \mathbb{N}_0^{3N}, \beta_j \in \mathbb{N}_0^3 \), we have \( \beta_j = 0 \) for all \( j \not\in Q_\alpha \). Let
\[
V_\alpha(x) = \sum_{j \in Q_\alpha} |x_j| + \sum_{j,k \not\in Q_\alpha, j < k} \frac{1}{x_j - x_k} + \sum_{j \in Q_\alpha, k \not\in Q_\alpha} \frac{1}{x_j - x_k}. \tag{2.4}
\]
We have that \( V_\alpha \in C^\infty(B_{3N}(x^0, \lambda_\alpha)) \); note that \( B_{3N}(x^0, \lambda_\alpha) \subset \mathbb{R}^{3N} \setminus \Sigma^\alpha \) by (2.1).

By the definition of \( \Sigma^\alpha \) (see (1.9) and (1.6)), if \( x = (x_1, \ldots, x_N) \not\in \Sigma^\alpha \), then \( |x_k| \neq 0 \) for all those \( k \in \{1, \ldots, N\} \) for which \( \alpha_k \neq 0 (\in \mathbb{N}_0^3) \) (that is, for \( k \in Q_\alpha \), and \( |x_k - x_j| \neq 0 \) for the same \( k \), and all \( j \neq k \).

Next, let
\[
G_\alpha(x) = -\left[ \sum_{j \not\in Q_\alpha} \frac{\zeta}{2} \Delta_x(\sqrt{|x_j|^2 + 1}) - \sum_{j,k \not\in Q_\alpha, j < k} \frac{1}{4} \Delta_x(\sqrt{|x_j - x_k|^2 + 1}) \right] = V(x) - V_\alpha(x) - \Delta_x F_\alpha(x). \tag{2.5}
\]
Since \( |\Delta_x(\sqrt{|x|^2 + 1})| \leq 3 \) for all \( x \in \mathbb{R}^3 \), there exists \( C = C(N, Z) > 0 \) such that
\[
|G_\alpha(x)| \leq C \quad \text{for all } x \in \mathbb{R}^{3N}. \tag{2.6}
\]
Also, \( \partial^3_x G_\alpha \equiv 0 \) for all \( \beta \in \mathbb{N}_0^{3N} \) satisfying \( 0 < \beta \leq \alpha \), by the same argument as above. Therefore, with
\[
K_\alpha(x) := G_\alpha(x) - |\nabla_x F_\alpha(x)|^2, \tag{2.7}
\]
using (2.3) and (2.6), there exists \( C = C(N, Z) > 0 \) such that
\[
|K_\alpha(x)| \leq C \quad \text{for all } x \in \mathbb{R}^{3N}, \tag{2.8}
\]
and
\[
\partial^3_x K_\alpha \equiv 0 \quad \text{for all } \beta \in \mathbb{N}_0^{3N} \quad \text{satisfying } 0 < \beta \leq \alpha. \tag{2.9}
\]
Define
\[
\psi_\alpha := e^{-F_\alpha} \psi, \tag{2.10}
\]
then, using (1.11), \( \psi_\alpha \) satisfies
\[
-\Delta_x \psi_\alpha - 2 \nabla_x F_\alpha \cdot \nabla_x \psi_\alpha + (V_\alpha + K_\alpha - E) \psi_\alpha = 0. 
\] (2.11)

Define rescaled functions by
\[
\psi_\alpha^\lambda(y) := \psi_\alpha(x^0 + \lambda y),
\] (2.12)
\[
V_\alpha^\lambda(y) := \lambda V_\alpha(x^0 + \lambda y),
\] (2.13)
\[
H_\alpha^\lambda(y) := (\nabla_x F_\alpha)(x^0 + \lambda y),
\] (2.14)
\[
K_\alpha^\lambda(y) := K_\alpha(x^0 + \lambda y)
\] (2.15)
for \( y = (y_1, \ldots, y_N) \in \mathbb{B}_{3N}(0, 1), y_i \in \mathbb{R}^3 \). Then, by (2.3) and (2.8),
\[
|K_\alpha^\lambda(y)|, |H_\alpha^\lambda(y)| \leq C = C(N, Z)
\] (2.16)
for all \( y \in \mathbb{B}_{3N}(0, 1) \), and
\[
\partial^\beta_y K_\alpha^\lambda = \partial^\beta_y H_\alpha^\lambda \equiv 0 \text{ for all } \beta \in \mathbb{N}_0^{3N} \text{ satisfying } 0 < \beta \leq \alpha. 
\] (2.17)

We have that \( V_\alpha^\lambda \in C^\infty(\mathbb{B}_{3N}(0, 1)) \), since, as noted above, \( V_\alpha \in C^\infty(\mathbb{B}_{3N}(x^0, \lambda_\alpha)) \). Furthermore, by the chain rule, for all \( \gamma \in \mathbb{N}_0^{3N}, \)
\[
(\partial^\gamma_y V_\alpha^\lambda)(y) = \lambda^{|\gamma|+1} (\partial^\gamma_x V_\alpha)(x^0 + \lambda y). 
\] (2.18)

Note that, for all \( \gamma = (\gamma_1, \ldots, \gamma_N) \in \mathbb{N}_0^{3N}, \gamma_i \in \mathbb{N}_0^3, \)
\[
|\partial^\gamma_x V_\alpha(x)| \leq \sum_{j \in Q_\alpha} \frac{Z \sqrt{2} \gamma_j!}{|x_j|} \left( \frac{8}{|x_j|} \right)^{|\gamma_j|}
\]
\[
+ \sum_{j \in Q_\alpha} \sum_{k=1, k \neq j}^N \frac{\sqrt{2} (\gamma_j! + \gamma_k!)}{|x_j - x_k|} \left( \frac{8}{|x_j - x_k|} \right)^{|\gamma_j|+|\gamma_k|}. 
\] (2.19)
(The exact value of the constant is immaterial; it can be found in [5, Lemma C.3, (C.7)].) By the definition of \( Q_\alpha, \) of \( \Sigma^\alpha = \Sigma^{Q_\alpha}, \) and of \( \lambda_\alpha, \)
we have that
\[
\lambda_\alpha \leq d(x^0, \Sigma^\alpha) \leq \left\{ \begin{array}{ll} |x_j^0| & \text{for all } j \in Q_\alpha, \\
\frac{1}{\sqrt{2}} |x_j^0 - x_k^0| & \text{for all } j \in Q_\alpha, k \neq j. \end{array} \right.
\] (2.20)

Note that \( x^0 + \lambda y = (x_1^0 + \lambda_1 y_1, \ldots, x_N^0 + \lambda_N y_N). \) Now, let \( R \in (0, 1), \)
and \( y \in \mathbb{B}_{3N}(0, R). \) Then \( |y_j|^2 + |y_k|^2 \leq |y|^2 < R^2 \) for all \( j, k \in \{1, \ldots, N\}, \) and so \( |y_j| + |y_k| < \sqrt{2} R. \)

Hence, for all \( y \in \mathbb{B}_{3N}(0, R), R \in (0, 1), \)
\[
|x_j^0 + \lambda y_j| \geq |x_j^0| - \lambda_\alpha |y_j| \geq (1 - R) \lambda_\alpha \quad \text{for all } j \in Q_\alpha,
\]
\[
|y_j| + |y_k| \geq |y_j| + |y_k| \geq \lambda_\alpha (\sqrt{2} - (|y_j| + |y_k|)) \geq \sqrt{2} (1 - R) \lambda_\alpha \quad \text{for all } j \in Q_\alpha, k \neq j. 
\]
Using this, (2.18) and (2.19) imply that for all $\gamma = (\gamma_1, \ldots, \gamma_N) \in \mathbb{N}_0^N$, and all $y \in B_{3N}(0, R)$, $R \in (0, 1)$,

$$
|\left(\partial_y V_\alpha^\lambda(y)\right)(y)| \leq \lambda^{|\gamma|+1} \sqrt{2Z} \left(\frac{8}{1-R}\right)^{|\gamma|} \lambda^{-|\gamma|-1} 
$$

(2.21)

$$
+ \frac{\sqrt{2}}{1-R} \sum_{j \in Q_\alpha} \sum_{k=1, k \neq j}^N \gamma_j! \gamma_k!(4 \sqrt{2})^{|\gamma_j|+|\gamma_k|} \lambda^{-|\gamma_j|-|\gamma_k|-1} 
$$

$$
\leq C_\gamma(R),
$$

with

$$
C_\gamma(R) = C_\gamma(R, N, Z) = \sqrt{2 \frac{8}{1-R}} N \left(\frac{8}{1-R}\right)^{|\gamma|} (Z + 2N - 1). (2.22)
$$

Here we used that $\gamma_j! \leq \gamma!$, $|\gamma| = \sum_{j=1}^N |\gamma_j|$, and that $\lambda \leq 1$.

The estimate (2.21) is the essential property of the potential $V$ for the proof to work. It is also satisfied for the potential $W$ given in (1.27); see Remark 1.7.

It follows from (2.11) that $\psi_\alpha^\lambda$, defined in (2.12), satisfies

$$
(\Delta y \psi_\alpha^\lambda)(y) = \lambda^2 (\Delta_x \psi_\alpha)(x^0 + \lambda y) - 2 \lambda H_\alpha^\lambda(y) \cdot (\nabla y \psi_\alpha^\lambda)(y)
$$

$$
+ \left[\lambda V_\alpha^\lambda(y) + \lambda^2 (K_\alpha^\lambda(y) - E)\right] \psi_\alpha^\lambda(y), \quad (2.23)
$$

that is, with $P = P(y, \partial_y)$ the operator

$$
P = -\Delta_y - 2 \lambda H_\alpha^\lambda(y) \cdot \nabla_y
$$

$$
+ \left[\lambda V_\alpha^\lambda(y) + \lambda^2 (K_\alpha^\lambda(y) - E)\right]
$$

we have

$$
(P \psi_\alpha^\lambda)(y) = 0 \quad \text{in} \ B_{3N}(0, 1). \quad (2.24)
$$

Note that for all $R \in (0, 1)$, by (2.16) and (2.21) (and $\lambda \leq 1$), the coefficients of $P$ are all in $L^\infty(B_{3N}(0, R))$, with norms bounded by some $C = C(R, N, Z, E)$; recall also (2.17) and (2.21).  

Proof of Theorem 1.1 for $p = \infty$ : We will use (2.25) and standard elliptic regularity (in the form of Theorem C.2 in Appendix C below) to prove the following lemma, from which the case $p = \infty$ of Theorem 1.1 follows.

Lemma 2.1. For all $\beta \in \mathbb{N}_0^N$, with $0 < \beta \leq \alpha$, all $\theta \in (0, 1)$, and all $R, r > 0$, $0 < r < R < 1$, there exists $C = C(r, R, \beta, \theta, E, N, Z)$ such
that
\[
\| \partial^\beta_x \psi^{\lambda_\alpha}_x \|_{C^{1,\theta}(B_{3N}(0,r))} \\
\leq C \left( \lambda_\alpha \| \psi^{\lambda_\alpha}_x \|_{L^\infty(B_{3N}(0,R))} + \| \nabla_y (\psi^{\lambda_\alpha}_x) \|_{L^\infty(B_{3N}(0,R))} \right).
\]  

We first prove that Theorem 1.1 follows from Lemma 2.1. In particular, (2.26) holds for $\beta = \alpha$. Note that for all $\gamma \in \mathbb{N}_0^N$,
\[
(\partial^\gamma_y \psi^{\lambda_\alpha}_x)(y) = \lambda_\alpha^{|\gamma|} (\partial^\gamma_y \psi^{\lambda_\alpha}_x)(x^0 + \lambda_\alpha y),
\]  

so for all $y \in B_{3N}(0, r)$, using (2.26),
\[
\| (\partial^\gamma_y \psi^{\lambda_\alpha}_x)(x^0 + \lambda_\alpha y) \| = \lambda_\alpha^{-|\gamma|} \| (\partial^\gamma_y \psi^{\lambda_\alpha}_x)(y) \|
\leq C \lambda_\alpha^{-|\gamma|} \left( \lambda_\alpha \| \psi^{\lambda_\alpha}_x \|_{L^\infty(B_{3N}(0,R))} + \| \nabla_y (\psi^{\lambda_\alpha}_x) \|_{L^\infty(B_{3N}(0,R))} \right)
= C \lambda_\alpha^{-|\gamma| + 1} \left( \| \psi^{\lambda_\alpha}_x \|_{L^\infty(B_{3N}(0, R \lambda_\alpha))} + \| \nabla_y \psi^{\lambda_\alpha}_x \|_{L^\infty(B_{3N}(0, R \lambda_\alpha))} \right).
\]  
The last equality follows from (2.27), used on $\nabla_y (\psi^{\lambda_\alpha}_x)$.

Now (see (2.10)), $\psi = e^{F_\alpha} \psi^{\lambda_\alpha}_x$, with $\partial_x F_\alpha \equiv 0$, and $\| F_\alpha \|_{L^\infty(\mathbb{R}^N)}$, $\| \nabla_x F_\alpha \|_{L^\infty(\mathbb{R}^N)} \leq C(N, Z)$ (see (2.3)). Hence, (2.28) gives that, for all $y \in B_{3N}(0, r)$,
\[
\| (\partial^\alpha_x \psi)(x^0 + \lambda_\alpha y) \| = \| (e^{F_\alpha} \partial^\alpha_x \psi^{\lambda_\alpha}_x)(x^0 + \lambda_\alpha y) \|
\leq C \lambda_\alpha^{-|\alpha| + 1} \left( \| \psi^{\lambda_\alpha}_x \|_{L^\infty(B_{3N}(0, R \lambda_\alpha))} + \| \nabla_x \psi^{\lambda_\alpha}_x \|_{L^\infty(B_{3N}(0, R \lambda_\alpha))} \right)
= C \lambda_\alpha^{-|\alpha|} \left( \| \psi^{\lambda_\alpha}_x \|_{L^\infty(B_{3N}(0, R \lambda_\alpha))} + \| \nabla_x \psi^{\lambda_\alpha}_x \|_{L^\infty(B_{3N}(0, R \lambda_\alpha))} \right).
\]  

Hence, the above proves that for all $\alpha \in \mathbb{N}_0^N$, $|\alpha| \geq 1$, and all $0 < r < R < 1$ there exists $C_\alpha(r, R) = C(\alpha, r, R, N, Z, E)$ such that for all $x^0 = (x_1^0, \ldots, x_N^0) \in \mathbb{R}^N \setminus \Sigma^\alpha$,
\[
\| \partial^\alpha_x \psi \|_{L^\infty(B_{3N}(x^0, r \lambda_\alpha))} \\
\leq C_\alpha(r, R) \lambda_\alpha^{-|\alpha|} \left( \| \psi \|_{L^\infty(B_{3N}(x^0, R \lambda_\alpha))} + \| \nabla \psi \|_{L^\infty(B_{3N}(x^0, R \lambda_\alpha))} \right).
\]  

Recall (see (2.1)) that $\lambda_\alpha = \min \{1, d_\alpha(x^0, \Sigma)\}$. This then proves (1.12), and therefore Theorem 1.1.

