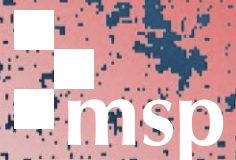


PROBABILITY and MATHEMATICAL PHYSICS

**THE DIAGONAL BEHAVIOUR OF THE
ONE-PARTICLE COULOMBIC DENSITY MATRIX**

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4:4
2023



THE DIAGONAL BEHAVIOUR OF THE ONE-PARTICLE COULOMBIC DENSITY MATRIX

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We obtain bounds for all derivatives of the nonrelativistic Coulombic one-particle density matrix $\gamma(x, y)$ near the diagonal $x = y$.

1. Introduction

Consider on $L^2(\mathbb{R}^{3N})$ the Schrödinger operator

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_0 + V, \quad \mathcal{H}_0 = -\Delta = -\sum_{k=1}^N \Delta_k, \\ V(\mathbf{x}) &= -Z \sum_{k=1}^N \frac{1}{|x_k|} + \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|}, \end{aligned} \quad (1-1)$$

describing an atom with N particles (e.g., electrons) with coordinates $\mathbf{x} = (x_1, x_2, \dots, x_N)$, $x_k \in \mathbb{R}^3$, $k = 1, 2, \dots, N$, and a nucleus with charge $Z > 0$. The notation Δ_k is used for the Laplacian with respect to the variable x_k . The operator $\mathcal{H}$ acts on the Hilbert space $L^2(\mathbb{R}^{3N})$ and by standard methods one proves that it is self-adjoint on the domain $D(\mathcal{H}) = W^{2,2}(\mathbb{R}^{3N})$; see, e.g., [25, Theorem X.16]. (Here and throughout the paper we use the standard notation $W^{l,p}$ for the Sobolev spaces, where l and p indicate the smoothness and summability respectively). Our methods allow consideration of the molecular Schrödinger operator, but we restrict our attention to the atomic case for simplicity. Let $\psi = \psi(\mathbf{x})$ be an eigenfunction of the operator $\mathcal{H}$ with an eigenvalue $E \in \mathbb{R}$, i.e., $\psi \in D(\mathcal{H})$ and

$$(\mathcal{H} - E)\psi = 0.$$

For each $j = 1, \dots, N$, we represent

$$\mathbf{x} = (x_j, \hat{\mathbf{x}}_j), \quad \text{where } \hat{\mathbf{x}}_j = (x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_N),$$

with obvious modifications if $j = 1$ or $j = N$. The one-particle density matrix is defined as the function

$$\gamma_0(x, y) = \sum_{j=1}^N \int_{\mathbb{R}^{3N-3}} \psi(x, \hat{\mathbf{x}}_j) \overline{\psi(y, \hat{\mathbf{x}}_j)} d\hat{\mathbf{x}}_j, \quad \text{a.e. } x \in \mathbb{R}^3, \text{ a.e. } y \in \mathbb{R}^3. \quad (1-2)$$

MSC2020: primary 35B65; secondary 35J10, 81V55.

Keywords: multiparticle system, Schrödinger equation, one-particle density matrix.

This function is one of the key objects in multiparticle quantum mechanics; see [6; 7; 23; 24; 28] for details and further references. If one assumes that all N particles are spinless fermions (resp. bosons), i.e., that the function ψ is antisymmetric (resp. symmetric) under the permutations $x_j \leftrightarrow x_k$, then the definition (1-2) simplifies to

$$\gamma_0(x, y) = N \int_{\mathbb{R}^{3N-3}} \psi(x, \hat{x}) \overline{\psi(y, \hat{x})} d\hat{x}, \quad \text{where } \hat{x} = \hat{x}_1.$$

Our results however do not require any symmetry assumptions. We are interested in the smoothness properties of the function (1-2). It is clear that for this purpose it suffices to study each term in (1-2) individually. Moreover, using permutations of the variables it is sufficient to focus just on one term on the right-hand side of (1-2):

$$\gamma(x, y) = \int_{\mathbb{R}^{3N-3}} \psi(x, \hat{x}) \overline{\psi(y, \hat{x})} d\hat{x}, \quad \hat{x} = (x_2, x_3, \dots, x_N). \quad (1-3)$$

Throughout we refer to this function as the *one-particle density matrix*. In [9] (see also [18]) the *one-particle density*

$$\rho(x) = \gamma(x, x) = \int_{\mathbb{R}^{3N-3}} |\psi(x, \hat{x})|^2 d\hat{x} \quad (1-4)$$

was shown to be a real-analytic function of $x \neq 0$. The real analyticity of the function $\gamma(x, y)$ as a function of two variables on the domain

$$= \{(x, y) : |x| |y| \neq 0, x \neq y\} \subset \mathbb{R}^3 \times \mathbb{R}^3, \quad (1-5)$$

was proved in [16]. The method used in [18] was later extended in [19] to prove analyticity for all k -particle densities and k -particle density matrices on the appropriate subsets. In particular, the one-particle density γ was proved to be analytic on the same domain (1-5). As was pointed out in [16], one does not expect analyticity in x and y to hold on the diagonal $x = y$. In fact, quantum chemistry calculations in [4] (see also [5]) show that for each $x \neq 0$, the function γ has the following behaviour:

$$\operatorname{Re} \gamma(x + v, x - v) - \gamma(x, x) = C(x) |v|^5 + \tilde{g}(x, v) \quad \text{as } v \rightarrow 0, \quad (1-6)$$

where $C(x)$ is some nonzero function, and the expansion of function $\tilde{g}(x, v)$ does not contain powers $|v|$, $|v|^3$ and $|v|^5$. Motivated in part by (1-6), in the current paper we aim to obtain explicit bounds for all partial derivatives of $\gamma(x, y)$ near the diagonal $x = y$ or the points $x = 0$ and $y = 0$. For the derivatives of γ we use the standard notation $\partial_x^m \partial_y^l \gamma(x, y)$, where $m, l \in \mathbb{N}_0$, $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. For two nonnegative numbers (or functions) X and Y depending on some parameters, we write $X \lesssim Y$ (or $Y \gtrsim X$) if $X \leq CY$ with some positive constant C independent of those parameters. The notation $B(x, R)$ is used for the open ball of radius R centred at the point x .

For $b \geq 0, t > 0$ we define

$$h_b(t) = \begin{cases} 1 & \text{if } b < 5, \\ \log(t^{-1} + 2) & \text{if } b = 5, \\ 1 + t^{5-b} & \text{if } b > 5. \end{cases} \quad (1-7)$$

The next theorem contains the main result.

Theorem 1.1. *Let ψ be an eigenfunction, and let $R > 0$ be fixed. Then for all $x \neq 0$, $y \neq 0$, $x \neq y$, and all $l, m \in \mathbb{Z}_0^3$ such that $|l| \geq 1$, $|m| \geq 1$, we have*

$$|\partial_x^l \partial_y^m \gamma(x, y)| \lesssim (1 + |x|^{2-|l|} + |y|^{2-|l|-|m|} + h_{|l|+|m|}(|x-y|)) \|\rho\|_{L^1(B(x,R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y,R))}^{\frac{1}{2}}. \quad (1-8)$$

Furthermore, for all $|l| \geq 1$,

$$|\partial_x^l \gamma(x, y)| + |\partial_y^l \gamma(x, y)| \lesssim (1 + |x|^{1-|l|} + |y|^{1-|l|} + h_{|l|}(|x-y|)) \|\rho\|_{L^1(B(x,R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y,R))}^{\frac{1}{2}}. \quad (1-9)$$

The implicit constants in (1-8) and (1-9) may depend on l, m and R , but are independent of x, y and the function ψ .

Remark 1.2. (1) [Theorem 1.1](#) naturally extends to the case of a molecule with several nuclei whose positions are fixed. The modifications are straightforward.

- (2) Observe that $\|\rho\|_{L^1(B(x,R))} \leq \|\psi\|_{L^2(\mathbb{R}^{3N})}^2$, $R > 0$, so that the right-hand sides of (1-8) and (1-9) are finite.
- (3) Comparing the derivatives $\partial_x^l \partial_y^m \gamma(x, y)$, $|l| \geq 1$, $|m| \geq 1$, and, for example, $\partial_x^n \gamma(x, y)$ of the same order, i.e., with $|m| + |l| = |n|$, we see from (1-8) and (1-9) that the derivative $\partial_x^n \gamma(x, y)$ is “allowed” to be more singular than $\partial_x^l \partial_y^m \gamma(x, y)$ at $x = 0$ or $y = 0$. This can be explained by the following intuitive argument. Taking one derivative does not make the function ψ (and hence the function $\gamma(x, y)$) “more singular”, as the bound (4-6) (or (4-7)) below shows. This property is exploited twice in (1-8) where the derivatives fall on each of the two variables at least once. This “saves” one order of singularity compared to (1-9) where all the derivatives fall on one variable.
- (4) The bound (1-9) for $|l| = 1$ implies that $\gamma(x, y)$ is a Lipschitz function on $\mathbb{R}^3 \times \mathbb{R}^3$.
- (5) The bounds (1-8), (1-9) ensure that $\gamma \in W_{\text{loc}}^{5,p}(\cdot)$ with arbitrary $p < \infty$; see (1-5) for the definition of $\cdot$. By [Proposition A.1](#) in the [Appendix](#), this implies that $\gamma \in W_{\text{loc}}^{5,p}(\mathbb{R}^3 \setminus \{0\}) \times (\mathbb{R}^3 \setminus \{0\})$, which means that $\gamma \in W_{\text{loc}}^{4,\theta}(\mathbb{R}^3 \setminus \{0\}) \times (\mathbb{R}^3 \setminus \{0\})$ for all $\theta < 1$. This result just barely misses the 4,1 -smoothness of the factor $|x-y|^5$ in the formula (1-6). In this sense [Theorem 1.1](#) is sharp, up to a log-term.
- (6) The one-electron density $\rho(x) = \gamma(x, x)$ is known to be real analytic for $x \neq 0$, see [\[9\]](#). As shown in [\[12\]](#), the function $\rho(x)$ satisfies the bound

$$|\partial_x^l \rho(x)| \lesssim (1 + |x|^{1-|l|}) \|\rho\|_{L^1(B(x,R))} \quad \text{for all } l \in \mathbb{Z}_0^3, \quad x \neq 0. \quad (1-10)$$

As in [Remark 1.2\(3\)](#) above, it is immediate from this bound that ρ is Lipschitz. This fact was first proved in [\[17\]](#). For $|l| \leq 4$ the bound (1-10) follows from (1-8) and (1-9).