It remains to prove Lemma 2.1. This will be done by induction in $|\beta|$.

First, using (2.16), (2.21) (with $\gamma = 0$), and $\lambda_\alpha \leq 1$, it follows from (2.25) and Theorem C.2 in Appendix C below that, for all $0 < r < R < 1$ and all $\theta \in (0, 1)$, we have
\[
\psi^{\lambda_\alpha}_x \in C^{1,\theta}_{\text{loc}}(B_{3N}(0, 1)) \quad \text{for all } \theta \in (0, 1),
\]  

and
\[
\| \psi^{\lambda_\alpha}_x \|_{C^{1,\theta}(B_{3N}(0,r))} \leq C \| \psi^{\lambda_\alpha}_x \|_{L^\infty(B_{3N}(0,R))}
\]  

(2.32)
for some constant $C = C(r, R, \theta, N, Z, E)$.

The induction base:

Let $\beta \in \mathbb{N}^3$, with $0 < \beta \leq \alpha$ and $|\beta| = 1$. Define $\varphi_{\alpha,\beta} = \lambda_\alpha^{-1} \partial_\beta \psi_\alpha$. Differentiating the equation (2.25) for $\psi_\alpha$, then multiplying with $\lambda_\alpha^{-1}$, we get that

\[
(P \varphi_{\alpha,\beta})(y) = g_{\alpha,\beta}^\lambda(y),
\]

\[
g_{\alpha,\beta}^\lambda(y) = -\left(\partial_\beta^2 V_\alpha(y)\right) \psi_\alpha(y).
\]

Here we also used (2.17).

From (2.21) (with $\gamma = \beta$) and (2.31) it follows that, for all $R \in (0, 1)$, $g_{\alpha,\beta}^\lambda \in L^\infty(B_{3N}(0, R))$, and that

\[
\|g_{\alpha,\beta}^\lambda\|_{L^\infty(B_{3N}(0, R))} \leq C_\beta \|\psi_\alpha\|_{L^\infty(B_{3N}(0, R))}.
\]

It therefore follows from Theorem C.2 that $\varphi_{\alpha,\beta}^\lambda \in C^{1,\theta}_{\text{loc}}(B_{3N}(0, 1))$ for all $\theta \in (0, 1)$, and that, for all $0 < r < R < 1$,

\[
\|\varphi_{\alpha,\beta}^\lambda\|_{C^{1,\theta}(B_{3N}(0, r))} \leq C\left(\|g_{\alpha,\beta}^\lambda\|_{L^\infty(B_{3N}(0, R))} + \|\varphi_{\alpha,\beta}^\lambda\|_{L^\infty(B_{3N}(0, R))}\right)
\]

\[
\leq C\left(\|\psi_\alpha\|_{L^\infty(B_{3N}(0, R))} + \|\varphi_{\alpha,\beta}^\lambda\|_{L^\infty(B_{3N}(0, R))}\right),
\]

for some constant $C = C(r, R, \theta, \beta, E, N, Z)$.

It follows from (2.36) and the fact that $\varphi_{\alpha,\beta}^\lambda = \lambda_\alpha^{-1} \partial_\beta \psi_\alpha$, $|\beta| = 1$, that, for all $0 < r < R < 1$, all $\theta \in (0, 1)$, and all $\beta \in \mathbb{N}^3$ with $0 < \beta \leq \alpha$, $|\beta| = 1$,

\[
\|\partial_\beta^2 \psi_\alpha\|_{C^{1,\theta}(B_{3N}(0, r))} \leq C\left(\lambda_\alpha \|\psi_\alpha\|_{L^\infty(B_{3N}(0, R))} + \|\nabla \psi_\alpha\|_{L^\infty(B_{3N}(0, R))}\right),
\]

for some $C = C(r, R, \theta, \beta, E, N, Z)$. This is (2.26).

The induction step:

Let now $j \in \mathbb{N}$, $1 \leq j \leq |\alpha|$, and assume (2.26) holds for all $\beta \in \mathbb{N}^3$, with $0 < \beta \leq \alpha$ and $|\beta| \leq j$, all $\theta \in (0, 1)$, and all $0 < r < R < 1$, with a constant $C = C(r, R, \theta, E, N, Z)$.

Let $\beta \leq \alpha$, with $|\beta| = j + 1$, and let (as before) $\varphi_{\alpha,\beta}^\lambda := \lambda_\alpha^{-1} \partial_\beta \psi_\alpha$. Differentiating the equation (2.25), then multiplying with $\lambda_\alpha^{-1}$, we get that

\[
P(\varphi_{\alpha,\beta}^\lambda)(y) = g_{\alpha,\beta}^\lambda,
\]

\[
g_{\alpha,\beta}^\lambda(y) = -\sum_{\gamma \leq \beta, |\gamma| \geq 1} \binom{\beta}{\gamma} \left[(\partial_\gamma V_\alpha(y)) \psi_\alpha(y)\right] (\partial_\gamma \psi_\alpha(y)).
\]

Again, we also used (2.17).
From (2.21) and the induction hypothesis (that is, (2.26) for \( \beta - \gamma \leq \alpha \) with \(|\beta - \gamma| \leq |\beta| - 1 = j\)) it follows that \( g_{\alpha,\beta}^{\lambda_0} \in L^\infty(B_{3N}(0,\tilde{r})) \) for all \( \tilde{r} \in (0,1) \), and that, for all \( 0 < r < R < 1 \),
\[
\|g_{\alpha,\beta}^{\lambda_0}\|_{L^\infty(B_{3N}(0,(r+R)/2))} \leq \sum_{\gamma \leq \beta,|\gamma| \geq 1} C_{\gamma,\beta} \|\partial^\gamma_y \psi_{\alpha}^{\lambda_0}\|_{L^\infty(B_{3N}(0,R))} \tag{2.39}
\]
\[
\leq C_\beta (\lambda_\alpha \|\psi_{\alpha}^{\lambda_0}\|_{L^\infty(B_{3N}(0,R))} + \|\nabla_y (\psi_{\alpha}^{\lambda_0})\|_{L^\infty(B_{3N}(0,R))}) .
\]

It therefore follows from Theorem C.2 (applied to (2.38)) that \( \varphi_{\alpha,\beta}^{\lambda_0} \in C^{1,\theta}_{loc}(B_{3N}(0,1)) \) for all \( \theta \in (0,1) \), and that, for all \( 0 < r < R < 1 \),
\[
\|\varphi_{\alpha,\beta}^{\lambda_0}\|_{C^{1,\theta}(B_{3N}(0,r))} \leq C (\|g_{\alpha,\beta}^{\lambda_0}\|_{L^\infty(B_{3N}(0,(r+R)/2))} + \|\varphi_{\alpha,\beta}^{\lambda_0}\|_{L^\infty(B_{3N}(0,(r+R)/2))})
\]
\[
\leq C (\|\varphi_{\alpha}^{\lambda_0}\|_{L^\infty(B_{3N}(0,R))} + \|\nabla_y (\psi_{\alpha}^{\lambda_0})\|_{L^\infty(B_{3N}(0,R))}) + \|\varphi_{\alpha,\beta}^{\lambda_0}\|_{L^\infty(B_{3N}(0,(r+R)/2))} ,
\]
for some constant \( C = C(r, R, \beta, \theta, E, N, Z) \).

Now write \( \beta = \beta_j + e_j \), \( |e_j| = 1 \), \( |\beta_j| = j \) (so \( \beta_j \leq \alpha \), \( |\beta_j| = j \)), and the definition of the \( C^{1,\theta} \)-norm,
\[
\|\varphi_{\alpha,\beta}^{\lambda_0}\|_{L^\infty(B_{3N}(0,(r+R)/2))} = \|\partial^\beta_y \varphi_{\alpha,\beta}^{\lambda_0}\|_{L^\infty(B_{3N}(0,(r+R)/2))} \leq \|\varphi_{\alpha,\beta}^{\lambda_0}\|_{C^{1,\theta}(B_{3N}(0,(r+R)/2))}
\]
\[
= \lambda_\alpha^{-1} \|\partial^\beta_y \psi_{\alpha}^{\lambda_0}\|_{C^{1,\theta}(B_{3N}(0,(r+R)/2))}
\]
\[
\leq C (\|\psi_{\alpha}^{\lambda_0}\|_{L^\infty(B_{3N}(0,R))} + \lambda_\alpha^{-1} \|\nabla_y (\psi_{\alpha}^{\lambda_0})\|_{L^\infty(B_{3N}(0,R))}) .
\]

It follows from (2.36), (2.41), and the fact that \( \varphi_{\alpha,\beta}^{\lambda_0} = \lambda_\alpha^{-1} \partial_y^\beta \psi_{\alpha}^{\lambda_0} \) that, for all \( 0 < r < R < 1 \),
\[
\|\partial^\beta_y \psi_{\alpha}^{\lambda_0}\|_{C^{1,\theta}(B_{3N}(0,r))} = \lambda_\alpha \|\varphi_{\alpha,\beta}^{\lambda_0}\|_{C^{1,\theta}(B_{3N}(0,r))} \tag{2.42}
\]
\[
\leq C \lambda_\alpha \{ \lambda_\alpha \|\psi_{\alpha}^{\lambda_0}\|_{L^\infty(B_{3N}(0,R))} + \|\nabla_y (\psi_{\alpha}^{\lambda_0})\|_{L^\infty(B_{3N}(0,R))} + \|\lambda_\alpha^{-1} \|\nabla_y (\psi_{\alpha}^{\lambda_0})\|_{L^\infty(B_{3N}(0,R))} \} .
\]

Using that \( \lambda_\alpha \leq 1 \), this proves that (2.26) holds for all \( \beta \in \mathbb{N}_0^3 \), with \( 0 < \beta \leq \alpha \) and \( |\beta| = j + 1 \), all \( \theta \in (0,1) \), and all \( R, r > 0 \), \( 0 < r < R < 1 \), and some constant \( C = C(r, R, \beta, \theta, N, Z, E) \). The lemma now follows by induction over \( j \).

This finishes the proof of Theorem 1.1 in the case \( p = \infty \). \( \square \)

**Proof of Theorem 1.1 for \( p \in (1, \infty) \):** Again, (2.25) and standard elliptic regularity (this time in the form of Theorem C.3 in Appendix C below) give the following lemma, from which the case \( p \in (1, \infty) \) of
Theorem 1.1 follows. This lemma is the substitute for Lemma 2.1 in the case \( p \in (1, \infty) \).

**Lemma 2.2.** For all \( p \in (1, \infty) \), all \( \beta \in \mathbb{N}_0^{3N} \), with \( 0 < \beta \leq \alpha \), and all \( R, r > 0 \), \( 0 < r < R < 1 \), there exists \( C = C(p, R, \beta, E, N, Z) \) such that

\[
\| \partial_{\alpha}^{\beta} \psi_{\alpha}^{\lambda_{\alpha}} \|_{W^{2,p}(B_{3N}(0, r))} \leq C\lambda_{\alpha} \| \psi_{\alpha}^{\lambda_{\alpha}} \|_{L^p(B_{3N}(0, R))} + \| \nabla_y (\psi_{\alpha}^{\lambda_{\alpha}}) \|_{L^p(B_{3N}(0, R))}.
\]

The proof of Lemma 2.2 follows that of Lemma 2.1 verbatim, except for substituting ‘Theorem C.3’ for ‘Theorem C.2’, ‘\( W^{2,p}_{loc} \)’ for ‘\( C^{1,\theta}_{loc} \)’, ‘\( W^{2,p}(B_{3N}(0, \cdot)) \)’ for ‘\( C^{1,\theta}(B_{3N}(0, \cdot)) \)’ (and leaving out \( \theta \) everywhere), and ‘\( L^p(B_{3N}(0, \cdot)) \)’ for ‘\( L^\infty(B_{3N}(0, \cdot)) \)’.

Similarly, the proof that Theorem 1.1 follows from Lemma 2.2 in the case \( p \in (1, \infty) \) mimics the one that Theorem 1.1 for \( p = \infty \) follows from Lemma 2.1 (substituting ‘\( L^p \)’ for ‘\( L^\infty \)’), and is left to the reader.

\[\square\]

3. **Proof of Corollaries 1.2 and 1.3**

**Proof of Corollary 1.2.** The inequality (1.15) follows from (1.14) by using (1.10), and that \( \Sigma \supseteq \Sigma^\alpha \).

It is obviously enough to prove (1.14) for all \( R \in (0, 1) \). Use that \( x \in B_{3N}(x, t) \) for all \( t > 0 \), the bound (1.12) (with \( R/4 \) and \( R/2 \) for \( R \in (0, 1) \)), that \( \lambda_{\alpha} \leq 1 \), and the *a priori* estimate for \( \nabla \psi \) in Theorem A.1 in Appendix A below (with \( R/2 \) and \( R \)), to get the inequalities

\[
|\partial^{\alpha} \psi(x)| \leq \| \partial^{\alpha} \psi \|_{L^\infty(B_{3N}(x, R\lambda_{\alpha}(x)/4))}
\leq C\lambda_{\alpha}(x)^{1-|\alpha|}\left(\| \psi \|_{L^\infty(B_{3N}(x, R/2))} + \| \nabla \psi \|_{L^\infty(B_{3N}(x, R/2))}\right)
\leq C\lambda_{\alpha}(x)^{1-|\alpha|}\| \psi \|_{L^\infty(B_{3N}(x, R))}.
\]

\[\square\]

**Proof of Corollary 1.3.** Note first that (1.18) follows from (1.17) (in the same way that (1.15) followed from (1.14) in the proof of Corollary 1.2).

To prove (1.17) note first that (1.16) implies that

\[
\| \psi \|_{L^\infty(B_{3N}(x, 1/2))} \leq C_0 e^{c_0/2} e^{-c_0|x|} \quad \text{for all } x \in \mathbb{R}^{3N}.
\]

Therefore (1.17) follows from (1.14) when \( d_\alpha(x, \Sigma) \leq 1 \). Secondly note that (since \( d_\alpha(x, \Sigma) \leq |x| \), see (1.10)) we have that

\[
d_\alpha(x, \Sigma)^{|\alpha|-1} e^{-c_0|x|/2} \leq |x|^{\alpha-1} e^{-c_0|x|/2},
\]

Therefore (1.17) follows from (1.14) when \( d_\alpha(x, \Sigma) \leq 1 \). Secondly note that (since \( d_\alpha(x, \Sigma) \leq |x| \), see (1.10)) we have that

\[
d_\alpha(x, \Sigma)^{|\alpha|-1} e^{-c_0|x|/2} \leq |x|^{\alpha-1} e^{-c_0|x|/2},
\]
and the right side is uniformly bounded for \( x \in \mathbb{R}^{3N} \). This proves that (1.17) also follows from (1.14) when \( d_\alpha(x, \Sigma) \geq 1 \). (Note that this also shows that we can take \( c_\alpha \) as close to \( c_0 \) as we like, at the expense of increasing \( C_\alpha \). Similarly for \( \tilde{C}_\alpha, \tilde{c}_\alpha \).) This finishes the proof of (1.17).

To prove (1.19) note that (see (1.10)), for all \( x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \),

\[
d_\alpha(x, \Sigma) = |x_j| \quad \text{for some} \ j \in \{1, \ldots, N\}
\]

or

\[
d_\alpha(x, \Sigma) = \frac{1}{\sqrt{2}} |x_j - x_k| \quad \text{for some} \ j, k \in \{1, \ldots, N\}.
\]

Hence, for all \( x \in \mathbb{R}^{3N} \) and all \( s \in \mathbb{R} \),

\[
d_\alpha(x, \Sigma)^s \leq \sum_{j=1}^N |x_j|^s + \sum_{1 \leq j < k \leq N} \left( \frac{1}{\sqrt{2}} |x_j - x_k| \right)^s.
\]

We use the notation of (1.29) and (1.30) and, for \( j, k \in \{1, \ldots, N\} \), define the orthogonal transformation \((y_j, y_k) = (x_j - x_k, x_j + x_k) / \sqrt{2}\). We denote the new coordinates in \( \mathbb{R}^{3N} \) by \( y \). Then it follows from (1.17) and (3.5) that, for \( |\alpha| \geq 1 \),

\[
\int_{\mathbb{R}^{3N} \setminus \Sigma^\alpha} \left| d_\alpha(x, \Sigma)^{|\alpha| - a} \partial^\alpha \psi(x) \right|^2 dx \leq C_\alpha \sum_{j=1}^N \left( \int_{\mathbb{R}^3} |x_j|^{2-2a} e^{-2c_\alpha|x_j|} dx_j \right) \left( \int_{\mathbb{R}^{3N-3}} e^{-2c_\alpha|\hat{x}_j|} d\hat{x}_j \right)
\]

\[
+ C_\alpha \sum_{1 \leq j < k \leq N} \left( \int_{\mathbb{R}^3} |y_j|^{2-2a} e^{-2c_\alpha|y_j|} dy_j \right) \left( \int_{\mathbb{R}^{3N-3}} e^{-2c_\alpha|\hat{y}_j|} d\hat{y}_j \right).
\]

Now note that the right side is finite for all \( a < 5/2 \). This finishes the proof of (1.19).

The same argument works for \( d(x, \Sigma) \) (use (1.18) instead of (1.17)).

\[\square\]

### 4. Proof of Theorem 1.5

**Proof.** Note that, with \( \lambda_\alpha(x) = \min\{1, d(x, \Sigma^\alpha)\} \), we have, for all \( x, y \in \mathbb{R}^{3N} \) and \( \epsilon \in (0, 1) \),

\[
|x - y| \leq \epsilon \lambda_\alpha(x) \Rightarrow (1 - \epsilon) \lambda_\alpha(x) \leq \lambda_\alpha(y) \leq (1 + \epsilon) \lambda_\alpha(x).
\]

This follows from

\[
|d(x, \Sigma^\alpha) - d(y, \Sigma^\alpha)| \leq |x - y|.
\]
Also, for all \(z \in \mathbb{R}^{3N}\), \(b > 0\),

\[
1 = C_N(b) \lambda_\alpha(z)^{-3N} \int_{\mathbb{R}^{3N}} \mathbf{1}_{[|z-u| \leq b \lambda_\alpha(z)]}(u) \, du ,
\]

with \(C_N(b) = b^{3N} \text{Vol}(B_{3N}(0,1))\). Note that, as a consequence of (4.1), for all \(z, u \in \mathbb{R}^{3N}\), all \(k \in \mathbb{R}\), and all \(\epsilon \in (0, 1)\),

\[
\lambda^k_\alpha(z) \mathbf{1}_{[|z-u| \leq \epsilon \lambda_\alpha(z)]}(u) \leq C(k, \epsilon) \lambda^k_\alpha(u) \mathbf{1}_{[|u-z| \leq \frac{\epsilon}{1-\epsilon} \lambda_\alpha(u)]}(z) .
\]

(4.4)

In the following we suppress that constants depend on \(N, \alpha\), and \(a\). Also, \(C\) might change from line to line.

Using (4.3), then (4.4) (both with \((z, u) = (x, y)\), and with \(b = \epsilon = 1/4\)), we get that

\[
\int_{\mathbb{R}^{3N} \setminus \Sigma^\alpha} \left| (\lambda_\alpha^{\alpha-a} \partial^\alpha \psi)(x) \right|^2 \, dx
\]

\[
= C \int_{\mathbb{R}^{3N} \setminus \Sigma^\alpha} \int_{\mathbb{R}^{3N}} \lambda_\alpha(y)^{-3N} \mathbf{1}_{[|y-x| \leq \lambda_\alpha(y)/4]}(y) \lambda_\alpha(x)^{2\alpha-2a} \left| \partial^\alpha \psi(x) \right|^2 \, dy \, dx
\]

\[
\leq C \int_{\mathbb{R}^{3N}} \int_{\mathbb{R}^{3N} \setminus \Sigma^\alpha} \lambda_\alpha(y)^{-3N} \mathbf{1}_{[|y-x| \leq \lambda_\alpha(y)/3]}(x) \lambda_\alpha(y)^{2\alpha-2a} \left| \partial^\alpha \psi(x) \right|^2 \, dx \, dy
\]

\[
= C \int_{\mathbb{R}^{3N}} \lambda_\alpha(y)^{-3N} \lambda_\alpha(y)^{2\alpha-2a} \left( \int_{\mathbb{R}^{3N} \setminus \Sigma^\alpha} \left| \partial^\alpha \psi(x) \right|^2 \, dx \right) \, dy
\]

\[
= C \int_{\mathbb{R}^{3N}} \lambda_\alpha(y)^{-3N} \lambda_\alpha(y)^{2\alpha-2a} \left\| \partial^\alpha \psi \right\|^2_{L^2(B_{3N}(y, \lambda_\alpha(y)/3))} \, dy .
\]

(4.5)

We also used that \(B_{3N}(y, \lambda_\alpha(y)/3) \setminus \Sigma^\alpha = B_{3N}(y, \lambda_\alpha(y)/3)\).

We now use the a priori estimate (1.12) in Theorem 1.1 (with \(p = 2\) and \(r = 1/3, R = 2/3\)), then (4.4) (this time with \((z, u) = (y, x)\) and \(\epsilon = 2/3\)), and finally (4.3) (again with \((z, u) = (x, y)\), but with \(b = 2\),
to get that
\[
\int_{\mathbb{R}^3N \setminus \Sigma^\alpha} \left| \left( \lambda^{[\alpha]} - a \partial^\alpha \psi \right)(x) \right|^2 \, dx \\
\leq C \int_{\mathbb{R}^3N} \lambda_\alpha(y)^{-3N} \lambda_\alpha(y)^{2-2a} \left\{ \|\psi\|^2_{L^2(B_{3N}(y,2\lambda_\alpha(y)/3))} + \|\nabla \psi\|^2_{L^2(B_{3N}(y,2\lambda_\alpha(y)/3))} \right\} \, dy \\
= C \int_{\mathbb{R}^3N} \lambda_\alpha(y)^{-3N} \lambda_\alpha(y)^{2-2a} \times \\
\times \left( \int_{\mathbb{R}^3N} 1_{\{|y-x|\leq 2\lambda_\alpha(y)/3\}}(x) \left( |\psi(x)|^2 + |\nabla \psi(x)|^2 \right) \, dx \right) \, dy \\
\leq C \int_{\mathbb{R}^3N} \lambda_\alpha(x)^{2-2a} \left( |\psi(x)|^2 + |\nabla \psi(x)|^2 \right) \times \\
\times \left( \int_{\mathbb{R}^3N} \lambda_\alpha(x)^{-3N} 1_{\{|x-y|\leq 2\lambda_\alpha(x)\}}(y) \, dy \right) \, dx \\
= C \int_{\mathbb{R}^3N} \lambda_\alpha^{2-2a}(x)(|\psi(x)|^2 + |\nabla \psi(x)|^2) \, dx \quad (4.6)
\]

Recall that \( \lambda_\alpha(x) \leq 1 \) for all \( x \in \mathbb{R}^3N \). Hence, if \( a \leq 1 \), it follows that

\[
\int_{\mathbb{R}^3N \setminus \Sigma^\alpha} \left| \left( \lambda^{[\alpha]} - a \partial^\alpha \psi \right)(x) \right|^2 \, dx \leq C \int_{\mathbb{R}^3N} \left( |\psi(x)|^2 + |\nabla \psi(x)|^2 \right) \, dx \\
= C\|\psi\|^2_{W^{-1,2}(\mathbb{R}^3N)} \leq C\|\psi\|^2_{W^{2,2}(\mathbb{R}^3N)} < \infty \quad (4.7)
\]
since \( \psi \in W^{2,2}(\mathbb{R}^3N) \), which proves (1.21) in this case.

If, on the other hand, \( a \in (1,5/2) \), we have that

\[
\int_{\mathbb{R}^3N \setminus \Sigma^\alpha} \left| \left( \lambda^{[\alpha]} - a \partial^\alpha \psi \right)(x) \right|^2 \, dx \quad (4.8)
\]

\[
\leq C \int_{\{d(x,\Sigma^\alpha) \leq 1\}} \lambda_\alpha^{2-2a}(x)(|\psi(x)|^2 + |\nabla \psi(x)|^2) \, dx \\
+ C \int_{\{d(x,\Sigma^\alpha) > 1\}} \lambda_\alpha^{2-2a}(x)(|\psi(x)|^2 + |\nabla \psi(x)|^2) \, dx \\
\leq C \int_{\{d(x,\Sigma^\alpha) \leq 1\}} d(x,\Sigma^\alpha)^{2-2a}(|\psi(x)|^2 + |\nabla \psi(x)|^2) \, dx + C\|\psi\|^2_{W^{2,2}(\mathbb{R}^3N)} ,
\]

by the same argument as above. It therefore remains to estimate the first term on the right side of (4.8). (At this point, compare with (3.6).)
Using (3.3), (3.4), and (3.5) we get that

\[
\int_{\{d(x, \Sigma^a) \leq 1\}} \left[ d(x, \Sigma^a)^{2-2a} \left( |\psi(x)|^2 + |\nabla \psi(x)|^2 \right) \right] dx \leq \sum_{j=1}^{N} \int_{\{|x_j| \leq 1\}} |x_j|^{2-2a} \left( |\psi(x)|^2 + |\nabla \psi(x)|^2 \right) dx
\]

\[
+ \sum_{1 \leq j < k \leq N} \int_{\{|x_j - x_k| \leq 1\}} \left( \frac{1}{\sqrt{2}} |x_j - x_k| \right)^{2-2a} \left( |\psi(x)|^2 + |\nabla \psi(x)|^2 \right) dx.
\]

It remains to show that each summand on the right side in (4.9) is finite for any \( a < \frac{5}{2} \). All summands will be treated in the same manner, so we just consider one of each of them.

For fixed \( \hat{x}_1 \in \mathbb{R}^{3N-3} \) we can estimate, since \( a < \frac{5}{2} \),

\[
\int_{\{|x_1| \leq 1\}} |x_1|^{2-2a} \left( |\psi(x_1, \hat{x}_1)|^2 + |\nabla \psi(x_1, \hat{x}_1)|^2 \right) dx_1
\]

\[
\leq \left\{ \|\psi\|_{L^\infty(B_{3N}((0,\hat{x}_1),2))}^2 + \|\nabla \psi\|_{L^\infty(B_{3N}((0,\hat{x}_1),2))}^2 \right\} \int_{\{|x_1| \leq 1\}} |x_1|^{2-2a} dx_1
\]

\[
\leq C(a)\|\psi\|_{L^2(B_{3N}((0,\hat{x}_1),4))}^2,
\]

where we used the \textit{a priori} estimate of Proposition A.2 below and the finiteness of the integral to get the last inequality.

Therefore we get

\[
\int_{\{|x_1| \leq 1\}} |x_1|^{2-2a} \left( |\psi(x)|^2 + |\nabla \psi(x)|^2 \right) dx
\]

\[
\leq C \int_{\mathbb{R}^{3N-3}} \left( \int_{\mathbb{R}^{3N}} |\psi(y)|^2 I_{\{|y-(0,\hat{x}_1)| \leq 4\}} dy \right) d\hat{x}_1
\]

\[
\leq C \int_{\mathbb{R}^{3N}} |\psi(y)|^2 \left( \int_{\mathbb{R}^{3N-3}} I_{\{|y_1-\hat{x}_1| \leq 4\}} d\hat{x}_1 \right) dy
\]

\[
= C \|\psi\|_{L^2(\mathbb{R}^{3N})}^2 < \infty.
\]

The last inequality follows since the inner integral is independent of \( y \).

Similarly, for fixed \( \hat{x}_{1,2} \in \mathbb{R}^{3N-6} \) (with \( x = (x_1, x_2, \hat{x}_{1,2}) \)), make the orthogonal transformation \( (y_1, y_2) = (x_1 - x_2, x_1 + x_2)/\sqrt{2} \) (see the
argument leading to (3.6)). Then we can estimate, since $a < \frac{5}{2}$,
\[
\int_{\{ |x_1 - x_2| \leq 1 \}} \left( \frac{1}{2} |x_1 - x_2| \right)^{2-2a} \left( |\psi(x)|^2 + |\nabla \psi(x)|^2 \right) dx_1 \, dx_2
\]
\[
= \int_{\mathbb{R}^3} \int_{\{ |y_1| \leq 1 \}} |y_1|^{2-2a} \left\{ |\psi\left( \frac{y_1 + y_2}{\sqrt{2}}, \frac{y_2 - y_1}{\sqrt{2}}, \tilde{x}_{1,2} \right)|^2 
+ |\nabla \psi\left( \frac{y_1 + y_2}{\sqrt{2}}, \frac{y_2 - y_1}{\sqrt{2}}, \tilde{x}_{1,2} \right)|^2 \right\} dy_1 \, dy_2
\]
\[
\leq \int_{\mathbb{R}^3} \left( \int_{\{ |y_1| \leq 1 \}} |y_1|^{2-2a} \, dy_1 \right) \left\{ \| \psi \|^2_{L^\infty(B_{3N}(\frac{y_2}{\sqrt{2}}, \frac{y_2}{\sqrt{2}}, \tilde{x}_{1,2}), 2))} 
+ \| \nabla \psi \|^2_{L^\infty(B_{3N}(\frac{y_2}{\sqrt{2}}, \frac{y_2}{\sqrt{2}}, \tilde{x}_{1,2}), 2))} \right\} dy_2
\]
\[
\leq C(a) \int_{\mathbb{R}^3} \| \psi \|^2_{L^2(B_{3N}(\frac{y_2}{\sqrt{2}}, \frac{y_2}{\sqrt{2}}, \tilde{x}_{1,2}), 4))} \, dy_2, \quad (4.12)
\]
where we again used the \textit{a priori} estimate of Proposition A.2 and the finiteness of the inner integral to get the last inequality.