- (7) There is an independent (indirect) argument indicating that $\gamma(x, y)$ should have a $|x-y|^5$ -singularity on the diagonal. More precisely, assume that $\gamma(x, y) = \gamma_1(x, y) + \gamma_2(x, y)|x-y|^b$ with some $b > 3$, where γ_1, γ_2 are smooth functions of x and y . Then one can show that necessarily $b = 5$. This argument is based on the analysis of spectral asymptotics of the (nonnegative) operator Γ with kernel $\gamma_0(x, y)$; see (1-2). It was shown in [\[26\]](#) that the eigenvalues $\lambda_k(\Gamma)$ have asymptotics of

order $k^{-8/3}$ as $k \rightarrow \infty$. On the other hand, according to the results on spectral asymptotics for integral operators with homogeneous kernels, see [3] (and also [26] for a summary), the singularity $|x - y|^b$, $b \neq 0, 2, 4, \dots$, would produce the spectral asymptotics of order $k^{-(1+b/3)}$. The exponent $1 + b/3$ coincides with $8/3$ exactly for $b = 5$, which proves the point.

- (8) Understanding the behaviour of $\gamma(x, y)$ at the diagonal has implications for the rate of convergence of approximation schemes for eigenfunctions ψ ; see, e.g., [4]. In particular, the eigenvalues of the operator Γ with kernel $\gamma_0(x, y)$ play a vital role in the convergence rates of the configurational interaction (CI) model, [28, Section 4.4]. See [14] for an example of a CI convergence result for the ground state of a Helium atom.

Our proofs have two main ingredients. At the heart of our method are regularity properties of the eigenfunction ψ . By the standard elliptic argument, the function ψ is real analytic away from the singularities of the potential (1-1), i.e., away from the particle coalescence points. According to T. Kato's seminal paper [20], at the coalescence points the function ψ is Lipschitz. More recent contributions to the study of the regularity of ψ include [1; 2; 9; 10; 11; 17]. A detailed analysis of smoothness properties of ψ was conducted in the recent paper [12], to which we also refer for further bibliography. In particular, this paper provides global pointwise bounds for partial derivatives of ψ . In the study of the one-particle density (1-4) conducted in [8; 9; 12] the key point was to obtain bounds for certain directional derivatives of ψ . Such derivatives are also critical for our analysis in the current paper, and we explain their importance below.

Let $R = \{1, 2, \dots, N\}$ be the set of all particle labels. A subset $P \subset R$ is called a *cluster*. For each cluster P we define the following *cluster (directional) derivative*:

$$m = \left(\sum_{k \in P} \partial_{x'_k} \right)^{m'} \left(\sum_{k \in P} \partial_{x''_k} \right)^{m''} \left(\sum_{k \in P} \partial_{x'''_k} \right)^{m'''} \quad (1-11)$$

Here $m = (m', m'', m''')$ with $m', m'', m''' \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$ and $x = (x', x'', x''')$ with $x', x'', x''' \in \mathbb{R}$. Such cluster derivatives were introduced in [8; 9] because they annihilate certain Coulomb terms in (1-1) which remain singular under usual partial derivatives. To illustrate this observe that for all $m \neq 0$,

$$m \frac{1}{|x_j - x_k|} = 0, \quad \text{if } j, k \in P \text{ or } j, k \notin P.$$

Therefore the potential (1-1) is infinitely smooth with respect to x as long as $x_j \neq 0$, $j = 1, 2, \dots, N$, and $x_j \neq x_k$, where $j \in P, k \notin P$ or $j \notin P, k \in P$. As a consequence, the function ψ is also infinitely smooth with respect to x for the same values of the coordinates; see [8], [9] or [16]. In particular, the cluster derivatives of ψ do not have singularities at the coalescence points $x_j = x_k$, if $j, k \in P$ or $j, k \notin P$. One of the pivotal points in [12] was the pointwise bound for the cluster derivative $m \psi(x)$ with explicit dependence on the distance of $x \in \mathbb{R}^{3N}$ to the coalescence set

$$\Sigma = \left\{ x \in \mathbb{R}^{3N} : \prod_{j \in P} |x_j| \prod_{k \in P, l \in P^c} |x_k - x_l| = 0 \right\}.$$

For our purposes we need bounds of such type for cluster derivatives involving an arbitrary finite number M of clusters $P_1, P_2, \dots, P_M$, i.e., for $\prod_{i=1}^{m_1} \prod_{j=2}^{m_2} \dots \prod_{M}^{m_M} \psi$; see [Corollary 4.6](#). This generalization is not immediate and requires substantial further work, which is done in [Sections 3](#) and [4](#).

The next step of the proof is to use the bounds obtained for cluster derivatives to estimate partial derivatives of the function [\(1-3\)](#). To this end we use a partition of unity consisting of smooth functions $\Phi(x, y, \hat{x})$ of $3N + 3$ variables that we call *extended cut-off functions*, and study the integrals

$$\gamma(x, y; \Phi) = \int_{\mathbb{R}^{3N-3}} \Phi(x, y, \hat{x}) \psi(x, \hat{x}) \overline{\psi(y, \hat{x})} d\hat{x}. \quad (1-12)$$

These extended cut-offs were introduced in [\[16\]](#) to establish the real analyticity of $\gamma(x, y)$ outside the diagonal. They generalize the cut-offs instrumental in the study of the density $\rho(x)$ in [\[8; 9\]](#).

The support of each extended cut-off divides the particles $x_2, x_3, \dots, x_N$ into three disjoint groups: the first two groups consist of particles that are “close” to the particles x and y respectively, and the third group contains the particles that are “far” from the first two groups. This partition naturally gives rise to two clusters, denoted P and S : cluster P labels the particles close to x , and cluster S the particles close to y . Thus, when differentiating the integral [\(1-12\)](#) with respect to x and y , under the integral these derivatives convert into the cluster derivatives ∂_P and ∂_S respectively. This general method of differentiating integrals such as [\(1-12\)](#) was developed in [\[8; 9; 16\]](#). We can illustrate it using the following simplified example. Let us differentiate with respect to x the integral

$$F(x) = \int f(x, \hat{x}) d\hat{x},$$

where the integration is conducted over the space $\mathbb{R}^{3N-3}$, and we assume for simplicity that $f \in C_0^\infty(\mathbb{R}^{3N})$. To this end under the integral we make the change of variables $\hat{x} = \hat{w} + \hat{z}$, where $\hat{z} = (z_2, z_3, \dots, z_N) \in \mathbb{R}^{3N-3}$ is defined by $z_j = x$, $j \in P$, and $z_j = 0$, $j \notin P$, for some cluster P such that $1 \in P$. Thus $F(x)$ rewrites as

$$F(x) = \int f(x, \hat{w} + \hat{z}) d\hat{w}.$$

Consequently, for all $l \in \mathbb{N}_0^3$, we have

$$\partial_x^l F(x) = \int (\partial^l f)(x, \hat{w} + \hat{z}) d\hat{w} = \int \partial^l f(x, \hat{x}) d\hat{x}.$$

In order to estimate the derivatives of the integral [\(1-12\)](#), we use the bounds for cluster derivatives of ψ linked to clusters P and S that are obtained in the first stage of the proof. Integrating these bounds in $\hat{x}$ leads to [\(1-8\)](#) and [\(1-9\)](#) thereby completing the proof; see [Section 6](#).

The paper is organized as follows. In [Section 2](#) we gather information about cut-off functions and clusters associated with them. Most of the required facts are borrowed from [\[16\]](#). [Section 3](#) considers the general elliptic equation of the form [\(3-1\)](#) in a ball $B(x_0, \ell) = \{x : |x - x_0| < \ell\} \subset \mathbb{R}^{3N}$. Here we study cluster derivatives of solutions of [\(3-1\)](#), and the main focus is on the explicit dependence of these estimates on the radius ℓ , see [Theorem 3.2](#). In [Section 4](#) these estimates are applied to the Schrödinger equation to derive the bounds for the cluster derivatives of ψ , summarized in [Corollary 4.6](#). Some estimates for integrals emerging in the proof of [Theorem 1.1](#) are gathered in [Section 5](#). The proof itself is completed in [Section 6](#). The [Appendix](#) contains an elementary extension property for the Sobolev spaces that was proved in [\[27\]](#).

Notation. We conclude the introduction with some general notational conventions.

Coordinates. As mentioned earlier, we use the following standard notation for the coordinates: $\mathbf{x} = (x_1, x_2, \dots, x_N)$, where $x_j \in \mathbb{R}^3$, $j = 1, 2, \dots, N$. As a rule we represent $\mathbf{x}$ in the form $\mathbf{x} = (x_1, \hat{\mathbf{x}})$ with $\hat{\mathbf{x}} = (x_2, x_3, \dots, x_N) \in \mathbb{R}^{3N-3}$.