Hence,
\[
\int_{\{ |x_1 - x_2| \leq 1 \}} \left( \frac{1}{2} |x_1 - x_2| \right)^{2-2a} \left( |\psi(x)|^2 + |\nabla \psi(x)|^2 \right) dx_1 \, dx_2 \, d\tilde{x}_{1,2}
\]
\[
\leq C \int_{\mathbb{R}^{3N}} |\psi(z)|^2 \left( \int_{\mathbb{R}^{3N-3}} \mathbf{1}_{\{ |x_2 - (\frac{y_2}{\sqrt{2}}, \frac{y_2}{\sqrt{2}}, \tilde{x}_{1,2})| \leq 4 \}} dy_2 \, d\tilde{x}_{1,2} \right) \, dz
\]
\[
\leq C \int_{\mathbb{R}^{3N}} |\psi(z)|^2 \left( \int_{\mathbb{R}^{3N-3}} \mathbf{1}_{\{ |(x_1, \tilde{x}_{1,2}) - (\frac{y_2}{\sqrt{2}}, \tilde{x}_{1,2})| \leq 4 \}} dy_2 \, d\tilde{x}_{1,2} \right) \, dz
\]
\[
= C \| \psi \|^2_{L^2(\mathbb{R}^{3N})} < \infty, \quad (4.13)
\]
where, again, the last inequality follows since the inner integral is independent of $z$.

This finishes the proof of (1.21) (for $\lambda_0$). The proof of (1.22) (for $\lambda$) is completely analogous (replace $\lambda_0$ by $\lambda$, and use (1.13) from Theorem 1.1 instead of (1.12), in the argument above).

This finishes the proof of Theorem 1.5. \hfill \Box

5. Proof of Proposition 1.10

Assume, without restriction, that $Q = \{1, \ldots, M\} \subseteq \{1, \ldots, N\}$, $M \leq N$. Fix $x^0 = (x^0_1, \ldots, x^0_N) \in \mathbb{R}^{3N} \setminus \Sigma_Q$ and
\[
\lambda_Q := \min\{1, d_Q(x^0, \Sigma)\} = \min\{1, d(x^0, \Sigma_Q)\}. \quad (5.1)
\]
For $\Sigma_Q$ and $d(x^0, \Sigma_Q)$, see (1.43)–(1.44). Recall that (in general) $\Sigma_Q \neq \Sigma^Q$. We proceed similarly to the proof of Theorem 1.1 but will exploit the structure of $\Sigma_Q$. 
Define, for \( x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \),

\[
F_Q(x) = \sum_{j \not\in Q} \left( -\frac{Z}{2}|x_j| + \frac{Z}{2}\sqrt{|x_j|^2 + 1} \right)
+ \sum_{j,k \not\in Q, j < k} \left( \frac{1}{4}|x_j - x_k| - \frac{1}{4}\sqrt{|x_j - x_k|^2 + 1} \right)
+ \sum_{j,k \in Q, j < k} \left( \frac{1}{4}|x_j - x_k| - \frac{1}{4}\sqrt{|x_j - x_k|^2 + 1} \right).
\]

(5.2)

Note that there exists \( C = C(N, Z) > 0 \) such that

\[
|F_Q(x)|, |\nabla_x F_Q(x)| \leq C \quad \text{for all} \quad x \in \mathbb{R}^{3N} \setminus \Sigma,
\]
and that \( \partial^\beta_{x_Q} F_Q \equiv 0 \) for all \( \beta \in \mathbb{N}_0^3, \beta \neq 0 \), by the definition of \( x_Q \) and \( \partial^\beta_{x_Q} \) (see (1.38)–(1.40)), since, such \( \beta \), and all \( i,j \),

\[
\partial^\beta_{x_i+x_j} |x_i - x_j| = 0;
\]

(5.4)

see also (1.42). Let

\[
V_Q(x) = \sum_{j \in Q} \frac{Z}{|x_j|} + \sum_{j \in Q} \sum_{k \not\in Q} \frac{1}{|x_j - x_k|}.
\]

(5.5)

Note that \( V_Q \in C^\infty(B_{3N}(x^0, \lambda_Q)) \), since \( x^0 \in \mathbb{R}^{3N} \setminus \Sigma_Q \), and \( \lambda_Q \leq d(x^0, \Sigma_Q) \) by (5.1).

Define

\[
\psi_Q := e^{-F_Q \psi}.
\]

(5.6)

Then, using \( H\psi = E\psi \), we get that \( \psi_Q \) satisfies the equation

\[
-\Delta \psi_Q - 2\nabla F_Q \cdot \nabla \psi_Q + (V_Q + K_Q - E)\psi_Q = 0,
\]

(5.7)

where

\[
K_Q = -|\nabla F_Q|^2 - \Delta \left\{ \sum_{j \not\in Q} \frac{Z}{2}\sqrt{|x_j|^2 + 1} - \sum_{j,k \not\in Q, j < k} \frac{1}{4}\sqrt{|x_j - x_k|^2 + 1} \right. \
- \left. \sum_{j,k \in Q, j < k} \frac{1}{4}\sqrt{|x_j - x_k|^2 + 1} \right\}.
\]

(5.8)

Notice that \( K_Q \) is bounded on \( \mathbb{R}^{3N} \setminus \Sigma \), and that \( \partial^\beta_{x_Q} K_Q \equiv 0 \) for all \( \beta \in \mathbb{N}_0^3, \beta \neq 0 \), just as above for \( F_Q \).
Define rescaled functions by
\[
\psi_Q^{\lambda}(y) := \psi_Q(x^0 + \lambda Q y),
\]
\[
V_Q^{\lambda}(y) := \lambda Q V_Q(x^0 + \lambda Q y),
\]
\[
H_Q^{\lambda}(y) := (\nabla_x F_Q)(x^0 + \lambda Q y),
\]
\[
K_Q^{\lambda}(y) := K_Q(x^0 + \lambda Q y)
\]
for \(y = (y_1, \ldots, y_N) \in B_{3N}(0,1), y_i \in \mathbb{R}^3\). Then, since \(K_Q\) and \(\nabla F_Q\) are bounded on \(\mathbb{R}^{3N} \setminus \Sigma\),
\[
|K_Q^{\lambda}(y)|, |H_Q^{\lambda}(y)| \leq C,
\]
for all \(y \in B_{3N}(0,1)\), and
\[
\partial_{y_Q}^{\beta}K_Q^{\lambda} = \partial_{y_Q}^{\beta}H_Q^{\lambda} \equiv 0 \text{ for all } \beta \in \mathbb{N}_0^3, \beta \neq 0.
\]
Here, \(y_Q\) and \(\partial_{y_Q}^{\beta}\) are defined as for \(x_Q\). Also, \(V_Q^{\lambda} \in C^\infty(B_{3N}(0,1))\), and, by estimates and arguments as in (2.18)–(2.21),
\[
|\partial_{y}^{\gamma}V_Q^{\lambda}(y)| = |\lambda|^{\gamma+1}(\partial_{x}V_Q)(x^0 + \lambda Q y)| \leq C_\gamma(R),
\]
for all \(R < 1, y \in B_{3N}(0,R)\).

It follows that, in \(B_{3N}(0,1)\),
\[
\left\{-\Delta_y - 2\lambda Q H_Q^{\lambda}(y) \cdot \nabla_y + \left[\lambda Q V_Q^{\lambda}(y) + \lambda^2 Q (K_Q^{\lambda}(y) - E)\right]\right\}\psi_Q^{\lambda} = 0.
\]

Compare with (2.24)–(2.25).

The proof of Proposition 1.10 follows by successive differentiation with respect to \(y_Q\) of the equation (5.16) for \(\psi_Q^{\lambda}\), and from applying elliptic regularity to the resulting equations. We state the relevant results for \(p = \infty\) and \(p < \infty\) as Lemmas 5.1 and 5.2 below. One can compare with Lemmas 2.1 and 2.2.

Lemma 5.1. For all \(\beta \in \mathbb{N}_0^3\), with \(\beta \neq 0\), all \(\theta \in (0,1)\), and all \(R, r > 0, 0 < r < R < 1\), there exists \(C = C(r, R, \beta, \theta, E, N, Z)\) such that
\[
\left\|\partial_{y_Q}^{\beta}\psi_Q^{\lambda}\right\|_{C^{1,\theta}(B_{3N}(0,r))} \leq C\left(\lambda Q \left\|\psi_Q^{\lambda}\right\|_{L^\infty(B_{3N}(0,R))} + \left\|\nabla_y (\psi_Q^{\lambda})\right\|_{L^\infty(B_{3N}(0,R))}\right).
\]

Lemma 5.2. For all \(p \in (1, \infty)\), all \(\beta \in \mathbb{N}_0^3\), with \(\beta \neq 0\), and all \(R, r > 0, 0 < r < R < 1\), there exists \(C = C(p, r, \beta, E, N, Z)\) such that
that
\[ \| \partial_{\beta}^{\lambda,\psi,\lambda} \|_{W^{2,p}(B_{3N}(0,r))} \leq C(\lambda, \| \psi_{\lambda} \|_{L^p(B_{3N}(0,R))}) \]  
(5.18)

Since the proofs of Lemmas 5.1 and 5.2 are completely analogous to the proofs of Lemmas 2.1 and 2.2, we omit them here. (Note the similarity, but also difference, between (5.14) and (2.17).) It is also simple to verify that Proposition 1.10 follows from Lemmas 5.1 and 5.2 and the definition of \( \psi_{\lambda} \) (see (5.9) and (5.6)). (Compare with the proof that Theorem 1.1 follows from Lemma 2.1, situated after Lemma 2.1.)

6. Proof of Theorem 1.8

\[ \text{Proof:} \] To prove (i), let \( \rho \) be as in the theorem. Note that it suffices to prove the statement for each \( \rho_j \) in (1.28). The proof is the same for each \( j \), and so we shall prove it for \( \rho_1 \), which, by abuse of notation, we shall denote \( \rho_1 \).

To prove (1.32), let \( x_1 \in \mathbb{R}^3 \setminus \{0\} \) and \( R \in (0,1) \) (the case \( R \geq 1 \) obviously follows from this case). Let \( 1 = \sum \chi_I \) be the partition of unity (on \( \mathbb{R}^{3N} \)) from Lemma B.1 in Appendix B below. Then
\[ \rho(x_1) = \sum_I \int_{\mathbb{R}^{3N-3}} \chi_I(x_1, \hat{x}_1) |\psi(x_1, \hat{x}_1)|^2 d\hat{x}_1 = \sum_I \rho_I(x_1), \]  
(6.1)
and so, for all \( \alpha \in \mathbb{N}_0^3 \) with \( |\alpha| \geq 1 \),
\[ (\partial_{\alpha}^{\rho})_I(x_1) = \sum_I (\partial_{\alpha}^{\rho_I}) (x_1), \]  
(6.2)
with
\[ (\partial_{\alpha}^{\rho_I})_I(x_1) = \partial_{\alpha}^{\rho_I} \left( \int_{\mathbb{R}^{3N-3}} \chi_I(x_1, \hat{x}_1) |\psi(x_1, \hat{x}_1)|^2 d\hat{x}_1 \right). \]  
(6.3)

It then suffices to prove the estimate in (1.32) for each \( \partial_{\alpha}^{\rho_I} \), since the sum in (6.2) is finite.

To this end, recall again the definition of \( \chi_I \) from (B.4) in Lemma B.1 below. Let \( Q := \{1\} \cup (\cup_{j=0}^{J-1} Q_j) \subseteq \{1, \ldots, N\} \). Re-numbering, we may assume that \( Q = \{1, \ldots, M\}, M \leq N \). In the integral in (6.3), make the change of variables
\[ y_j = x_j - x_1, \ j = 2, \ldots, M. \]  
(6.4)
Then (re-naming $y_j$ to $x_j$ again)

$$
\int_{\mathbb{R}^{3N-3}} \chi_I(x_1, \hat{x}_1) |\psi(x_1, \hat{x}_1)|^2 \, d\hat{x}_1
$$

(6.5)

$$
= \int_{\mathbb{R}^{3N-3}} (\chi_I |\psi|^2)(x_1, x_2 + x_1, \ldots, x_M + x_1, x_{M+1}, \ldots, x_N) \, d\hat{x}_1
$$

$$
= \int_{\mathbb{R}^{3N-3}} \widetilde{\chi}_I(x) |\psi|^2(x_1, x_2 + x_1, \ldots, x_1 + x_M, x_{M+1}, \ldots, x_N) \, d\hat{x}_1,
$$

with $\widetilde{\chi}_I$ as in (B.21) in Lemma B.4 below (see (B.4) for $\chi_I$). By Leibniz’ rule

$$(\partial_{x_1}^\alpha \rho_I)(x_1) = \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} \int_{\mathbb{R}^{3N-1}} (\partial_{x_1}^\beta \widetilde{\chi}_I(x)) \times
$$

(6.6)

$$
\times \left( \partial_{x_1}^{\alpha-\beta} \{ |\psi|^2(x_1, x_2 + x_1, \ldots, x_M, x_{M+1}, \ldots, x_N) \} \right) \, d\hat{x}_1.
$$

Differentiating under the integral sign can be justified as in [27, p. 97]. Again by Leibniz’ rule, and the chain rule,

$$
\partial_{x_1}^{\alpha-\beta} \{ |\psi|^2(x_1, x_2 + x_1, \ldots, x_1 + x_M, x_{M+1}, \ldots, x_N) \}
$$

(6.7)

$$
= \sum_{\sigma \leq \alpha-\beta} \binom{\alpha-\beta}{\sigma} \partial_{x_1}^{\sigma} \{ \psi(x_1, x_2 + x_1, \ldots, x_1 + x_M, x_{M+1}, \ldots, x_N) \}
$$

$$
\times \partial_{x_1}^{\alpha-\beta-\sigma} \{ \psi(x_1, x_2 + x_1, \ldots, x_1 + x_M, x_{M+1}, \ldots, x_N) \}.
$$

Note that, by the chain rule and (1.39), for $s = 1, 2, 3$,

$$
\partial_{x_1}^{s} \{ \psi(x_1, x_2 + x_1, \ldots, x_1 + x_M, x_{M+1}, \ldots, x_N) \}
$$

(6.8)

$$
= \sum_{j=1}^{M} (\partial_{x_j} \psi)(x_1, x_2 + x_1, \ldots, x_1 + x_M, x_{M+1}, \ldots, x_N)
$$

$$
= \sqrt{M} (\partial_{x_Q}^{s} \psi)(x_1, x_2 + x_1, \ldots, x_1 + x_M, x_{M+1}, \ldots, x_N),
$$

and, by iteration, for $\sigma \in \mathbb{N}_0^3$,

$$
\partial_{x_1}^{\sigma} \{ \psi(x_1, x_2 + x_1, \ldots, x_1 + x_M, x_{M+1}, \ldots, x_N) \}
$$

(6.9)

$$
= M^{\sigma/2} (\partial_{x_Q}^{s} \psi)(x_1, x_2 + x_1, \ldots, x_1 + x_M, x_{M+1}, \ldots, x_N).
$$

Now apply (6.7) and (6.9) in (6.6) above. Then estimate $\partial_{x_1}^\beta \widetilde{\chi}_I(x)$ using Lemma B.4 below. (For $|\beta| = |\alpha| \geq 1$, use (B.23) or (B.24) with $n = 1$; for $\beta < \alpha$, use (B.22).) Then re-change variables ($y_j = x_j + x_1$, $j = 2, \ldots, M$) and re-name them back to $x_j$, to obtain (for
some \( j \in \{2, \ldots, N\} \)

\[
| (\partial_{x_1}^\alpha \rho_I)(x_1) | \leq C |x_1|^{1-|\alpha|} \int_{\mathbb{R}^{3N-3}} |x_j|^{-1} |\psi(x)|^2 \, d\hat{x}_1 \tag{6.10}
\]

\[
+ C \sum_{\beta < \alpha} |x_1|^{-|\beta|} \left( \sum_{\sigma \leq \alpha - \beta} \int_{\mathbb{R}^{3N-3}} 1_{\text{supp} \chi_I}(x) \left| (\partial_{xQ}^\sigma \psi)(x) \right| \left| (\partial_{xQ}^{\alpha-\beta-\sigma} \psi)(x) \right| d\hat{x}_1 \right).
\]

By Lemma B.2 below, and the fact that \( x_1 \neq 0 \), it follows that if \( x \in \text{supp} \chi_I \), then \( x \in \mathbb{R}^{3N} \setminus \Sigma_Q \) (see (1.43)). Also note that (see (1.44)), for all \( x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \),

\[
d_Q(x, \Sigma) = |x_j| \quad \text{for some } j \in Q = \{1, \ldots, M\}
\]

or

\[
d_Q(x, \Sigma) = \frac{1}{\sqrt{2}} |x_j - x_k| \quad \text{for some } j \in Q, k \in \{M + 1, \ldots, N\}.
\]

In both case, it follows from Lemma B.2 that if \( x \in \text{supp} \chi_I \), then

\[
d_Q(x, \Sigma)^{1-|\sigma|} \leq C |x_1|^{1-|\sigma|}. \tag{6.11}
\]

Also, if \( |x_1| \leq 1 \), then \( d_Q(x, \Sigma) \leq |x_1| \leq 1 \) (since \( 1 \in Q \) and \( |x_1| \leq 1 \); see also (1.44)), so, from (6.11),

\[
\lambda_Q(x)^{1-|\sigma|} \leq C r(x_1)^{1-|\sigma|}. \tag{6.12}
\]

(Recall that \( \lambda_Q(x) = \min \{1, d_Q(x, \Sigma)\} \) and \( r(x_1) = \min \{1, |x_1|\} \).) On the other hand, if \( |x_1| \geq 1 \), then either \( \lambda_Q(x) = d_Q(x, \Sigma) \), so that, by (6.11), and assuming \( \sigma \neq 0 \), then

\[
\lambda_Q(x)^{1-|\sigma|} \leq C |x_1|^{1-|\sigma|} \leq C r(x_1)^{1-|\sigma|}, \tag{6.13}
\]

or, \( \lambda_Q(x) = 1 \), in which case (6.12) holds trivially if \( \sigma \neq 0 \) (since \( C \geq 1 \) and \( 1 - |\sigma| \leq 0 \)).

In conclusion, if \( x \in \text{supp} \chi_I \), then (6.12) holds for all \( \sigma \neq 0 \).

Hence, applying the estimate (1.46) in Proposition 1.10 (with \( p = \infty, r = R/8, R = R/4 \) (!)) for each point \( x \in \mathbb{R}^{3N} \) for which the integrand in the second integral in (6.10) is non-zero, and then the a priori estimate in Theorem A.1 below (with \( R = R/4 \) (!)) for \( \nabla \psi \), we
get that
\[ |(\partial_{x_1}^\alpha \rho_I)(x_1)| \leq C r(x_1)^{1-|\alpha|} \int_{\mathbb{R}^3 \setminus \{0\}} |x_1|^{-1} |\psi(x)|^2 \, d\bar{x}_1 \]
\[ + C \sum_{\beta < \alpha} r(x_1)^{-|\beta|} \left\{ r(x_1)^{1-|\alpha|-|\beta|} \int_{\mathbb{R}^3 \setminus \{0\}} |\psi(x)| \|\psi\|_{L^\infty(B_{3N}(x,R/2))} \, d\bar{x}_1 \right\} \]
\[ + \sum_{0 < \sigma < \alpha} r(x_1)^{1-|\sigma|} r(x_1)^{1-((|\alpha|-|\beta|)-|\sigma|)} \int_{\mathbb{R}^3 \setminus \{0\}} \|\psi\|^2_{L^\infty(B_{3N}(x,R/2))} \, d\bar{x}_1 \}.
\]
(The term in the second line comes from \( \sigma = 0 \) and \( \sigma = \alpha - \beta \).) At this point we can finish the proof using Proposition A.3 below (with \( R = R/2, R = R \)) to get
\[ |(\partial_{x_1}^\alpha \rho_I)(x_1)| \leq C r(x_1)^{1-|\alpha|} \int_{B_3(x_1,R)} \rho(y) \, dy \]
\[ \leq C r(x_1)^{1-|\alpha|} \|\rho\|_{L^1(\mathbb{R}^3)} = C r(x_1)^{1-|\alpha|} \|\psi\|^2_{L^2(\mathbb{R}^3)}, \]
for all \( x_1 \in \mathbb{R}^3 \setminus \{0\} \) (and \( \alpha \neq 0 \)). This finishes the proof of (1.32), and hence of (i).

To prove (ii), for \( p \in [1, \infty) \), let \( \alpha \in [0, \frac{p+3}{p}) \). Then, since \( r(x) = \min\{1, |x|\} \),
\[ \int_{\mathbb{R}^3 \setminus \{0\}} \left[ r(x)^{|\alpha|-a} \partial^\alpha \rho(x) \right]^p \, dx \]
\[ = \int_{B_3(0,1) \setminus \{0\}} \left[ |x|^{|\alpha|-a} \partial^\alpha \rho(x) \right]^p \, dx + \int_{\mathbb{R}^3 \setminus B_3(0,1)} |\partial^\alpha \rho(x)|^p \, dx. \]
Now, by (1.32) (for \( R = 1 \)),
\[ \int_{B_3(0,1) \setminus \{0\}} \left[ |x|^{|\alpha|-a} \partial^\alpha \rho(x) \right]^p \, dx \leq C \int_{B_3(0,1)} \left( |x|^{1-a} \int_{B_3(x,1)} \rho(y) \, dy \right)^p \, dx \]
\[ \leq C \|\rho\|^p_{L^1(\mathbb{R}^3)} \int_{B_3(0,1)} |x|^{p(1-a)} \, dx \leq C_\alpha(a,p) \|\psi\|_{L^2(\mathbb{R}^3)}^{2p} \]
\[ \leq C \|\psi\|_{L^2(\mathbb{R}^3)}^{2p} < \infty, \]
since \( a < \frac{p+3}{p} \) and by the definition (1.28) of \( \rho \).

Furthermore, by (1.32), for all \( x \in \mathbb{R}^3 \setminus B_3(0,1) \),
\[ |\partial^\alpha \rho(x)|^{p-1} \leq C \left( \int_{B_3(x,1)} \rho(y) \, dy \right)^{p-1} \leq C \|\psi\|_{L^2(\mathbb{R}^3)}^{2(p-1)} \],
again, by the definition of \( \rho \). Hence, again by (1.32) and Fubini,

\[
\int_{\mathbb{R}^3 \setminus B_3(0,1)} |\partial^\alpha \rho(x)|^p \, dx \leq C \|\psi\|_{L^p(\mathbb{R}^3N)}^{2(p-1)} \int_{\mathbb{R}^3 \setminus B_3(0,1)} |\partial^\alpha \rho(x)| \, dx \tag{6.19}
\]

\[
\leq C \|\psi\|_{L^p(\mathbb{R}^3N)}^{2(p-1)} \int_{\mathbb{R}^3} \left( \int_{B_3(x,1)} \rho(y) \, dy \right) \, dx
\]

\[
= C \|\psi\|_{L^p(\mathbb{R}^3N)}^{2(p-1)} \int_{\mathbb{R}^3} \rho(y) \left( \int_{\mathbb{R}^3} 1_{|x-y| \leq 1} \, dy \right) \, dx = C_\alpha(p) \|\psi\|_{L^2(\mathbb{R}^3N)}^{2p}.
\]

It then follows from (6.16), (6.17), and (6.19) that

\[
\int_{\mathbb{R}^3 \setminus \{0\}} \left[ r(x)|\alpha| - \partial^\alpha \rho(x) \right]^p \, dx \leq C_\alpha(a,p) \|\psi\|_{L^2(\mathbb{R}^3N)}^{2p} < \infty. \tag{6.20}
\]

This proves (iii).

To prove (iii), note that, for \(|x_1| \leq 1\), the estimate (1.35) follows from (1.32). For \(|x_1| > 1\), it follows from [12, Theorem 1 (1.10)] (using that, for all \( \delta > 0 \) and all \( \alpha \in \mathbb{N}_3^+ \) with \(|\alpha| \geq 1\), the function \( e^{-\delta|x_1|} |x_1|^{|\alpha|-1} \) is uniformly bounded for \(|x_1| \geq 1\)).

This finishes the proof of Theorem 1.8. \( \square \)

**Appendix A. Some new a priori estimates**

In this appendix we state and prove a few results related to the a priori estimate proved in [27, Theorem 1.2] (see also the discussion in [39, (19.17)])

We start by recalling that estimate.

**Theorem A.1** ([27, Theorem 1.2]). Let \( \psi \) be as in (1.2). For all \( R \in (0, \infty) \), there exists \( C > 0 \) such that

\[
\sup_{y \in B(x, R)} |\nabla \psi(y)| \leq C \sup_{y \in B(x, 2R)} |\psi(y)| \tag{A.1}
\]

for all \( x \in \mathbb{R}^{3N} \).

The proof of (A.1) is based on an ‘Ansatz’ (see also (A.9) below) for the solution of the eigenvalue equation, and then on using elliptic regularity on the resulting equation. The objective of this Appendix is the following strengthening of Theorem A.1:

**Proposition A.2.** Let \( H \) be the operator in (1.1). For all \( 0 < r < R \) and \( E \in \mathbb{C} \) there exists \( C = C(r, R, E) \) (and also depending on \( N, Z \)) such that if \( H \psi = E \psi, \psi \in W^{2,2}_{\text{loc}}(\mathbb{R}^{3N}) \), then

\[
\|\psi\|_{L^\infty(B_{3N}(x_0, r))} + \|\nabla \psi\|_{L^\infty(B_{3N}(x_0, r))} \leq C \|\psi\|_{L^2(B_{3N}(x_0, R))} \tag{A.2}
\]
for all $x_0 \in \mathbb{R}^{3N}$.

**Proof.** Define, for $x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N}$,

$$
\tilde{F}(x) = \sum_{j=1}^{N} \left( -\frac{Z_2}{2}|x_j| + \frac{Z_2}{2}\sqrt{|x_j|^2 + 1} \right) \\
+ \sum_{1 \leq j < k \leq N} \left( \frac{1}{4}|x_j - x_k| - \frac{1}{4}\sqrt{|x_j - x_k|^2 + 1} \right). \tag{A.3}
$$

Note that there exists $C = C(N, Z) > 0$ such that (for $\Sigma$, see (1.3))

$$
|\tilde{F}(x)|, |\nabla_x \tilde{F}(x)| \leq C \quad \text{for all } x \in \mathbb{R}^{3N} \setminus \Sigma. \tag{A.4}
$$

Next, let (for $V$, see (1.1))

$$
\tilde{G}(x) = -\left[ \sum_{j=1}^{N} \frac{Z_2}{2}\Delta_x(\sqrt{|x_j|^2 + 1}) - \sum_{1 \leq j < k \leq N} \frac{1}{4}\Delta_x(\sqrt{|x_j - x_k|^2 + 1}) \right] \\
= V(x) - \Delta_x \tilde{F}(x). \tag{A.5}
$$

Since $|\Delta_x(\sqrt{|x|^2 + 1})| \leq 3$ for all $x \in \mathbb{R}^3$, there exists $C = C(N, Z) > 0$ such that

$$
|\tilde{G}(x)| \leq C \quad \text{for all } x \in \mathbb{R}^{3N}. \tag{A.6}
$$

Therefore, with

$$
\tilde{K}(x) := \tilde{G}(x) - |\nabla_x \tilde{F}(x)|^2 - E, \tag{A.7}
$$

using (A.4) and (A.6), there exists $C = C(N, Z, E) > 0$ such that

$$
|\tilde{K}(x)| \leq C \quad \text{for all } x \in \mathbb{R}^{3N} \setminus \Sigma. \tag{A.8}
$$

Define

$$
\tilde{\psi} := e^{-\tilde{F}}\psi, \tag{A.9}
$$

then, (using that $H\psi = E\psi$), $\tilde{\psi}$ satisfies the equation

$$
-\Delta_x \tilde{\psi} - 2\nabla_x \tilde{F} \cdot \nabla_x \tilde{\psi} + \tilde{K}\tilde{\psi} = 0, \tag{A.10}
$$

with

$$
\nabla_x \tilde{F}, \tilde{K} \in L^\infty(\mathbb{R}^{3N}). \tag{A.11}
$$

Note that since $\psi \in W^{2,2}_{\text{loc}}(\mathbb{R}^{3N})$, we have that $\tilde{\psi} \in W^{2,2}_{\text{loc}}(\mathbb{R}^{3N})$. This follows from (A.4) and Hardy’s inequality (note that any second order derivative of $\tilde{F}$ behaves like $|x_j|^{-1}$ and $|x_j - x_k|^{-1}$).
It follows from Theorem C.2 in Appendix C that \( \tilde{\psi} \in C^{1,\theta}_{\text{loc}}(\mathbb{R}^{3N}) \) for all \( \theta \in (0,1) \). In particular, since this, (A.4), (A.8), and (A.10) then implies that
\[
-\Delta_x \tilde{\psi} = 2\nabla_x \tilde{F} \cdot \nabla_x \tilde{\psi} - \tilde{K} \tilde{\psi} \in L^p_{\text{loc}}(\mathbb{R}^{3N}) \quad \text{for all} \quad p \in [1, \infty] , \quad (A.12)
\]
it follows from Theorem C.4 that \( \tilde{\psi} \in W^{2,p}_{\text{loc}}(\mathbb{R}^{3N}) \) for all \( p \in [2, \infty) \).