For $N \geq 3$ it is also useful to introduce the notation for $\hat{\mathbf{x}}$ with x_j , $j \geq 2$, taken out. Let

$$\tilde{\mathbf{x}}_j = (x_2, \dots, x_{j-1}, x_{j+1}, \dots, x_N), \quad (1-13)$$

so that $\hat{\mathbf{x}} = (x_j, \tilde{\mathbf{x}}_j)$ and $\mathbf{x} = (x_1, x_j, \tilde{\mathbf{x}}_j)$.

Clusters. Let $R = \{1, 2, \dots, N\}$. A subset $P \subset R$ is called a *cluster*. We denote $|P| = \text{card } P$, $P^c = R \setminus P$, $P^* = P \setminus \{1\}$. If $P = \emptyset$, then $|P| = 0$ and $P^c = R$.

For M clusters $P_1, \dots, P_M$ we write $\mathbf{P} = \{P_1, P_2, \dots, P_M\}$, and call $\mathbf{P}$ a *cluster set*. Clusters $P_1, P_2, \dots, P_M$ in a cluster set are not assumed to be all disjoint or distinct.

Derivatives. Let $\mathbb{R}_0^3 = \mathbb{R}^3 \cup \{0\}$. If $x = (x', x'', x''') \in \mathbb{R}^3$ and $m = (m', m'', m''') \in \mathbb{R}_0^3$, then the derivative ∂_x^m is defined in the standard way:

$$\partial_x^m = \partial_{x'}^{m'} \partial_{x''}^{m''} \partial_{x'''}^{m'''}$$

This notation extends to $x \in \mathbb{R}^d$ with an arbitrary dimension $d \geq 1$ in the obvious way. Denote also

$$\partial^{\mathbf{m}} = \partial_{x_1}^{m_1} \partial_{x_2}^{m_2} \dots \partial_{x_N}^{m_N}, \quad \mathbf{m} = (m_1, m_2, \dots, m_N) \in \mathbb{R}_0^{3N}.$$

Let $\mathbf{P} = \{P_1, P_2, \dots, P_M\}$ be a cluster set, and let $\mathbf{m} = (m_1, m_2, \dots, m_M)$, $m_k \in \mathbb{R}_0^3$, $k = 1, 2, \dots, M$. Then we denote

$$\mathbf{m}_{\mathbf{P}} = \begin{pmatrix} m_1 & m_2 & \dots & m_M \\ 1 & 2 & \dots & M \end{pmatrix},$$

where each individual cluster derivative is defined as in (1-11). It is easy to see that the cluster derivatives satisfy the Leibniz rule. We use this fact without further comments throughout.

Supports. For any smooth function $f = f(\mathbf{x})$, we define $\text{supp}_0 f = \{\mathbf{x} : f(\mathbf{x}) \neq 0\}$. It is clear that the closure $\overline{\text{supp}_0 f}$ coincides with the support $\text{supp } f$ defined in the standard way. With this definition we immediately get the useful property that

$$\text{supp}_0(fg) = \text{supp}_0 f \cap \text{supp}_0 g.$$

Bounds. As explained earlier, for two nonnegative numbers (or functions) X and Y depending on some parameters, we write $X \lesssim Y$ (or $Y \gtrsim X$) if $X \leq CY$ with some positive constant C independent of those parameters. If $X \lesssim Y$ and $Y \lesssim X$, then $X \asymp Y$. To avoid confusion we often make explicit comments on the nature of (implicit) constants in the bounds. In particular, all constants (implicit or explicit) may depend on the eigenvalue E , the number of particles N and the charge Z .

2. Cut-off functions and clusters

2A. Admissible cut-off functions. Let

$$\xi \in {}_0^\infty(\mathbb{R}) : 0 \leq \xi(t) \leq 1, \quad \xi(t) = \begin{cases} 1 & \text{if } |t| \leq 1, \\ 0 & \text{if } |t| \geq 2. \end{cases} \quad (2-1)$$

Now for $\varepsilon > 0$ we define two radially symmetric functions $\zeta \in {}_0^\infty(\mathbb{R}^3)$, $\theta \in {}_0^\infty(\mathbb{R}^3)$ as follows:

$$\zeta(x) = \zeta_\varepsilon(x) = \xi\left(\frac{4N}{\varepsilon}|x|\right), \quad \theta(x) = \theta_\varepsilon(x) = 1 - \zeta_\varepsilon(x), \quad x \in \mathbb{R}^3, \quad (2-2)$$

so that

$$\zeta(x) = 0 \quad \text{for } x \notin B(0, \varepsilon(2N)^{-1}), \quad \theta(x) = 0 \quad \text{for } x \in B(0, \varepsilon(4N)^{-1}).$$

The dependence of the cut-offs on the parameter ε is important, but it is not always reflected in the notation.

Our next step is to build out of the functions ζ_ε and θ_ε cut-off functions of $3N$ variables. Let $\{f_{jk}\}$, $1 \leq j, k \leq N$, be a set of functions such that each of them is one of the functions ζ_ε or θ_ε , and $f_{jk} = f_{kj}$. We call functions of the form

$$\phi(\mathbf{x}) = \prod_{1 \leq j < k \leq N} f_{jk}(x_j - x_k). \quad (2-3)$$

admissible cut-off functions or simply *admissible cut-offs*. Such cut-offs (or, more precisely, a slightly more general version thereof) were used in [8; 9; 16]. We need only a subset of their properties established in [9; 16].

As in [8; 9; 16], we associate with the function ϕ a cluster $Q(\phi)$ defined next.

Definition 2.1. For an admissible cut-off ϕ , let $I(\phi) \subset \{(j, k) \in \mathbb{R} \times \mathbb{R} : j \neq k\}$ be the index set such that $(j, k) \in I(\phi)$, if and only if $f_{jk} = \zeta$. We say that two indices $j, k \in \mathbb{R}$, are ϕ -linked to each other if either $j = k$, or $(j, k) \in I(\phi)$, or there exists a sequence of pairwise distinct indices $j_1, j_2, \dots, j_s$, $1 \leq s \leq N - 2$, all distinct from j and k , such that $(j, j_1), (j_s, k) \in I(\phi)$ and $(j_p, j_{p+1}) \in I(\phi)$ for all $p = 1, 2, \dots, s - 1$.

The cluster $Q(\phi)$ associated with the cut-off ϕ is defined as the set of all indices that are ϕ -linked to index 1.

It follows from the above definition that $Q(\phi)$ always contains the index 1. Note also that the notion of being linked defines an equivalence relation on $\mathbb{R}$, and the cluster $Q(\phi)$ is nothing but the equivalence class containing index 1. On the support of the admissible cut-off ϕ the variables x_j , indexed by $j \in Q(\phi)$, are “close” to each other and are “far” from the remaining variables. In order to quantify these facts below we define a number of subsets in $\mathbb{R}^{3N}$ and $\mathbb{R}^{3N-3}$.

For any cluster P we introduce the following sets depending on the parameter $\varepsilon > 0$:

$$X(\varepsilon) = \begin{cases} \mathbb{R}^{3N} & \text{for } |P| = 0 \text{ or } N, \\ \{\mathbf{x} \in \mathbb{R}^{3N} : |x_j - x_k| > \varepsilon, \forall j \in P, k \in P^c\} & \text{for } 0 < |P| < N. \end{cases}$$

The set $X(\varepsilon)$ separates the points x_k and x_j labeled by the clusters P and P^c respectively. Note that $X(\varepsilon) = X^c(\varepsilon)$. Define also the sets separating x_k 's from the origin:

$$T(\varepsilon) = \begin{cases} \mathbb{R}^{3N} & \text{for } |P| = 0, \\ \{\mathbf{x} \in \mathbb{R}^{3N} : |x_j| > \varepsilon, \forall j \in P\} & \text{for } |P| > 0. \end{cases}$$

It is also convenient to introduce corresponding sets in the space $\mathbb{R}^{3N-3}$:

$$\widehat{X}(\mathbf{x}, \varepsilon) = \{\hat{\mathbf{x}} \in \mathbb{R}^{3N-3} : (\mathbf{x}, \hat{\mathbf{x}}) \in X(\varepsilon)\} \quad \text{for all } \mathbf{x} \in \mathbb{R}^3, \quad (2-4)$$

and

$$\widehat{T}(\varepsilon) = \begin{cases} \mathbb{R}^{3N-3} & \text{for } |P^*| = 0, \\ \{\hat{\mathbf{x}} \in \mathbb{R}^{3N-3} : |x_j| > \varepsilon, \forall j \in P^*\} & \text{for } |P^*| > 0. \end{cases} \quad (2-5)$$

Observe that $\widehat{T}(\varepsilon) = \widehat{T}^*(\varepsilon)$.

The support of the admissible cut-off ϕ is easily described with the help of the sets introduced above. The next proposition is adapted from [9, Lemma 4.3(i); 16, Lemmata 4.2, 4.3].

Proposition 2.2. *For $P = Q(\phi)$ the inclusion*

$$\text{supp}_0 \phi \subset X(\varepsilon(4N-1))$$

holds.

Moreover, if $j \in Q(\phi)$, then $|x_1 - x_j| < \varepsilon/2$ for all $\mathbf{x} \in \text{supp}_0 \phi$. If $|x_1| > \varepsilon$, then

$$\text{supp}_0 \phi(x_1, \cdot) \subset \widehat{T}(\varepsilon/2).$$

We do not use Proposition 2.2 directly in this paper, but present it in order to demonstrate the relevance of the associated cluster $Q(\phi)$.