It now follows from Theorem C.3 (used on (A.10), with \( p = 2 \)) that for all \( \tilde{R}, \tilde{r} > 0 \) there exists a constant \( C = C(\tilde{r}, \tilde{R}) \) (depending also on \( N, Z, E \) through (A.4) and (A.8)) such that, for all \( x_0 \in \mathbb{R}^{3N} \),
\[
\| \tilde{\psi} \|_{W^{2,2}(B_{3N}(x_0, \tilde{r}))} \leq C \| \tilde{\psi} \|_{L^2(B_{3N}(x_0, \tilde{R}))} . \quad (A.13)
\]

Hence, by Theorem C.1(i) (Sobolev embedding; with \( k = 2, n = 3N \), and \( p = p_1 = 2, q = p_1^* = 6N/(3N - 4) > 2 + 8/3N = p_1 + 8/3N \)), and then (A.13), there exists a constant \( C = C(\tilde{r}, \tilde{R}) \) such that
\[
\| \tilde{\psi} \|_{L^{p_1}(B_{3N}(x_0, \tilde{r}))} \leq C \| \tilde{\psi} \|_{L^2(B_{3N}(x_0, \tilde{R}))} < \infty . \quad (A.14)
\]

Now, using Theorem C.3 again, but this time with \( p = p_2 = p_1^* \), and then (A.14), we therefore get that, for all \( \tilde{r} \in (0, \tilde{r}) \), there exists a constant \( C = C(\tilde{r}, \tilde{R}) > 0 \), such that
\[
\| \tilde{\psi} \|_{W^{2,p_2}(B_{3N}(x_0, \tilde{r}))} \leq C \| \tilde{\psi} \|_{L^2(B_{3N}(x_0, \tilde{R}))} , \quad (A.15)
\]
with \( p_2 > p_1 + 8/3N = 2 + 8/3N \). (Of course the constant \( C \) changes every time.)

We repeat this: Sobolev embedding, in the form of Theorem C.1(i) (always with \( k = 2, n = 3N \); next time with \( W^{2,p_2} \) and \( L^{p_2^*} \), \( p_2^* > p_2 + 8/3N \)), and then Theorem C.3 (with \( p = p_3 = p_2^* \)) as long as \( 2p_2 < 3N \).

Note that \( 2 = p_2 < p_2 < p_3 < \cdots \), with
\[
p_{i+1} = p_i^* = 3Np_i/(3N - 2p_i) > p_i + 2p_i^*/3N > p_i + 8/3N , \quad i = 1, 2, \ldots .
\]

Hence, we reach \( p_M \) satisfying \( 2p_M < 3N < 2p_M^* \) in maximally \( (3N - 2)/(8/3N) + 1 = (9N^2 - 6N + 8)/8 \) steps (that is, \( M \) is smaller equal this number). As above, the radius of the smaller ball decreases each time (above, from \( \tilde{r} \) to \( \tilde{r} \)). However, splitting the original difference \((R - r)/2 = R - (R + r)/2 \) in \( M + 1 \) equally large parts (we use Theorem C.3 \( M + 1 \) times), we get: For all \( 0 < r < R \) there exists a constant \( C = C(r, R) > 0 \) such that
\[
\| \tilde{\psi} \|_{W^{2,p_M^*}(B_{3N}(x_0, (r+R)/2))] \leq C \| \tilde{\psi} \|_{L^2(B_{3N}(x_0, R))} , \quad (A.16)
\]
with \( 2p_M < 3N < 2p_M^* \).
Now use Theorem C.1(ii) (Morrey’s Theorem): With \( k = 2, p = p_M^*, n = 3N \) (so \( kp > n \)), to get, for some \( \theta \in (0, 1) \),
\[
\|\tilde{\psi}\|_{C^0(B_{3N}(x_0, (r+R)/2))} \leq C\|\tilde{\psi}\|_{W^{2,p_M^*}(B_{3N}(x_0, (r+R)/2))}.
\] (A.17)
Using (A.16), and that \( \|\tilde{\psi}\|_{L^\infty} \leq \|\tilde{\psi}\|_{C^\theta} \), this implies that, for all \( 0 < r < R \),
\[
\|\tilde{\psi}\|_{L^\infty(B_{3N}(x_0, (r+R)/2))} \leq C\|\tilde{\psi}\|_{L^2(B_{3N}(x_0, R))},
\] (A.18)
for some \( C = C(r, R) > 0 \).
Hence, using (A.10)–(A.11), Theorem C.2 (used on (A.10)), and (A.18) give that, for all \( \theta \in (0, 1) \),
\[
\|\tilde{\psi}\|_{C^{1,\theta}(B_{3N}(x_0, r))} \leq C\|\tilde{\psi}\|_{L^\infty(B_{3N}(x_0, (r+R)/2))}
\leq C\|\tilde{\psi}\|_{L^2(B_{3N}(x_0, R))}.
\] (A.19)
Hence (since \( \|\tilde{\psi}\|_{L^\infty} + \|\nabla\tilde{\psi}\|_{L^\infty} \leq \|\tilde{\psi}\|_{C^{1,\theta}} \)), (A.2) follows, but with \( \tilde{\psi} \) instead of \( \psi \). It remains to recall that \( \psi = e^{\tilde{F}}\tilde{\psi} \) (see (A.9)) with \( \tilde{F} \) (globally) Lipschitz (see also (A.4)), to arrive at (A.2) for \( \psi \).

As a consequence of Propostion A.2, we get the following, which is of independent interest:

**Proposition A.3.** For \( N \geq 2 \), let \( H \) be the operator in (1.1). Then for all \( 0 < r < R \) and all \( E \in \mathbb{R} \) there exists a constant \( C = C(r, R, E) > 0 \) such that if \( H\psi = E\psi, \psi \in W^{2,2}(\mathbb{R}^{3N}) \), and if \( \rho \) is the associated one-electron density as in (1.28), then, for all \( x_1 \in \mathbb{R}^3 \),
\[
\int_{\mathbb{R}^{3N-3}} \|\psi\|^2_{L^\infty(B_{3N}(x_1, x_1, r))} d\hat{x}_1 \leq C \int \rho(y_1) dy_1, \]
(A.20)
\[
\int_{\mathbb{R}^{3N-3}} \|\nabla\psi\|^2_{L^\infty(B_{3N}(x_1, x_1, r))} d\hat{x}_1 \leq C \int \rho(y_1) dy_1, \]
(A.21)
\[
\rho(x_1) = \int_{\mathbb{R}^{3N-3}} |\psi(x_1, \hat{x}_1)|^2 d\hat{x}_1 \leq C \int \rho(y_1) dy_1, \]
(A.22)
and
\[
|\nabla\rho(x_1)| = \left| \int_{\mathbb{R}^{3N-3}} \nabla x_1 (|\psi(x_1, \hat{x}_1)|^2) d\hat{x}_1 \right| \leq C \int \rho(y_1) dy_1, \]
(A.23)
in the sense that, for all \( v \in \mathbb{R}^3 \), the directional derivative (exists and) satisfies
\[
|v \cdot \nabla\rho(x_1)| \leq C|v| \int \rho(y_1) dy_1. \]
(A.24)
Furthermore, for all $b \in [0, 3]$ and $R > 0$ there exists $C = C(b, R, E) > 0$ such that
\[
\int_{\mathbb{R}^{3N-3}} |x_2|^{-b} |\psi(x_1, \hat{x}_1)|^2 \, d\hat{x}_1 \leq C \int_{B_3(x_1, R)} \rho(y_1) \, dy_1. \tag{A.25}
\]

**Remark A.4.** Note that, for all $x_1 \in \mathbb{R}^3$, $R > 0$,
\[
\int_{B_3(x_1, R)} \rho(y_1) \, dy_1 \leq \|\rho\|_{L^1(\mathbb{R}^3)} = \|\psi\|_{L^2(\mathbb{R}^{3N})}^2 < \infty. \tag{A.26}
\]

In particular, it follows from (A.23) that $\rho$ is globally Lipschitz: $\rho \in C^{0,1}(\mathbb{R}^3)$. This was already known [27, Theorem 1.11 (i)].

**Proof.** We start by proving (A.20) and (A.21) from which the other estimates will follow in a simple manner. Using (A.2) and Fubini’s Theorem,
\[
\int_{\mathbb{R}^{3N-3}} \|\psi\|_{L^\infty(B_{3N}((x_1, \hat{x}_1), r))}^2 \, d\hat{x}_1 \leq C \int_{\mathbb{R}^{3N-3}} \|\psi\|_{L^2(B_{3N}((x_1, \hat{x}_1), R))}^2 \, d\hat{x}_1
\]
\[
= C \int_{\mathbb{R}^N} |\psi(y)|^2 \left( \int_{\{y - (x_1, \hat{x}_1) \leq R\}} \, d\hat{x}_1 \right) \, dy. \tag{A.27}
\]
Now, for all $y = (y_1, \hat{y}_1) \in \mathbb{R}^{3N}$,
\[
\int_{\{y - (x_1, \hat{x}_1) \leq R\}} \, d\hat{x}_1 \leq |\{y_1 - x_1 \leq R\}| \int_{\{y_1 - \hat{x}_1 \leq R\}} \, d\hat{x}_1, \tag{A.28}
\]
and the last integral equals the volume of $B_{3N-3}(0, R)$ for all $\hat{y}_1 \in \mathbb{R}^{3N-3}$. Inserting this in (A.27) and using the definition of $\rho$ in (1.28) finishes the proof of (A.20). The proof of (A.21) is similar.

To prove (A.22) notice that
\[
\int_{\mathbb{R}^{3N-3}} |\psi(x_1, \hat{x}_1)|^2 \, d\hat{x}_1 \leq \int_{\mathbb{R}^{3N-3}} \|\psi\|_{L^\infty(B_{3N}((x_1, \hat{x}_1), R/2))}^2 \, d\hat{x}_1
\]
and use (A.20) with $r = R/2$.

To prove (A.23) we differentiate and estimate, to get that
\[
|\nabla_{x_1} (|\psi(x_1, \hat{x}_1)|^2)| \leq 2 \|\psi\|_{L^\infty(B_{3N}((x_1, \hat{x}_1), R/2))} \|\nabla \psi\|_{L^\infty(B_{3N}((x_1, \hat{x}_1), R/2))}. \tag{A.29}
\]
Here (A.29) should be understood in terms of directional derivatives in the same way as in (A.24). From [27, Proposition 1.5] we know that the directional derivatives of $\psi$ exist.

At this point we can use (A.2) and finish the estimate as above.

To prove (A.25) it suffices, using (A.22), to estimate
\[
\int_{\{|x_2| \leq R/4\}} |x_2|^{-b} |\psi(x_1, \hat{x}_1)|^2 \, d\hat{x}_1.
\]
We argue in a similar fashion as above, with \( \hat{x}_{1,2} = (x_3, \ldots, x_N) \). Since \((x_1, x_2, \hat{x}_{1,2}) \in B_{3N}((x_1, 0, \hat{x}_{1,2}), R/2) \) for all \(|x_2| \leq R/4\), we get from Fubini’s Theorem and (A.2) that

\[
\int_{\{|x_2| \leq R/4\}} |x_2|^{-b} |\psi(x_1, \hat{x}_1)|^2 d\hat{x}_1 \\
\leq \int_{\mathbb{R}^{3N-6}} \left( \int_{\{|x_2| \leq R/4\}} |x_2|^{-b} dx_2 \right) \|\psi\|^2_{L^\infty(B_{3N}((x_1, 0, \hat{x}_{1,2}), R/2))} d\hat{x}_{1,2} \\
\leq C(b, R) \int_{\mathbb{R}^{3N-6}} \|\psi\|^2_{L^2(B_{3N}((x_1, 0, \hat{x}_{1,2}), R))} d\hat{x}_{1,2} \\
= C(b, R) \int_{\mathbb{R}^{3N}} |\psi(y)|^2 \left( \int_{\{|y-(x_1,0,\hat{x}_{1,2})| \leq R\}} d\hat{x}_{1,2} \right) dy. \quad (A.30)
\]

Here we also used that \( b \in [0, 3) \). Now, for all \( y = (y_1, y_2, \hat{y}_{1,2}) \in \mathbb{R}^{3N}, \)

\[
\int_{\{|y-(x_1,0,\hat{x}_{1,2})| \leq R\}} d\hat{x}_{1,2} \leq 1_{\{|y_1-x_1| \leq R\}} \int_{\{|\hat{y}_{1,2}-\hat{x}_{1,2}| \leq R\}} d\hat{x}_{1,2}, \quad (A.31)
\]

and the last integral equals the volume of \( B_{3N-6}(0, R) \) for all \( \hat{y}_{1,2} \in \mathbb{R}^{3N-6} \). Inserting this in (A.30) and using the definition of \( \rho \) in (1.28) finishes the proof of (A.25). \( \square \)

**Appendix B. A partition of unity**

In this appendix we gather various facts about a particular partition of unity (on \( \mathbb{R}^{3N} \)), needed when studying the electron density \( \rho \); see Section 6.

We denote by \( C_b^\infty(\Omega) \) the set of all smooth functions on \( \Omega \) which are bounded together with all their derivatives.

Let \( \chi_1, \chi_2 \in C_b^\infty(\mathbb{R}), 0 \leq \chi_i \leq 1, i = 1, 2, \chi_1, \chi_2 \) both monotone, with

\[
\chi_1(t) = \begin{cases} 
1, & t \leq 1/4, \\
0, & t \geq 3/4,
\end{cases} \quad \text{and} \quad \chi_2(t) = \begin{cases} 
0, & t \leq 1/4, \\
1, & t \geq 3/4,
\end{cases} \quad (B.1)
\]

and

\[
\chi_1(t) + \chi_2(t) = 1 \quad \text{for all } t \in \mathbb{R}. \quad (B.2)
\]

The partition of unity depends on an index \( I \in X \), where \( X = \bigcup_{J=0}^{N-1} X_J \), with the \( X_J \)'s to be described below. Here

\[
X_{J=0} = \{(0, \{2, \ldots, N\}, \emptyset)\},
\]
and the corresponding function in the partition of unity is (with \( x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \)),

\[
\chi_{(0,\{2,\ldots,N\},\emptyset)}(x) = \prod_{j \in \{2,\ldots,N\}} \chi_1 \left( \frac{|x_j|}{|x_1|} \right). \tag{B.3}
\]

For \( J \geq 1 \), \( X_J \) consists of all elements of the form \((J, P_J, Q_{J-1}, \ldots, Q_0)\) with \( Q_0, Q_1, \ldots, Q_{J-1}, P_J \subset \{2, \ldots, N\} \) disjoint, and \( P_J \cup \left( \bigcup_{s=0}^{J-1} Q_s \right) = \{2, \ldots, N\} \) (possibly \( P_J = \emptyset \) or \( Q_s = \emptyset \), \( s \geq 1 \)). The corresponding function is (with \( \prod_{j \in \emptyset} = 1 \))

\[
\chi_I(x) = \chi_{(J,P_J,Q_{J-1},\ldots,Q_0)}(x) \tag{B.4}
\]

\[
= \left[ \prod_{j \in P_J} \chi_1 \left( \frac{4^J|x_j|}{|x_1|} \right) \right] \left[ \prod_{j \in Q_{J-1}} \chi_2 \left( \frac{4^{J-1}|x_j|}{|x_1|} \right) \chi_1 \left( \frac{4^{J-2}|x_j|}{|x_1|} \right) \right] \times
\]

\[
\times \cdots \times \left[ \prod_{j \in Q_s} \chi_2 \left( \frac{4^s|x_j|}{|x_1|} \right) \chi_1 \left( \frac{4^{s-1}|x_j|}{|x_1|} \right) \right] \times \cdots \times
\]

\[
\times \left[ \prod_{j \in Q_0} \chi_2 \left( \frac{4^0|x_j|}{|x_1|} \right) \chi_1 \left( \frac{4^0|x_j|}{|x_1|} \right) \right] \left[ \prod_{j \in Q_0} \chi_2 \left( \frac{4^0|x_j|}{|x_1|} \right) \right] \right]. \tag{B.8}
\]

**Lemma B.1.** Let \( \chi_1 \) and \( \chi_2 \) be as above (see (B.1)–(B.2)), then (as functions of \( x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \)),

\[
1 = \sum_I \chi_I, \tag{B.5}
\]

where the sum is over a subset of \( X \).

**Proof:** To ease notation, let, for \( x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \),

\[
\chi_{i,j}^s(x) = \chi_i \left( \frac{4^s|x_j|}{|x_1|} \right), \quad i = 1, 2, j = 2, \ldots, N, s = 0, 1, 2, \ldots. \tag{B.6}
\]

Note that, by (B.1), for all \( j \) and \( s = 1, 2, \ldots \),

\[
\chi_{1,j}^s \chi_{1,j}^{s-1} = \chi_{1,j}^s. \tag{B.7}
\]

Using (B.2) we have (again, with \( \prod_{j \in \emptyset} = 1 \))

\[
1 = \prod_{j=2}^{N} \left[ \chi_{1,j}^0 + \chi_{2,j}^0 \right] = \sum_{p_0 \cup q_0 = \{2, \ldots, N\}, p_0 \cap q_0 = \emptyset} \left[ \prod_{j \in p_0} \chi_{1,j}^0 \right] \left[ \prod_{j \in q_0} \chi_{2,j}^0 \right]. \tag{B.8}
\]
The term in (B.8) with \( q_0 = \emptyset \) equals
\[
\prod_{j \in \{2, \ldots, N\}} \chi_{1,j} \cdot \chi_{2,j} = \chi_{1,\emptyset,\{2, \ldots, N\},\emptyset} \cdot \chi_{2,\emptyset,\{2, \ldots, N\},\emptyset}.
\] (B.9)

The term in (B.8) with \( p_0 = \emptyset \) equals
\[
\prod_{j \in \{2, \ldots, N\}} \chi_{1,j} \cdot \chi_{2,j} = \chi_{1,\emptyset,\{2, \ldots, N\},\emptyset} \cdot \chi_{2,\emptyset,\{2, \ldots, N\},\emptyset}.
\] (B.10)

For all other terms \( \chi_{p_0,q_0} = \left[ \prod_{j \in p_0} \chi_{1,j} \right] \left[ \prod_{j \in q_0} \chi_{2,j} \right] \) in (B.8) we have \( q_0 \neq \emptyset \neq p_0 \), and so \( 0 < \#p_0 < \#\{2, \ldots, N\} = N - 1 \). In each of these terms, insert a factor of (recall (B.6) and (B.2))
\[
1 = \prod_{j \in p_0} \left[ \chi_{1,j} + \chi_{2,j} \right],
\] (B.11)

and multiply out, to get
\[
\chi_{p_0,q_0} = \left[ \prod_{j \in p_0} \chi_{1,j} \right] \cdot 1 \cdot \left[ \prod_{j \in q_0} \chi_{2,j} \right]
= \sum_{q_1 \cup p_1 = p_0, q_1 \cap p_1 = \emptyset} \left[ \prod_{j \in p_0} \chi_{1,j} \right] \left[ \prod_{j \in q_1} \chi_{1,j} \right] \left[ \prod_{j \in q_0} \chi_{1,j} \right] \left[ \prod_{j \in q_0} \chi_{2,j} \right].
\] (B.12)

By (B.7), \( \chi_{1,j} \chi_{1,j} = \chi_{1,j} \) for all \( j \in p_1 \subseteq p_0 \), and so, since \( p_0 = q_1 \cup p_1 \), each of the terms in the sum in (B.12) is of the form
\[
\chi_{p_1,q_1,q_0} = \left[ \prod_{j \in p_1} \chi_{1,j} \right] \left[ \prod_{j \in q_1} \chi_{2,j} \chi_{1,j} \right] \left[ \prod_{j \in q_0} \chi_{2,j} \right].
\] (B.13)

As before, the term with \( p_1 = \emptyset \) (that is, \( q_1 = p_0 \)) equals
\[
\left[ \prod_{j \in q_1} \chi_{2,j} \chi_{1,j} \right] \left[ \prod_{j \in q_0} \chi_{2,j} \right] = \chi_{2,\emptyset, q_1, q_0},
\] (B.14)

and the term with \( q_1 = \emptyset \) (that is, \( p_1 = p_0 \)) equals
\[
\left[ \prod_{j \in p_1} \chi_{1,j} \right] \left[ \prod_{j \in q_0} \chi_{2,j} \right] = \chi_{1,p_1, q_0}.
\] (B.15)

For the rest of the terms in (B.13), we have \( q_1 \neq \emptyset \neq p_1 \), and so \( 0 < \#p_1 < \#p_0 < N - 1 \), that is, \( 0 < \#p_1 < N - 2 \). For each of these terms \( \chi_{p_1,q_1,q_0} \) (with \( p_1 \cup q_1 \cup q_0 = \{2, \ldots, N\}, p_1, q_1, q_0 \) disjoint), insert a factor of
\[
1 = \prod_{j \in p_1} \left[ \chi_{1,j} + \chi_{2,j} \right],
\] (B.16)
and proceed as above, using (B.7) with \( s = 2 \), to write \( \chi_{p_1, q_1, q_0} \) as a sum (over \( p_2, q_2 \) with \( p_2 \cup q_2 = p_1, p_2 \cap q_2 = \emptyset \)) of terms of the form

\[
\chi_{p_2, q_2, q_1, q_0} = \left[ \prod_{j \in p_2} \chi_{1,j}^2 \right] \left[ \prod_{j \in q_2} \chi_{2,j}^2 \chi_{1,j}^1 \right] \left[ \prod_{j \in q_1} \chi_{2,j}^1 \chi_{1,j}^0 \right] \left[ \prod_{j \in q_0} \chi_{2,j}^0 \right]. \tag{B.17}
\]

Again, the terms with \( p_2 = \emptyset \) or \( q_2 = \emptyset \) have (see (B.4)) the correct form (namely, with \( J = 3, P_3 = p_2, Q_i = q_i, i = 0, 1, 2, I = (3, \emptyset, Q_2, Q_1, Q_0) \in X_3 \), and, respectively, with \( J = 2, P_2 = p_2, Q_i = q_i, i = 0, 1, I = (2, P_2, Q_1, Q_0) \in X_2 \)). Furthermore, for all other terms \( \chi_{p_2, q_2, q_1, q_0} \) in (B.17), we have \( q_2 \neq \emptyset \neq p_2 \), hence, \( 0 < \#p_2 < \#p_1 < N - 2 \), that is, \( 0 < \#p_2 < N - 3 \). Continuing like this, we get a sum of terms of the form in (B.4), with the size of \( p_j \) diminishing at each step, until \( \#p_k = 1 \) (which occurs for \( k = N - 3 \)). Then the above two possibilities—\( p_k = \emptyset \) or \( q_k = \emptyset \)—are the only two, and we are done.

The localization functions \( \chi_I \) above are constructed in order to have the following lemma, bounding certain terms in the Coulomb-potential by \( |x_1|^{-1} \), on the support of \( \chi_I \).

**Lemma B.2.** Let \( \chi_1 \) and \( \chi_2 \) be as in (B.1)–(B.2), and define \( \chi_I \) as in (B.4).

Then there exists a constant \( C = C(N) > 0 \) such that for all \( \mathbf{x} = (x_1, \ldots, x_N) \in \text{supp} \chi_I \):

\[
|x_j|^{-1} \leq C|x_1|^{-1} \quad \text{for all } j \in \bigcup_{j=0}^{J-1} Q_j, \tag{B.18}
\]

\[
|x_1 - x_j|^{-1} \leq C|x_1|^{-1} \quad \text{for all } j \in (\bigcup_{j=1}^{J-1} Q_j) \cup P_J, \tag{B.19}
\]

\[
|x_j - x_k|^{-1} \leq C|x_1|^{-1} \quad \text{for all } j \in P_J, k \in \bigcup_{j=0}^{J-1} Q_j. \tag{B.20}
\]

**Proof:** To prove (B.18) note that, since \( \chi_I(\mathbf{x}) \neq 0 \), for all the stated \( j \)'s we have \( \chi_2(4^s|x_j|/|x_1|) \neq 0 \) for some \( s \in \{1, \ldots, J-1\} \), \( J \leq N \). Hence, by (B.1),

\[
|x_j| \geq \frac{1}{4} \frac{1}{4^s} |x_1| \geq \frac{1}{4} \frac{1}{4^N} |x_1| = c_N |x_1|,
\]

which proves (B.18).

To prove (B.19), note that, for \( j \in P_J \), we have \( \chi_1(4^t|x_j|/|x_1|) \neq 0 \). Hence, by (B.1), \( |x_j| \leq \frac{1}{4} |x_1| \), and so \( |x_1 - x_j| \geq \frac{1}{4} |x_1| \) for these \( j \).

On the other hand, for \( j \in Q_1 \cup \ldots \cup Q_{J-1} \), \( \chi_1(4^{s-1}|x_j|/|x_1|) \neq 0 \) for some \( s \in \{1, \ldots, J-1\} \), \( J \leq N \). Hence, by (B.1), \( |x_j| \leq \frac{3}{4^{s-1}} |x_1| \leq \frac{3}{4} |x_1| \), and so (B.19) holds also for these \( j \)'s.
Finally, to prove (B.20), note that for the stated \( j \)'s, we have \( |x_j| \leq \frac{3}{4} \frac{1}{4^j} |x_1| \), and for the stated \( k \)'s, we have, for some \( s \in \{1, \ldots, J - 1\} \),
\[
|x_k| \geq \frac{1}{4} \frac{1}{4^s} |x_1| \geq \frac{1}{4} \frac{1}{4^{J-1}} |x_1|.
\]
Therefore,
\[
|x_j - x_k| \geq |x_k| - |x_j| \geq \frac{1}{4} \frac{1}{4^s} |x_1| - \frac{3}{4} \frac{1}{4^j} |x_1| = \frac{1}{4} \frac{1}{4^s} |x_1| \geq \frac{1}{4} \frac{1}{4^N} |x_1| = c_N |x_1| ,
\]
which proves (B.20). \( \square \)

**Remark B.3.** This last argument is the reason why we need \( 4^J \) in the \( \chi_1 \) in the \( P_J \)-factor, and at most \( 4^J - 1 \) in the \( \chi_2 \) in the \( Q_s \)-factors, in (B.4).

The next lemma uses the previous one, to control derivatives with respect to \( x_1 \) of (a slightly changed version of) the localization functions \( \chi_I \).

**Lemma B.4.** Let \( \chi_1 \) and \( \chi_2 \) be as in (B.1)–(B.2), and let \( \chi_I \) be as in Lemma B.1. For \( \mathbf{x} = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \), define \( \tilde{\mathbf{x}} = (\tilde{x}_1, \ldots, \tilde{x}_N) \) with
\[
\tilde{x}_j = \begin{cases} 
  x_j, & \text{if } j = 1 \text{ or } j \in P_J, \\
  x_1 + x_j, & \text{else.} 
\end{cases}
\]
Define finally
\[
\tilde{\chi}_I(\mathbf{x}) = \chi_I(\tilde{\mathbf{x}}). \tag{B.21}
\]

Then, for all \( \beta \in \mathbb{N}_0^3 \) there exists a constant \( C = C(I, \beta) \) such that, for all \( \mathbf{x} = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \),
\[
|\partial_{x_1}^{\beta} \tilde{\chi}_I(\mathbf{x})| \leq C |x_1|^{-|\beta|}. \tag{B.22}
\]

Furthermore, if \( |\beta| \geq 1 \), then there exists \( j \in \{2, \ldots, N\} \) and a constant \( C = C(I, \beta, j) \) such that, for all \( \mathbf{x} = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \) and all \( n \in \mathbb{N}_0 \),
\[
|\partial_{x_1}^{\beta} \tilde{\chi}_I(\mathbf{x})| \leq C |x_j|^{-n} |x_1|^{n-|\beta|} \tag{B.23}
\]
or
\[
|\partial_{x_1}^{\beta} \tilde{\chi}_I(\mathbf{x})| \leq C |x_1 + x_j|^{-n} |x_1|^{n-|\beta|}. \tag{B.24}
\]
Proof: First note that, by Leibniz’ rule, to prove (B.22) it suffices to prove that for all $\gamma \in \mathbb{N}^3$, there exists a constant such that
\[
| (\partial^\gamma_{x_1} f)(x_1) | \leq C |x_1|^{-|\gamma|} \tag{B.25}
\]
for $f$ any of the functions
\[
\chi_1 \left( \frac{4^k |x_j|}{|x_1|} \right), \quad \chi_1 \left( \frac{4^k |x_1 + x_j|}{|x_1|} \right), \quad \chi_2 \left( \frac{4^k |x_1 + x_j|}{|x_1|} \right), \tag{B.26}
\]
($k \in \{0, \ldots, N\}, j \neq 1$). By the choice of $\chi_1$ and $\chi_2$, the bound (B.25) is trivial for $\gamma = 0$ (with $C = 1$). In particular, (B.22) trivially holds if $\beta = 0$ (again, with $C = 1$).

Secondly, note that in each case, for any $\gamma \in \mathbb{N}^3 \setminus \{0\}$,
\[
(\partial^\gamma_{x_1} f)(x_1) = \sum_{\substack{1 \leq m \leq |\gamma| \\gamma_1 + \ldots + \gamma_m = |\gamma|}} c_{m, \gamma} \chi_i^{(m)}(g(x_1)) (\partial^\gamma_{x_1} g)(x_1) \cdots (\partial^\gamma_{x_1} g)(x_1), \tag{B.27}
\]
with $i = 1$ or 2, and $g(x_1)$ either $\frac{4^k |x_j|}{|x_1|}$ or $\frac{4^k |x_1 + x_j|}{|x_1|}$. On $\text{supp}(\chi_i^{(m)} \circ g)$ ($m \geq 1$) we have, in all cases (see (B.1))
\[
\frac{1}{4} \leq g(x_1) \leq \frac{3}{4}. \tag{B.28}
\]
Hence, if $g(x_1) = \frac{4^k |x_j|}{|x_1|}$, then for any $\gamma \in \mathbb{N}^3 \setminus \{0\}$, on $\text{supp}(\chi_i^{(m)} \circ g)$,
\[
| (\partial^\gamma_{x_1} g)(x_1) | \leq c_{\gamma, k} |x_j| |x_1|^{-1-|\gamma|} \leq \tilde{c}_{\gamma, k} |x_1|^{-|\gamma|}. \tag{B.29}
\]
On the other hand, if $g(x_1) = \frac{4^k |x_1 + x_j|}{|x_1|}$, then for any $\gamma \in \mathbb{N}^3 \setminus \{0\}$, again on $\text{supp}(\chi_i^{(m)} \circ g)$,
\[
| (\partial^\gamma_{x_1} g)(x_1) | = \left| \sum_{\sigma \leq |\gamma|} \binom{\gamma}{\sigma} (\partial^\sigma_{x_1} |x_1 + x_j|) (\partial^{\gamma-\sigma}_{x_1} |x_1|^{-1}) \right|
\leq \sum_{\sigma \leq |\gamma|} c_{\gamma, \sigma} |x_1 + x_j|^{-|\sigma|} |x_1|^{-1-|\gamma|+|\sigma|} \leq \tilde{c}_{\gamma, k} |x_1|^{-|\gamma|}. \tag{B.30}
\]
In both (B.29) and (B.30), the second inequality follows from (B.28).