2B. Extended cut-offs. In our analysis the central role is played by another class of cut-off functions. These cut-offs are functions of $3N+3$ variables and they are defined as follows: for each $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$, $\hat{\mathbf{x}} \in \mathbb{R}^{3N-3}$ let

$$\Phi(\mathbf{x}, \mathbf{y}, \hat{\mathbf{x}}) = \prod_{2 \leq j \leq N} g_j(\mathbf{x} - \mathbf{x}_j) \prod_{2 \leq j \leq N} h_j(\mathbf{y} - \mathbf{x}_j) \prod_{2 \leq k < l \leq N} f_{kl}(\mathbf{x}_k - \mathbf{x}_l), \quad (2-6)$$

where each of the functions g_j, h_j and $f_{jk} = f_{kj}$ is one of the cut-offs θ or ζ defined in (2-2). We call such functions *extended cut-offs*. Each extended cut-off uniquely defines two admissible cut-offs:

$$\phi(\mathbf{x}, \hat{\mathbf{x}}) = \prod_{2 \leq j \leq N} g_j(\mathbf{x} - \mathbf{x}_j) \prod_{2 \leq k < l \leq N} f_{kl}(\mathbf{x}_k - \mathbf{x}_l), \quad (2-7)$$

$$\mu(\mathbf{y}, \hat{\mathbf{x}}) = \prod_{2 \leq j \leq N} h_j(\mathbf{y} - \mathbf{x}_j) \prod_{2 \leq k < l \leq N} f_{kl}(\mathbf{x}_k - \mathbf{x}_l); \quad (2-8)$$

see definition (2-3). We say that the pair ϕ, μ and the extended cut-off Φ are associated to each other. We denote by $P = Q(\phi)$ and $S = Q(\mu)$ the clusters associated with ϕ and μ respectively.

We recall that the functions ϕ , μ and Φ all depend on the parameter ε . Thus whenever necessary we include ε in the notation and write, for example, $\Phi(x, y, \hat{x}; \varepsilon)$. Note however that the clusters P and S associated with the admissible cut-offs ϕ and μ do not depend on ε .

Below we list some useful properties of the extended cut-offs Φ and associated admissible ϕ , μ adapted from [16, Lemmata 4.6, 4.8].

Proposition 2.3. *If $P^* \cap S$ is nonempty and $|x - y| > \varepsilon$, then $\Phi(x, y, \hat{x}; \varepsilon) = 0$ for all $\hat{x} \in \mathbb{R}^{3N-3}$.*

In the estimates further on we assume, as a rule, that $|x - y| > \varepsilon$, so due to Proposition 2.3 from now on we may suppose that $P^* \subset S^c$ (which is equivalent to $S^* \subset P^c$). Under this condition we obtain the following information about the support of the extended cut-off Φ :

Proposition 2.4. *If $P^* \subset S^c$, then for all $x, y \in \mathbb{R}^3$ we have*

$$\text{supp}_0 \Phi(x, y, \cdot; \varepsilon) \subset \widehat{X}_{x, \varepsilon(4N-1)} \cap \widehat{X}_{S^*, x, \varepsilon(4N-1)} \cap \widehat{X}_{S, y, \varepsilon(4N-1)} \cap \widehat{X}_{S^*, y, \varepsilon(4N-1)}. \quad (2-9)$$

If, in addition $|x| > \varepsilon$, $|y| > \varepsilon$, then

$$\text{supp}_0 \Phi(x, y, \cdot; \varepsilon) \subset \widehat{T}_{S^*}(\varepsilon/2) \cap \widehat{T}_S(\varepsilon/2). \quad (2-10)$$

To complete this section we need to make a remark on the cluster derivatives of the extended cut-offs. For any cluster $Q \subset R$ we denote by $\frac{m}{x, Q} \Phi(x, y, \hat{x})$ the cluster derivative of Φ as a function of the variables $(x, \hat{x})$, i.e.,

$$\frac{m}{x, Q} \Phi(x, y, \hat{x}) = \frac{m}{Q} \tilde{\Phi}_y(x, \hat{x}), \quad \text{where } \tilde{\Phi}_y(x, \hat{x}) := \Phi(x, y, \hat{x}). \quad (2-11)$$

Similarly we define the derivative $\frac{m}{y, Q} \Phi(x, y, \hat{x})$. It immediately follows from the definition of $\Phi(x, y, \hat{x})$ that for any clusters Q_1, Q_2 and all $\mathbf{m} = (m_1, m_2) \in \mathbb{N}_0^2$, the bound

$$|\frac{m_1}{x, Q_1} \frac{m_2}{y, Q_2} \Phi(x, y, \hat{x}; \varepsilon)| \lesssim \begin{cases} 1 & \text{if } |\mathbf{m}| = 0, \\ \varepsilon^{-|\mathbf{m}|} \mathcal{M}_\varepsilon(x, y, \hat{x}) & \text{if } |\mathbf{m}| \geq 1, \end{cases} \quad (2-12)$$

holds, where

$$\mathcal{M}_\varepsilon(x, y, \hat{x}) = \sum_{2 \leq j \leq N} \xi_{N\varepsilon^{-1}|x - x_j|} + \sum_{2 \leq j \leq N} \xi_{N\varepsilon^{-1}|y - x_j|} + \sum_{2 \leq j < k \leq N} \xi_{N\varepsilon^{-1}|x_j - x_k|}; \quad (2-13)$$

see (2-1) for the definition of the function ξ .

3. Regularity estimates

3A. $\mathcal{C}^{1,\theta}$ -regularity for elliptic equations. In what follows we rely on the well-known $\mathcal{C}^{1,\theta}$ -regularity bounds for solutions of second order elliptic equations on bounded domains. This type of regularity is discussed, e.g., in [21, Chapter 3; 13, Chapter 8]. To be precise, therein one can find bounds even in the space $\mathcal{C}^{1,\theta}$.

with a suitable $\theta \in (0, 1)$, but we are not concerned with the Hölder properties. Moreover, in this paper we do not need the most general form of the equation. For our purposes it suffices to consider the equation

$$\Delta + \mathbf{a}(x) \cdot \nabla + b(x)u = g, \quad (3-1)$$

on an open ball $B \subset \mathbb{R}^d$, where all the coefficients are $L^\infty(B)$ -functions. The proposition below provides some convenient sup-norm bounds for the weak solution and its first derivatives. Since the proof is quite short, we provide it for the sake of completeness. It is similar to the argument in [12, Proposition A.2].

Proposition 3.1. *Let $B_R = B(x_0, R) \subset \mathbb{R}^d$ for some $x_0 \in \mathbb{R}^d$ and $R > 0$. Suppose that $u \in W^{1,2}(B_R)$ is a weak solution of (3-1), where $\mathbf{a}, b, g \in L^\infty(B_R)$, and*

$$\|\mathbf{a}\|_{L^\infty(B_R)} + \|b\|_{L^\infty(B_R)} \leq M,$$

with some constant $M > 0$. Then for any $r \in (0, R)$ the function u belongs to $W^{2,2}(B_r) \cap {}^{-1}(\overline{B_r})$ and

$$\|u\|_{{}^{-1}(\overline{B_r})} \lesssim \|u\|_{L^2(B_R)} + \|g\|_{L^\infty(B_R)}, \quad (3-2)$$

with an implicit constant that depends only on the constant M , dimension d and the radii r and R .

Proof. The inclusion $u \in W^{2,2}(B_r)$ is a direct consequence of the standard interior regularity result given in, for example, [13, Theorem 8.8].

In order to prove that the weak solution $u \in W^{1,2}(B_R)$ has the ${}^{-1}$ -regularity in B_r we repeatedly apply the following elementary fact.

Assume that $u \in W^{1,p}(B_\rho)$ with some $p \in (1, \infty)$ and $\rho \leq R$. Then for any $\nu < \rho$ the following is true:

(1) If $p \leq d$, then $u \in W^{1,q}(B_\nu)$ with $q = p(1 + d^{-1})$ and

$$\begin{aligned} \|u\|_{W^{1,q}(B_\nu)} &\lesssim \|u\|_{L^p(B_\rho)} + \|g\|_{L^p(B_\rho)} \\ &\lesssim \|u\|_{W^{1,p}(B_\rho)} + \|g\|_{L^\infty(B_\rho)}. \end{aligned} \quad (3-3)$$

(2) If $p > d$, then $u \in {}^{-1}(\overline{B_\nu})$ and

$$\begin{aligned} \|u\|_{{}^{-1}(\overline{B_\nu})} &\lesssim \|u\|_{L^p(B_\rho)} + \|g\|_{L^p(B_\rho)} \\ &\lesssim \|u\|_{W^{1,p}(B_\rho)} + \|g\|_{L^\infty(B_\rho)}. \end{aligned} \quad (3-4)$$

Indeed, under the assumption $u \in W^{1,p}(B_\rho)$, by interior L^p -estimates (see, e.g., [13, Theorem 9.11]) we have $u \in W^{2,p}(B_\nu)$ and the standard bound holds:

$$\|u\|_{W^{2,p}(B_\nu)} \lesssim \|u\|_{L^p(B_\rho)} + \|g\|_{L^p(B_\rho)}. \quad (3-5)$$

If $p < d$, then we use the bounded embedding $W^{2,p} \subset W^{1,q}$, for all $q \in [p, p^*]$, $p^* = dp(d - p)^{-1}$. In particular, the value $q = p(1 + d^{-1})$ belongs to the interval $[p, p^*]$, which proves (3-3). If $p = d$, then $W^{2,p} \subset W^{1,q}$ for all $q \in [p, \infty)$, and hence for $q = p(1 + d^{-1})$ in particular. Hence (3-3) holds again.

If $p > d$, then we use the embedding $W^{2,p} \subset {}^{-1}$, so that (3-5) leads to (3-4).

Let us proceed with the proof of (3-2). If $d = 1$, then the solution $u \in W^{1,2}(R)$ satisfies (3-4) with $p = 2$, which immediately implies (3-2). Suppose that $d \geq 2$, and define the sequence

$$q_n = 2(1 + d^{-1})^n, \quad n = 0, 1, \dots$$

Let $k \geq 1$ be the index such that $q_{k-1} \leq d$ and $q_k > d$. Pick finitely many numbers $r_n > 0$ such that

$$r < r_k < r_{k-1} < \dots < r_1 < r_0 = R.$$

Since $u \in W^{1,2}(B_R)$ we can apply the bound (3-3) with $v = r_1$, $\rho = R$ and $p = q_0 = 2$, $q = q_1$. Repeating this step successively for $\rho = r_n$, $v = r_{n+1}$ and $p = q_n$, $q = q_{n+1}$ for all $n = 1, \dots, k$, we arrive at the bound

$$\begin{aligned} \|u\|_{W^{1,q_k}(B_{r_k})} &\lesssim \|u\|_{W^{1,q_{k-1}}(B_{r_{k-1}})} + \|g\|_{L^\infty(B_{r_{k-1}})} \lesssim \dots \\ &\lesssim \|u\|_{W^{1,q_1}(B_{r_1})} + \|g\|_{L^\infty(B_{r_1})} \lesssim \|u\|_{L^2(B_R)} + \|g\|_{L^\infty(B_R)}. \end{aligned}$$

As $q_k > d$, we can now use (3-4) which gives

$$\begin{aligned} \|u\|_{W^{1,q_k}(B_{r_k})} &\lesssim \|u\|_{W^{1,q_k}(B_{r_k})} + \|g\|_{L^\infty(B_{r_k})} \\ &\lesssim \|u\|_{L^2(B_R)} + \|g\|_{L^\infty(B_R)}. \end{aligned}$$

This completes the proof of (3-2).

3B. Cluster derivatives. The next result is tailored for later use with the multiparticle Schrödinger equation. We assume in (3-1) that $d = 3N$ and the variable $\mathbf{x}$ is given by $\mathbf{x} = (x_1, x_2, \dots, x_N)$.

Now we obtain better regularity properties of the weak solution of (3-1) assuming some additional smoothness of the coefficients with respect to cluster derivatives. Precisely, consider a weak solution u of (3-1) in the ball $B(\mathbf{x}_0, R\ell)$ with some $\mathbf{x}_0 \in \mathbb{R}^{3N}$, $R > 0$, $\ell \in (0, 1]$. Suppose that for a cluster set $= \{P_1, P_2, \dots, P_M\}$ the coefficients $\mathbf{a}$ and $\mathbf{b}$ in (3-1) satisfy the bounds

$$|\mathbf{a}(\mathbf{x})| + |\mathbf{b}(\mathbf{x})| \lesssim \ell^{|\mathbf{m}|}, \quad \mathbf{x} \in B(\mathbf{x}_0, R\ell), \quad (3-6)$$

for all $\mathbf{m} \in \mathbb{N}_0^{3M}$, with constants potentially depending on $\mathbf{m}$, R and $\mathbf{x}_0$, but not on ℓ . In the next theorem we obtain bounds for the cluster derivatives $\mathbf{m}u$ with explicit dependence on the parameter $\ell \in (0, 1]$.

Theorem 3.2. Assume the conditions (3-6), and let u be a weak solution of (3-1) in $B(\mathbf{x}_0, R\ell)$ with the right-hand side $g = 0$. Then for all $\mathbf{m} \in \mathbb{N}_0^{3M}$ and all $r < R$ the cluster derivatives $\mathbf{m}u$ belong to $L^\infty(B(\mathbf{x}_0, r\ell))$. Furthermore, if $|\mathbf{m}| + k \geq 1$, where $k = 0, 1$, then for all $v \in (r, R)$ we have

$$\|\nabla^k \mathbf{m}u\|_{L^\infty(B(\mathbf{x}_0, r\ell))} \lesssim \ell^{1-|\mathbf{m}|+k} \ell \|u\|_{L^\infty(B(\mathbf{x}_0, v\ell))} + \|\nabla u\|_{L^\infty(B(\mathbf{x}_0, v\ell))}. \quad (3-7)$$

If $|\mathbf{m}| \geq 2$, then also

$$\|\mathbf{m}u\|_{L^\infty(B(\mathbf{x}_0, r\ell))} \lesssim \ell^{2-|\mathbf{m}|} \max_{l: |l|=2} \|\mathbf{l}u\|_{L^\infty(B(\mathbf{x}_0, v\ell))} + \|\nabla u\|_{L^\infty(B(\mathbf{x}_0, v\ell))} + \|u\|_{L^\infty(B(\mathbf{x}_0, v\ell))}. \quad (3-8)$$

The implicit constants in (3-7) and (3-8) may depend on the constants r , v , R , order $\mathbf{m}$ of the derivative, cluster set, and the constants in (3-6). In particular, if the constants in (3-6) are independent of $\mathbf{x}_0$, then so are the constants in (3-7) and (3-8).

In this paper we need the bound (3-7) only. Nevertheless, the bound (3-8) may be of independent interest.

The idea of the proof follows an argument in [12]. Namely, we rescale the problem by introducing the function

$$w(\mathbf{y}) = u(\mathbf{x}_0 + \ell \mathbf{y}), \quad \mathbf{y} \in B(\mathbf{0}, R),$$

and the coefficients

$$(\mathbf{y}) = \mathbf{a}(\mathbf{x}_0 + \ell \mathbf{y}), \quad \beta(\mathbf{y}) = b(\mathbf{x}_0 + \ell \mathbf{y}).$$

After the scaling (3-1) takes the form

$$\Delta w + 2\ell \cdot \nabla w + \ell^2 \beta w = 0. \quad (3-9)$$

Note that by (3-6),

$$|{}^m(\mathbf{y})| + |{}^m\beta(\mathbf{y})| \lesssim 1, \quad \mathbf{y} \in B(\mathbf{0}, R) \quad (3-10)$$

for all $\mathbf{m} \in \mathbb{N}_0^{3M}$.

We are interested in the bounds for the function $w_{\mathbf{m}} = {}^m w$ for $\mathbf{y} \in B(\mathbf{0}, R)$. For the sake of brevity throughout the proof we use the notation $B_r = B(\mathbf{0}, r)$ for $r > 0$.

Lemma 3.3. *Let $\ell \leq 1$. Suppose that w is a weak solution of (3-9). Then for all $\mathbf{m} \in \mathbb{N}_0^{3M}$ and all $r < R$ the cluster derivatives $w_{\mathbf{m}}$ belong to $C^1(\overline{B_r})$. Furthermore, if $|\mathbf{m}| \geq 1$, then for all $v \in (r, R)$ we have*

$$\|w_{\mathbf{m}}\|_{C^1(\overline{B_r})} \lesssim \ell^2 \|w\|_{L^\infty(B_v)} + \|\nabla w\|_{L^\infty(B_v)}. \quad (3-11)$$

If $|\mathbf{m}| \geq 2$, then also

$$\|w_{\mathbf{m}}\|_{C^1(\overline{B_r})} \lesssim \max_{l: |l|=2} \|{}^l w\|_{L^\infty(B_v)} + \ell \|\nabla w\|_{L^\infty(B_v)} + \ell^2 \|w\|_{L^\infty(B_v)}. \quad (3-12)$$

Proof. We begin the proof with a formal manipulation assuming that all the cluster derivatives $w_{\mathbf{m}}$ exist and are as smooth as necessary. Applying the operator m to (3-9) and using (3-10) we obtain the following equation for the function $w_{\mathbf{m}}$:

$$\Delta w_{\mathbf{m}} + 2\ell \cdot \nabla w_{\mathbf{m}} + \ell^2 \beta w_{\mathbf{m}} = g_{\mathbf{m}}, \quad (3-13)$$

with

$$g_{\mathbf{m}} = 2\ell \sum_{\substack{0 \leq \mathbf{q} \leq \mathbf{m} \\ |\mathbf{q}| \leq |\mathbf{m}| - 1}} \binom{\mathbf{m}}{\mathbf{q}} ({}^{\mathbf{m}-\mathbf{q}}) \cdot \nabla w_{\mathbf{q}} - \ell^2 \sum_{\substack{0 \leq \mathbf{q} \leq \mathbf{m} \\ |\mathbf{q}| \leq |\mathbf{m}| - 1}} \binom{\mathbf{m}}{\mathbf{q}} ({}^{\mathbf{m}-\mathbf{q}} \beta) w_{\mathbf{q}}.$$

It follows from (3-10) that

$$\|g_{\mathbf{m}}\|_{L^\infty(B_\rho)} \lesssim \sum_{\mathbf{q}: 0 \leq \mathbf{q} \leq |\mathbf{m}| - 1} T_{\mathbf{q}}(\ell, \rho), \quad T_{\mathbf{q}}(\ell, \rho) = \ell \|\nabla w_{\mathbf{q}}\|_{L^\infty(B_\rho)} + \ell^2 \|w_{\mathbf{q}}\|_{L^\infty(B_\rho)} \quad (3-14)$$

for all $\rho < R$.

Now we need to justify the above formal calculations. First note that since w is a weak solution of (3-9), by Proposition 3.1 it belongs to $W^{2,2}(B_\rho) \cap {}^{-1}(\overline{B_\rho})$ for all $\rho < R$, so that $T_0(\ell, \rho) = \ell \|\nabla w\|_{L^\infty(B_\rho)} + \ell^2 \|w\|_{L^\infty(B_\rho)}$ is finite, and as a result, for $|\mathbf{m}| = 1$ we have

$$\|g_{\mathbf{m}}\|_{L^\infty(B_\rho)} \lesssim T_0(\ell, \rho) = \ell \|\nabla w\|_{L^\infty(B_\rho)} + \ell^2 \|w\|_{L^\infty(B_\rho)}, \quad 0 < \rho < R. \quad (3-15)$$

By Proposition 3.1, for all $\mathbf{m}$ such that $|\mathbf{m}| = 1$ and all $r < \rho$, we conclude that $w_{\mathbf{m}} \in W^{2,2}(B_r) \cap {}^{-1}(\overline{B_r})$ and

$$\begin{aligned} \|w_{\mathbf{m}}\|_{{}^{-1}(\overline{B_r})} &\lesssim \|w_{\mathbf{m}}\|_{L^\infty(B_\rho)} + \|g_{\mathbf{m}}\|_{L^\infty(B_\rho)} \\ &\lesssim \|\nabla w\|_{L^\infty(B_\rho)} + \|g_{\mathbf{m}}\|_{L^\infty(B_\rho)} \lesssim \|\nabla w\|_{L^\infty(B_\rho)} + \ell^2 \|w\|_{L^\infty(B_\rho)}. \end{aligned}$$

This proves (3-11) for $|\mathbf{m}| = 1$.