Hence, (B.27), (B.29), (B.30), and the fact that all derivatives of $\chi_1$ and $\chi_2$ are globally bounded, imply that
\[
| (\partial^\gamma_{x_1} f)(x_1) | \leq \sum_{\substack{1 \leq m \leq |\gamma| \\gamma_1 + \ldots + \gamma_m = |\gamma|}} \tilde{c}_{m, \gamma} |x_1|^{-|\gamma_1|} \cdots |x_1|^{-|\gamma_m|} = C |x_1|^{-|\gamma|}. \tag{B.31}
\]
This finishes the proof of (B.25) in the case $|\gamma| \geq 1$, and hence the proof of (B.22).

To prove that (B.23) or (B.24) hold when $|\beta| \geq 1$, notice that in this case at least one of the functions in the product in (B.21) (that is, in (B.26)) gets differentiated (that is, $|\gamma| \geq 1$). For this one, do as above, but use additionally (B.28) to get, for all $n \in \mathbb{N}$,

$$\leq \frac{|x_1|^n}{|x_j|^n} \quad \text{or} \quad \leq \frac{|x_1|^n}{|x_1 + x_j|^n}. \quad \text{(B.32)}$$

(As before, on supp($\chi_{(m)}^{(n)} \circ g$)). Applying this in (B.29) or (B.30) yields (B.23) or (B.24). \hfill \Box

**Appendix C. Needed a priori estimates**

In this section we collect needed results from the literature.

We start by Sobolev embedding.

**Theorem C.1** ([6, Theorem 6 p. 284], [1, 4.12 Theorem p. 85]). Let $\Omega \subset \mathbb{R}^n$ be open and bounded, and let $k \in \mathbb{N}, p \geq 1$.

(i) Assume $\Omega$ satisfies an interior cone condition. Then, for any $k, p$ with $kp < n$, we have the continuous embedding

$$W^{k,p}(\Omega) \hookrightarrow L^q(\Omega) \quad \text{for all } q \in [p, p^*], \text{ with } p^* := np/(n - kp). \quad \text{(C.1)}$$

Moreover, there exists a constant $C = C(k, p, n, \Omega)$ such that

$$\|u\|_{L^q(\Omega)} \leq C\|u\|_{W^{k,p}(\Omega)} \quad \text{for all } u \in W^{k,p}(\Omega). \quad \text{(C.2)}$$

(ii) Assume $\Omega$ is locally Lipschitz. Then for $kp > n$, we have the continuous embedding

$$W^{k,p}(\Omega) \hookrightarrow C^{k-1-[n/p],\theta}(\Omega) \quad \text{for all } \theta \in [0, \theta_0], \quad \text{(C.3)}$$

$$\theta_0 = \begin{cases} \lfloor n/p \rfloor + 1 - (n/p), & \text{if } n/p \text{ is not an integer,} \\ \text{any positive number less than } 1 \text{ if } n/p \text{ is an integer.} \end{cases}$$

Moreover, there exists a constant $C = C(k, p, n, \theta, \Omega)$ such that

$$\|u\|_{C^{k-1-[n/p],\theta}(\Omega)} \leq C\|u\|_{W^{k,p}(\Omega)} \quad \text{for all } u \in W^{k,p}(\Omega). \quad \text{(C.4)}$$

Next, we list some results on elliptic regularity.

The following is adapted from [21, Theorem 8.32] by choosing $a^{ij} = \delta_{ij}, b^i = f^i = 0, i, j = 1, \ldots, n$. 


Theorem C.2 ([21, Theorem 8.32]). Let \( \theta \in (0, 1) \), and let \( u \in C^{1,\theta}(\Omega) \) be a weak solution of
\[
( - \Delta + c(x) \cdot \nabla + d(x)) u = g
\]
(C.5)
in a bounded domain \( \Omega \subset \mathbb{R}^n \), with \( c, d, g \in L^\infty(\Omega) \), with
\[
\max_{i=1,\ldots,n} \{ \| c_i \|_{L^\infty(\Omega)}, \| d \|_{L^\infty(\Omega)} \} \leq K.
\]
(C.6)
Then for any subdomain \( \Omega' \subset \subset \Omega \) we have
\[
\| u \|_{C^{1,\theta}(\Omega')} \leq C(\| u \|_{L^\infty(\Omega)} + \| g \|_{L^\infty(\Omega)}),
\]
(C.7)
for \( C = C(n, K, d') \) where \( d' = \text{dist}(\Omega', \Omega) \).

The following is adapted from [21, Theorem 9.11] by choosing \( a^{ij} = \delta_{ij}, i, j = 1, \ldots, n \).

Theorem C.3 ([21, Theorem 9.11]). Let \( \Omega \) be an open set in \( \mathbb{R}^n \) and \( u \in W^{2,p}_{\text{loc}}(\Omega) \cap L^p(\Omega) \), \( 1 < p < \infty \), a strong solution of the equation
\[
( - \Delta + b(x) \cdot \nabla + c(x)) u = f
\]
(C.8)
in \( \Omega \) with \( b, c \in L^\infty(\Omega) \), \( f \in L^p(\Omega) \), with
\[
\max_{i=1,\ldots,n} \{ \| b_i \|_{L^\infty(\Omega)}, \| c \|_{L^\infty(\Omega)} \} \leq \Lambda.
\]
(C.9)
Then for any subdomain \( \Omega' \subset \subset \Omega \),
\[
\| u \|_{W^{2,p}(\Omega')} \leq C(\| u \|_{L^p(\Omega)} + \| f \|_{L^p(\Omega)}),
\]
(C.10)
where \( C \) depends on \( n, p, \Lambda, \Omega', \) and \( \Omega \).

Theorem C.4 ([22, Lemma 2.4.1.4]). Let \( \Omega \) be an open and bounded set in \( \mathbb{R}^n \), let \( 2 \leq p < \infty \), and let \( u \in W^{2,2}(\Omega) \) be a strong solution of the equation
\[
- \Delta u = f
\]
(C.11)
in \( \Omega \) with \( f \in L^p(\Omega) \). Then \( u \in W^{2,p}_{\text{loc}}(\Omega) \).

REFERENCES

[1] Robert A. Adams and John J. F. Fournier, *Sobolev spaces*, second ed., Pure and Applied Mathematics (Amsterdam), vol. 140, Elsevier/Academic Press, Amsterdam, 2003.

[2] Reinhart Ahlrichs, Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and John D. Morgan III, *Bounds on the decay of electron densities with screening*, Phys. Rev. A (3) 23 (1981), no. 5, 2106–2117.

[3] Bernd Ammann, Catarina Carvalho, and Victor Nistor, *Regularity for Eigenfunctions of Schrödinger Operators*, Lett. Math. Phys. 101 (2012), no. 1, 49–84.
[4] Werner A. Bingel, *The Behaviour of the First-Order Density Matrix at the Coulomb Singularities of the Schrödinger Equation*, Z. Naturforsch. **18 a** (1963), 1249–1253.

[5] Anna Dall’Acqua, Søren Fournais, Thomas Østergaard Sørensen, and Edgardo Stockmeyer, *Real analyticity away from the nucleus of pseudorelativistic Hartree–Fock orbitals*, Anal. PDE **5** (2012), no. 3, 657–691.

[6] Lawrence C. Evans, *Partial Differential Equations*, second ed., Graduate Studies in Mathematics, vol. 19, American Mathematical Society, Providence, RI, 2010.

[7] Heinz-Jürgen Flad, Wolfgang Hackbusch, and Reinhold Schneider, *Best N-term approximation in electronic structure calculations. I. One-electron reduced density matrix*, M2AN Math. Model. Numer. Anal. **40** (2006), no. 1, 49–61.

[8] Heinz-Jürgen Flad and Gohar Harutyunyan, *Ellipticity of quantum mechanical Hamiltonians in the edge algebra*, Discrete Contin. Dyn. Syst. (2011), no. Dynamical systems, differential equations and applications. 8th AIMS Conference. Suppl. Vol. I, 420–429.

[9] Heinz-Jürgen Flad, Gohar Harutyunyan, Reinhold Schneider, and Bert-Wolfgang Schulze, *Explicit Green operators for quantum mechanical Hamiltonians. I. The hydrogen atom*, Manuscripta Math. **135** (2011), no. 3–4, 497–519.

[10] Heinz-Jürgen Flad, Gohar Harutyunyan, and Bert-Wolfgang Schulze, *Explicit Green operators for quantum mechanical Hamiltonians. II. Edge type singularities of the helium atom*, ArXiv e-prints 1801.07552 (2018), 50 pp.

[11] Heinz-Jürgen Flad, Reinhold Schneider, and Bert-Wolfgang Schulze, *Asymptotic regularity of solutions to Hartree-Fock equations with Coulomb potential*, Math. Methods Appl. Sci. **31** (2008), no. 18, 2172–2201.

[12] Søren Fournais, Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and Thomas Østergaard Sørensen, *The Electron Density is Smooth Away from the Nuclei*, Comm. Math. Phys. **228** (2002), no. 3, 401–415.

[13] Søren Fournais, Maria Hoffmann-Ostenhof, and Thomas Hoffmann-Ostenhof, *Sharp Regularity Results for Coulombic Many-electron Wave Functions*, Mathematical Results in Quantum Mechanics (Taxco, 2001), Contemp. Math., vol. 307, Amer. Math. Soc., Providence, RI, 2002, pp. 143–148.

[14] Søren Fournais, *Analyticity of the density of electronic wavefunctions*, Ark. Mat. **42** (2004), no. 1, 87–106.

[15] Søren Fournais, *Sharp Regularity Results for Coulombic Many-electron Wave Functions*, Comm. Math. Phys. **255** (2005), no. 1, 183–227.

[16] Søren Fournais, *Analytic Structure of Many-Body Coulombic Wave Functions*, Commun. Math. Phys. **289** (2009), no. 1, 291–310.

[17] Søren Fournais, *Analytic structure of solutions to multiconfiguration equations*, J. Phys. A: Math. Theor. **42** (2009), 315208.

[18] Søren Fournais, Maria Hoffmann-Ostenhof, and Thomas Østergaard Sørensen, *Third Derivative of the One-Electron Density at the Nucleus*, Ann. Henri Poincaré **9** (2008), no. 7, 1387–1412.

[19] Søren Fournais, Thomas Østergaard Sørensen, Maria Hoffmann-Ostenhof, and Thomas Hoffmann-Ostenhof, *Non-Isotropic Cusp Conditions and Regularity of the Electron Density of Molecules at the Nuclei*, Ann. Henri Poincaré **8** (2007), no. 4, 731–748.
[20] Richard Froese and Ira Herbst, *Exponential Bounds and Absence of Positive Eigenvalues for N-Body Schrödinger Operators*, Comm. Math. Phys. **87** (1982), no. 3, 429–447.

[21] David Gilbarg and Neil S. Trudinger, *Elliptic Partial Differential Equations of Second Order*, Classics in Mathematics, Springer-Verlag, Berlin, 2001, Reprint of the 1998 edition.

[22] Pierre Grisvard, *Elliptic Problems in Nonsmooth Domains*, Monographs and Studies in Mathematics, vol. 24, Pitman (Advanced Publishing Program), Boston, MA, 1985.

[23] Maria Hoffmann-Ostenhof and Thomas Hoffmann-Ostenhof, “Schrödinger inequalities” and asymptotic behavior of the electron density of atoms and molecules, Phys. Rev. A (3) **16** (1977), no. 5, 1782–1785.

[24] ———, *Local properties of solutions of Schrödinger equations*, Comm. Partial Differential Equations **17** (1992), no. 3-4, 491–522.

[25] Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, Reinhart Ahlrichs, and John D. Morgan III, *On the exponential fall off of wavefunctions and electron densities*, Mathematical problems in theoretical physics (Proc. Internat. Conf. Math. Phys., Lausanne, 1979), Lecture Notes in Phys., vol. 116, Springer, Berlin-New York, 1980, pp. 62–67.

[26] Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and Nikolai Nadirashvili, *Interior Hölder estimates for solutions of Schrödinger equations and the regularity of nodal sets*, Comm. Partial Differential Equations **20** (1995), no. 7-8, 1241–1273.

[27] Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and Thomas Østergaard Sørensen, *Electron Wavefunctions and Densities for Atoms*, Ann. Henri Poincaré **2** (2001), no. 1, 77–100.

[28] Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and Hanns Stremnitzer, *Local Properties of Coulombic Wave Functions*, Comm. Math. Phys. **163** (1994), no. 1, 185–215.

[29] Maria Hoffmann-Ostenhof and Ruedi Seiler, *Cusp conditions for eigenfunctions of n-electron systems*, Phys. Rev. A (3) **23** (1981), no. 1, 21–23.

[30] Lars Hörmander, *Linear Partial Differential Operators*, Third revised printing. Die Grundlehren der mathematischen Wissenschaften, Band 116, Springer-Verlag New York Inc., New York, 1969.

[31] Robert Jastrow, *Many-body Problem with Strong Forces*, Phys. Rev. **98** (1955), 1479–1484.

[32] Thierry Jecck, *A New Proof of the Analyticity of the Electronic Density of Molecules*, Lett. Math. Phys. **93** (2010), no. 1, 73–83.

[33] Tosio Kato, *Fundamental Properties of Hamiltonian Operators of Schrödinger Type*, Trans. Amer. Math. Soc. **70** (1951), 195–211.

[34] ———, *On the Eigenfunctions of Many-Particle Systems in Quantum Mechanics*, Comm. Pure Appl. Math. **10** (1957), 151–177.

[35] Jean Leray, *Sur les Solutions de l’Équation de Schrödinger Atomique et le Cas Particulier de deux Electrons*, Trends and Applications of Pure Mathematics to Mechanics (Palaiseau, 1983), Lecture Notes in Phys., vol. 195, Springer, Berlin, 1984, pp. 235–247.

[36] Paul G. Mezey, *The holographic electron density theorem and quantum similarity measures*, Molecular Physics **96** (1999), no. 2, 169–178.
[37] Barry Simon, *Exponential decay of quantum wave functions*,
http://www.math.caltech.edu/simon/Selecta/ExponentialDecay.pdf,
Online notes, part of Barry Simon’s Online Selecta at
http://www.math.caltech.edu/simon/selecta.html.

[38] _____, *Schrödinger semigroups*, Bull. Amer. Math. Soc. (N.S.) 7 (1982), no. 3,
447–526.

[39] _____, *Tosio Kato’s Work on Non–Relativistic Quantum Mechanics*, ArXiv
e-prints 1711.00528 (2017), 215 pp.

[40] Erich Steiner, *Charge Densities in Atoms*, J. Chem. Phys. 39 (1963), no. 9,
2365–2366.

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