Using the above observation as the induction base, we now prove that $w_{\mathbf{m}}$ is indeed well-defined for all $\mathbf{m} \in \mathbb{Z}_0^{3M}$ and that it is a weak solution of (3-13). To provide the induction step assume that for some $k = 1, \dots$, and all $\mathbf{m}$, $1 \leq |\mathbf{m}| \leq k$, the function $w_{\mathbf{m}}$ is a weak solution of (3-13) in B_ρ for all $\rho < R$ (and hence belongs to $W^{2,2}(B_r) \cap {}^{-1}(\overline{B_r})$, $r < \rho$, by Proposition 3.1), and that it satisfies (3-11). Let us prove that the same is true for the function $w_{\mathbf{n}}$ for all $\mathbf{n}$ such that $|\mathbf{n}| = k + 1$.

First note that for all $\rho < \nu < R$ the function $g_{\mathbf{n}}$ satisfies the bound

$$\|g_{\mathbf{n}}\|_{L^\infty(B_\rho)} \lesssim \ell \|\nabla w\|_{L^\infty(B_\nu)} + \ell^2 \|w\|_{L^\infty(B_\nu)}. \quad (3-16)$$

Indeed, in the bound (3-14) for $T_0(\ell, \rho)$ we use the estimate (3-15). For $T_q(\ell, \rho)$ with $1 \leq |q| \leq k$ we use (3-11) to obtain the estimate

$$T_q(\ell, \rho) \lesssim \ell \|w_q\|_{{}^{-1}(\overline{B_\rho})} \lesssim \ell \|\nabla w\|_{L^\infty(B_\nu)} + \ell^3 \|w\|_{L^\infty(B_\nu)}.$$

In view of (3-14), this gives (3-16) for $g_{\mathbf{n}}$, as required. Furthermore, as $w_{\mathbf{m}} \in W^{2,2}(B_\rho)$ for all $|\mathbf{m}| \leq k$, we have $w_{\mathbf{n}} \in W^{1,2}(B_\rho)$. Now, integrating (3-9) against the function $(-1)^{k+1} {}^{\mathbf{n}}\eta$, with an arbitrary $\eta \in {}_0^\infty(B_\rho)$ we obtain

$$\begin{aligned} 0 &= (-1)^{k+1} \int \nabla w \cdot \nabla {}^{\mathbf{n}}\eta \, dy + (-1)^{k+1} 2\ell \int \cdot \nabla w {}^{\mathbf{n}}\eta \, dy + (-1)^{k+1} \ell^2 \int \beta w {}^{\mathbf{n}}\eta \, dy \\ &= \int \nabla w_{\mathbf{n}} \cdot \nabla \eta \, dy + 2\ell \int \cdot \nabla w_{\mathbf{n}} \eta \, dy + \ell^2 \int \beta w_{\mathbf{n}} \eta \, dy - \int g_{\mathbf{n}} \eta \, dy, \end{aligned}$$

and hence $w_{\mathbf{n}}$ is a weak solution of (3-13) in B_ρ . Since the coefficients and the right-hand side of (3-13) are bounded uniformly in ℓ , by Proposition 3.1, $w_{\mathbf{n}} \in W^{2,2}(B_r) \cap {}^{-1}(\overline{B_r})$ for all $r < \rho$ and

$$\begin{aligned} \|w_{\mathbf{n}}\|_{{}^{-1}(\overline{B_r})} &\lesssim \|w_{\mathbf{n}}\|_{L^\infty(B_\rho)} + \|g_{\mathbf{n}}\|_{L^\infty(B_\rho)} \\ &\lesssim \|w_{\mathbf{n}}\|_{L^\infty(B_\rho)} + \ell \|\nabla w\|_{L^\infty(B_\nu)} + \ell^2 \|w\|_{L^\infty(B_\nu)}, \end{aligned} \quad (3-17)$$

where we have also used (3-16). Let $\mathbf{m}$, $|\mathbf{m}| = k$, be such that $|\mathbf{n} - \mathbf{m}| = 1$. Therefore, by (3-11),

$$\|w_{\mathbf{n}}\|_{L^\infty(B_\rho)} \lesssim \|\nabla w_{\mathbf{m}}\|_{L^\infty(B_\rho)} \lesssim \|\nabla w\|_{L^\infty(B_\nu)} + \ell^2 \|w\|_{L^\infty(B_\nu)}.$$

Together with (3-17) this leads to

$$\|w_n\|_{1(\bar{B}_r)} \lesssim \|\nabla w\|_{L^\infty(B_v)} + \ell^2 \|w\|_{L^\infty(B_v)},$$

as required. It remains to conclude that by induction, the bound (3-11) holds for all $\mathbf{m} \in \binom{3M}{0}$.

The proof of (3-12) is also conducted by induction. Assume that $|\mathbf{m}| = 2$. From (3-17) we get that

$$\begin{aligned} \|w_{\mathbf{m}}\|_{1(\bar{B}_r)} &\lesssim \|w_{\mathbf{m}}\|_{L^\infty(B_\rho)} + \ell \|\nabla w\|_{L^\infty(B_v)} + \ell^2 \|w\|_{L^\infty(B_v)} \\ &\lesssim \max_{l:|l|=2} \|\ell^l w\|_{L^\infty(B_v)} + \ell \|\nabla w\|_{L^\infty(B_v)} + \ell^2 \|w\|_{L^2(B_v)} \end{aligned} \quad (3-18)$$

for all $r < \rho < v < R$, which gives (3-12). The bound (3-18) serves as the induction base. Let us now provide the induction step. Suppose that (3-12) holds for all $\mathbf{m}$ such that $2 \leq |\mathbf{m}| \leq k$ with some $k = 2, 3, \dots$. Let us prove that it holds for all w_n where $|\mathbf{n}| = k + 1$. Let $\mathbf{m}, |\mathbf{m}| = k$, be such that $|\mathbf{n} - \mathbf{m}| = 1$. Thus (3-12) for $w_{\mathbf{m}}$ implies that

$$\|w_n\|_{L^\infty(B_\rho)} \lesssim \|\nabla w_{\mathbf{m}}\|_{L^\infty(B_\rho)} \lesssim \max_{l:|l|=2} \|\ell^l w\|_{L^\infty(B_v)} + \ell \|\nabla w\|_{L^\infty(B_v)} + \ell^2 \|w\|_{L^2(B_v)}.$$

Substituting this inequality in (3-17), we obtain (3-12) for w_n .

Consequently, (3-12) holds for all $\mathbf{m} \in \binom{3M}{0}$, $|\mathbf{m}| \geq 2$.

We would like to point out one fact which was not needed in the above proof but deserves mentioning. The bound (3-11) for $|\mathbf{m}| = 1$ and bound (3-12) for $|\mathbf{m}| \geq 2$ imply (3-11) for all $|\mathbf{m}| \geq 2$. Indeed, by (3-11) with $|\mathbf{q}| = 1$, we have

$$\max_{l:|l|=2} \|\ell^l w\|_{L^\infty(B_\rho)} \lesssim \sum_{|\mathbf{q}|=1} \|\nabla w_{\mathbf{q}}\|_{L^\infty(B_\rho)} \lesssim \|\nabla w\|_{L^\infty(B_v)} + \ell^2 \|w\|_{L^\infty(B_v)}$$

for all $\rho < v < R$. After substitution in (3-12) this gives (3-11) for all $|\mathbf{m}| \geq 2$, as claimed.

Proof of Theorem 3.2. Since

$$\nabla^k w_{\mathbf{m}}(\mathbf{y}) = \ell^{|\mathbf{m}|+k} (\nabla^k w_{\mathbf{m}})(\mathbf{x}_0 + \ell \mathbf{y}), \quad k = 0, 1, \quad \mathbf{m} \in \binom{3M}{0},$$

the bound (3-11) for $|\mathbf{m}| \geq 1$ rewrites as (3-7). If $\mathbf{m} = \mathbf{0}$ and $|k| = 1$, then (3-7) is trivial.

The bound (3-8) is obtained from (3-12) in the same way.

4. The Schrödinger equation

4A. Reduction of the Schrödinger equation. Here we apply the bounds obtained in the previous section to the Schrödinger equation

$$\Delta \psi + (V - E)\psi = 0, \quad (4-1)$$

where the potential V is defined in (1-1). Throughout this section we do not impose the condition $\psi \in L^2(\mathbb{R}^{3N})$, but consider local solutions of (4-1). In order to reduce (4-1) to the equation of the form (3-1) we use the representation $\psi = e^F \phi$ with a function F such that $F, \nabla F \in L^\infty_{\text{loc}}(\mathbb{R}^{3N})$.

In the mathematical physics literature the function e^F is often called a *Jastrow factor*; see, e.g., [15]. As pointed out by a referee, it appears that the first use of such Jastrow factors in the mathematical study of Coulombic wavefunctions was in [22]. The purpose of having a Jastrow factor (such as, e.g., in (4-3)) is to isolate the main singularity of the solution ψ , i.e., to ensure that ϕ is more regular than ψ . For example, it was shown in [17] that $\phi \in W_{\text{loc}}^{1,1}(\mathbb{R}^{3N})$ for all $\epsilon \in (0, 1)$. In [10], extracting yet another Jastrow factor that we do not specify here, allowed one to get $\phi \in W_{\text{loc}}^{1,1}(\mathbb{R}^{3N})$.

After the substitution (4-1) rewrites as

$$\Delta\phi - 2\nabla F \cdot \nabla\phi + (V - \Delta F - |\nabla F|^2 - E)\phi = 0. \quad (4-2)$$

More precisely, if $\psi \in W_{\text{loc}}^{1,2}(\mathbb{R}^{3N})$ is a weak solution of (4-1), then we also have $\phi \in W_{\text{loc}}^{1,2}(\mathbb{R}^{3N})$ and ϕ is a weak solution of (4-2). We choose to define F as in [17; 8; 9; 12]:

$$F(\mathbf{x}) = \sum_{j=1}^N \left(\frac{Z}{2}|x_j| + \frac{1}{4} \sum_{j < k \leq N} |x_j - x_k| \right) + \sum_{k=1}^N \left(\frac{Z}{2}\sqrt{|x_j|^2 + 1} - \frac{1}{4} \sum_{j < k \leq N} \sqrt{|x_j - x_k|^2 + 1} \right), \quad (4-3)$$

which has the property that

$$F, \nabla F \in L^\infty(\mathbb{R}^{3N}). \quad (4-4)$$

In fact, the original choice of F as used in [17, Proposition 1.5] is given by the first sum on the right-hand side, which has a bounded gradient. We follow [17, Proof of Theorem 1.2] and [8; 9; 12] to include the second term which is added to ensure that F itself is bounded on $\mathbb{R}^{3N}$. Thus both conditions (4-4) are satisfied. Due to the straightforward identities

$$\Delta|x_j - x_k| = \frac{4}{|x_j - x_k|}, \quad \Delta|x_j| = \frac{2}{|x_j|},$$

we have

$$\Delta \left[\sum_{j=1}^N \left(\frac{Z}{2}|x_j| + \frac{1}{4} \sum_{j < k \leq N} |x_j - x_k| \right) \right] = V(\mathbf{x}).$$

Therefore

$$\nabla^k (-\Delta F + V) \in L^\infty(\mathbb{R}^{3N}) \quad \text{for all } k = 0, 1, \dots \quad (4-5)$$

Using the factorization $\psi = e^F \phi$ it was shown in [17, Theorem 1.2] that, for any positive r, R such that $r < R$, the bound

$$\|\nabla\psi\|_{L^\infty(B(\mathbf{x}_0, r))} \lesssim \|\psi\|_{L^\infty(B(\mathbf{x}_0, R))}. \quad (4-6)$$

holds. The next lemma was proved in [12, Proposition A.2], but we provide a somewhat different (shorter) argument that uses only Proposition 3.1.

Lemma 4.1. *Let $\psi \in W_{\text{loc}}^{1,2}(\mathbb{R}^{3N})$ be a weak solution of (4-1). Then $\psi \in W_{\text{loc}}^{1,\infty}(\mathbb{R}^{3N})$ and for all numbers $r > 0$ and $R > 0$ such that $r < R$ we have*

$$\|\psi\|_{L^\infty(B(\mathbf{x}_0, r))} + \|\nabla\psi\|_{L^\infty(B(\mathbf{x}_0, r))} \lesssim \|\psi\|_{L^2(B(\mathbf{x}_0, R))}, \quad (4-7)$$

where the implicit constant does not depend on ψ and $\mathbf{x}_0 \in \mathbb{R}^{3N}$, but depends on r and R .

Proof. The function $\phi = e^{-F} \psi$ is a weak solution of (4-2) in $B(\mathbf{x}_0, R)$ with arbitrary $\mathbf{x}_0 \in \mathbb{R}^{3N}$ and $R > 0$. As established above, the coefficients in this equation are uniformly bounded on $\mathbb{R}^{3N}$. According to Proposition 3.1, $\phi \in W^{1,2}(\mathbb{R}^{3N})$ and for any pair of radii $r, R, r < R$, we have the bound

$$\|\phi\|_{L^\infty(B_r)} + \|\nabla \phi\|_{L^\infty(B_r)} \lesssim \|\phi\|_{L^2(B_R)}, \quad (4-8)$$

where $B_R = B(\mathbf{x}_0, R)$, and the implicit constant is independent of $\mathbf{x}_0$. Since F and ∇F satisfy (4-4), we can write for ψ that

$$\|\psi\|_{L^\infty(B_r)} \lesssim \|\phi\|_{L^\infty(B_r)}, \quad \|\phi\|_{L^2(B_R)} \lesssim \|\psi\|_{L^2(B_R)} \quad \text{and} \quad \|\nabla \psi\|_{L^\infty(B_r)} \lesssim \|\nabla \phi\|_{L^\infty(B_r)} + \|\phi\|_{L^\infty(B_r)}.$$

Therefore (4-8) implies (4-7), as required.

4B. Cluster derivatives of ψ : application of Theorem 3.2. For a cluster $P \subset \{1, 2, \dots, N\}$ introduce the set

$$\Sigma = \left\{ \mathbf{x} \in \mathbb{R}^{3N} : \prod_{j \in P} |x_j| \prod_{k \in P^c} |x_k| = 0 \right\},$$

and the distance

$$d(\mathbf{x}) = \min \left\{ |x_j|, \frac{1}{\sqrt{2}} |x_j - x_k| : j \in P, k \in P^c \right\}, \quad \lambda(\mathbf{x}) = \min\{1, d(\mathbf{x})\}. \quad (4-9)$$

The paper [12] contains bounds for cluster derivatives $\nabla^m \psi$ (see, e.g., [12, Proposition 1.10]) outside the set Σ , depending explicitly on the distance d . We need a generalization of this result to cluster sets $\Sigma = \{\Sigma_1, \Sigma_2, \dots, \Sigma_M\}$. Define

$$\Sigma = \bigcup_{j=1}^M \Sigma_j$$

and

$$d(\mathbf{x}) = \min_j d_j(\mathbf{x}), \quad \lambda(\mathbf{x}) = \min\{1, d(\mathbf{x})\}. \quad (4-10)$$

The presence of the factor $1/\sqrt{2}$ in the definition (4-9) is convenient since it ensures that the function d is Lipschitz with Lipschitz constant = 1:

Lemma 4.2. *For all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{3N}$ we have*

$$|d(\mathbf{x}) - d(\mathbf{y})| \leq |\mathbf{x} - \mathbf{y}|. \quad (4-11)$$

The same inequality holds for the function $\lambda(\mathbf{x})$.

Proof. It suffices to prove the inequality just for one cluster P . Let $j \in P, k \in P^c$, and estimate:

$$\begin{aligned} |x_j| &\leq |y_j| + |\mathbf{x} - \mathbf{y}|, \\ |x_j - x_k| &\leq |y_j - y_k| + |\mathbf{x} - \mathbf{y}| \leq |y_j - y_k| + \sqrt{2} |\mathbf{x} - \mathbf{y}|. \end{aligned}$$

For the last inequality we used the elementary fact that if $a^2 + b^2 \leq c^2$ for some positive a, b and c , then $a + b \leq \sqrt{2}c$. Taking the minimum (4-9), we get $d(\mathbf{x}) \leq d(\mathbf{y}) + |\mathbf{x} - \mathbf{y}|$, which gives (4-11). The function λ trivially satisfies the same inequality.

Our objective is to find L^∞ -bounds for the cluster derivatives $\nabla^m \psi$ outside the set Σ . Let us fix $\mathbf{x}_0 \in \mathbb{R}^{3N} \setminus \Sigma$, and denote

$$\lambda = \lambda(\mathbf{x}_0).$$

Observe that for any $R \in (0, 1)$ the inclusion $B(\mathbf{x}_0, R\lambda) \subset \mathbb{R}^{3N} \setminus \Sigma$ holds. Indeed, by [Lemma 4.2](#),

$$|\lambda(\mathbf{x}) - \lambda| \leq |\mathbf{x} - \mathbf{x}_0| < R\lambda, \quad \mathbf{x} \in B(\mathbf{x}_0, R\lambda),$$

which implies that

$$0 < (1 - R)\lambda \leq \lambda(\mathbf{x}) \leq (1 + R)\lambda \quad \text{for all } \mathbf{x} \in B(\mathbf{x}_0, R\lambda), \quad (4-12)$$

and hence proves the claim. In the next theorem we estimate the derivatives $\nabla^m \psi$ in the ball $B(\mathbf{x}_0, R\lambda)$.

Theorem 4.3. *Let $\mathbf{x}_0 \in \mathbb{R}^{3N} \setminus \Sigma$ and let $\lambda = \lambda(\mathbf{x}_0)$. Then for any r, R such that $0 < r < R < 1$, and for all $\mathbf{m} \in \mathbb{N}_0^{3N}$, the cluster derivatives $\nabla^m \psi$ belong to $L^\infty(B(\mathbf{x}_0, R\lambda))$. Moreover, if $|\mathbf{m}| + k \geq 1$ with $k = 0, 1$, then*

$$\|\nabla^k \nabla^m \psi\|_{L^\infty(B(\mathbf{x}_0, r\lambda))} \lesssim \lambda^{1-|\mathbf{m}|+k} \|\psi\|_{L^\infty(B(\mathbf{x}_0, R\lambda))} + \|\nabla \psi\|_{L^\infty(B(\mathbf{x}_0, R\lambda))}, \quad (4-13)$$

with an implicit constant depending on r, R , but independent of $\mathbf{x}_0 \in \mathbb{R}^{3N} \setminus \Sigma$.

For a single cluster P the bound (4-13), even for arbitrary L^p -norms with $p \in (1, \infty]$, was proved in [\[12, Proposition 1.10\]](#). The proof in [\[12\]](#) does not immediately generalize to arbitrary cluster sets. As in [\[12\]](#) we use the reduction to (4-2). In [\[12\]](#) the choice of the Jastrow factor depended on the cluster P , whereas we use the standard function (4-3) independent of the cluster set. To check that the coefficients in (4-2) satisfy the conditions of [Theorem 3.2](#), we start with the following elementary observation.

Lemma 4.4. *Let $g \in C^\infty(\mathbb{R}^3 \setminus \{0\})$ be such that*

$$|\partial^m g(x)| \lesssim |x|^{-|m|} \quad \text{for all } m \in \mathbb{N}_0^3.$$

Then for any cluster set and any $j, k = 1, 2, \dots, N$, we have

$$|\nabla^m g(x_j)| + |\nabla^m g(x_j - x_k)| \lesssim d(\mathbf{x})^{-|m|}$$

for all $\mathbf{x} \in \mathbb{R}^{3N} \setminus \Sigma$.

Proof. For simplicity we prove the lemma for one cluster, which is denoted P . Assume that $m \in \mathbb{N}_0^3$, $|m| \geq 1$. It is clear that $D^m g(x_j - x_k) = 0$ if $j, k \in P$ or $j, k \in P^c$. If $j \in P, k \in P^c$ or $k \in P, j \in P^c$, then

$$|\nabla^m g(x_j - x_k)| = |\partial_x^m g(x)|_{x=x_j - x_k} \lesssim |x_j - x_k|^{-|m|} \lesssim d(\mathbf{x})^{-|m|},$$

as claimed. In the same way we get the required estimate for $\nabla^m g(x_j)$.

Corollary 4.5. *Let F be the function (4-3). Then for any cluster set Σ we have for all $\mathbf{x} \notin \Sigma$ and all $\mathbf{m}$ that*

$$|\mathbf{m} \nabla F(\mathbf{x})| + |\mathbf{m} |\nabla F(\mathbf{x})|^2| \lesssim d(\mathbf{x})^{-|\mathbf{m}|}. \quad (4-14)$$

If $|\mathbf{m}| \geq 1$, then

$$|\mathbf{m} e^{F(\mathbf{x})}| \lesssim \lambda(\mathbf{x})^{1-|\mathbf{m}|}. \quad (4-15)$$

Proof. For the first sum in (4-3) the required bound for ∇F immediately follows from Lemma 4.4. The second sum in (4-3) is a smooth function whose derivatives have the same decay far from Σ as those of the first sum. For $|\nabla F|^2$ we use the Leibniz rule, which leads again to (4-14).

To prove the bound (4-15) observe that the derivative $\mathbf{m} e^F$ can be written as a sum of finitely many terms of the form

$$(\mathbf{k}_1 F)^{n_1} (\mathbf{k}_2 F)^{n_2} \dots (\mathbf{k}_s F)^{n_s} e^F,$$

where $1 \leq |\mathbf{k}_1| < |\mathbf{k}_2| < \dots < |\mathbf{k}_s| \leq |\mathbf{m}|$, $n_j \geq 1$, and $|\mathbf{k}_1| n_1 + |\mathbf{k}_2| n_2 + \dots + |\mathbf{k}_s| n_s = |\mathbf{m}|$. Each such term can be estimated by

$$d(\mathbf{x})^{n_1(1-|\mathbf{k}_1|)+n_2(1-|\mathbf{k}_2|)+\dots+n_s(1-|\mathbf{k}_s|)} = d(\mathbf{x})^{n_1+n_2+\dots+n_s-|\mathbf{m}|} \leq \lambda(\mathbf{x})^{1-|\mathbf{m}|},$$

as required.

Proof of Theorem 4.3. In view of (4-2), the function $\phi = e^{-F} \psi$ satisfies (3-1) where

$$\mathbf{a} = -2\nabla F, \quad \mathbf{b} = V - \Delta F - |\nabla F|^2 - E.$$

Let us fix a number $R_1 \in (R, 1)$. By virtue of (4-5) and (4-14), thus defined coefficients $\mathbf{a}$ and $\mathbf{b}$ satisfy the bound

$$|\mathbf{m} \mathbf{a}(\mathbf{x})| + |\mathbf{m} \mathbf{b}(\mathbf{x})| \lesssim 1 + d(\mathbf{x})^{-|\mathbf{m}|} \lesssim \lambda(\mathbf{x})^{-|\mathbf{m}|} \lesssim \lambda^{-|\mathbf{m}|}, \quad \mathbf{x} \in B(\mathbf{x}_0, R_1 \lambda),$$

where $\lambda = \lambda(\mathbf{x}_0)$. For the last inequality we have used (4-12). Thus the condition (3-6) is fulfilled with $\ell = \lambda \leq 1$. Consequently, by Theorem 3.2, $\mathbf{m} \phi \in {}^{1-|\mathbf{m}|}(\overline{B(\mathbf{x}_0, r\lambda)})$ for all $r < R_1$. Moreover, if $|\mathbf{m}| + k \geq 1$, where $k = 0, 1$, then for $r < R$ we have

$$\|\nabla^k \mathbf{m} \phi\|_{L^\infty(B(\mathbf{x}_0, r\lambda))} \lesssim \lambda^{1-|\mathbf{m}|+k} \lambda \|\phi\|_{L^\infty(B(\mathbf{x}_0, R\lambda))} + \|\nabla \phi\|_{L^\infty(B(\mathbf{x}_0, R\lambda))}. \quad (4-16)$$

Now we need to replace ϕ with the function $\psi = e^F \phi$. Let us prove (4-13) with $k = 0$, $|\mathbf{m}| \geq 1$. By the Leibniz rule,

$$\begin{aligned} \mathbf{m}(e^F \phi) &= \sum_{0 \leq \mathbf{q} \leq \mathbf{m}} \binom{\mathbf{m}}{\mathbf{q}} \mathbf{m} - \mathbf{q}(e^F) \mathbf{q} \phi \\ &= \sum_{\substack{0 \leq \mathbf{q} \leq \mathbf{m} \\ 0 < |\mathbf{q}| < |\mathbf{m}|}} \binom{\mathbf{m}}{\mathbf{q}} \mathbf{m} - \mathbf{q}(e^F) \mathbf{q} \phi + \mathbf{m}(e^F) \phi + e^F \mathbf{m} \phi. \end{aligned}$$

By (4-15) and (4-16), for $\mathbf{x} \in B(\mathbf{x}_0, r\lambda)$ the first sum is bounded by

$$\lambda^{2-|\mathbf{m}|} \lambda \|\phi\|_{L^\infty(B(\mathbf{x}_0, R\lambda))} + \|\nabla \phi\|_{L^\infty(B(\mathbf{x}_0, R\lambda))}.$$

The second term is estimated with the help of (4-15) by

$$\lambda^{1-|m|} \|\phi\|_{L^\infty(B(x_0, R\lambda))}.$$

Using (4-16) the third term is estimated by

$$\lambda^{1-|m|} \lambda \|\phi\|_{L^\infty(B(x_0, R\lambda))} + \|\nabla\phi\|_{L^\infty(B(x_0, R\lambda))}.$$

Consequently,

$$\| \nabla^m \psi \|_{L^\infty(B(x_0, R\lambda))} \lesssim \lambda^{1-|m|} \|\phi\|_{L^\infty(B(x_0, R\lambda))} + \|\nabla\phi\|_{L^\infty(B(x_0, R\lambda))}. \quad (4-17)$$

It remains to note that in view of (4-4),

$$|\phi| \lesssim |\psi|, \quad |\nabla\phi| \lesssim |\psi| + |\nabla\psi|,$$

so that the right-hand side of (4-17) is estimated by the right-hand side of (4-13) with $k = 0$.

The case $k = 1$ is done in the same way.

Later on we use Theorem 4.3 in a slightly different form:

Corollary 4.6. *For all $m \in \mathbb{Z}_0^{3M}$ the cluster derivatives $\nabla^m \psi$ belong to $L^1(\mathbb{R}^{3N} \setminus \Sigma)$, and under the condition $|m| + k \geq 1$ with $k = 0, 1$, for all $x \in \mathbb{R}^{3N} \setminus \Sigma$ and all $R > 0$, we have*

$$|\nabla^k \nabla^m \psi(x)| \lesssim \lambda(x)^{1-|m|-k} f_\infty(x; R), \quad (4-18)$$

$$f_\infty(x; R) = \|\psi\|_{L^\infty(B(x, R))} + \|\nabla\psi\|_{L^\infty(B(x, R))}. \quad (4-19)$$

The implicit constant in (4-18) is independent of ψ and x , but may depend on R .

Proof. Let $R_1 = \min\{1/2, R\}$. Then it follows from (4-13) that

$$|\nabla^k \nabla^m \psi(x)| \lesssim \lambda(x)^{1-|m|-k} f_\infty(x; R_1 \lambda(x)) \leq \lambda(x)^{1-|m|-k} f_\infty(x; R).$$

Here we have used the fact that $\lambda(x) \leq 1$. This completes the proof.

5. Auxiliary integral bounds

Here we derive several integral bounds that are instrumental in the proof of the main result in Section 6.

Let $\psi \in L^2(\mathbb{R}^{3N})$ be an eigenfunction. Along with the notation (4-19) it is convenient to introduce for arbitrary $R > 0$ also

$$f_2(x) = f_2(x; R) = \|\psi\|_{L^2(B(x, R))}.$$

According to (4-7), for any $R > 0$ we have

$$f_\infty(x; R) \lesssim f_2(x; 2R), \quad (5-1)$$

with an implicit constant depending on R .

The next lemma provides bounds for integrals involving the functions $f_\infty(x)$ and $f_2(x)$, and is an adaptation of inequalities given in [12, Proposition A.3], with similar proofs. Recall that the function $\mathcal{M}_\varepsilon(x, y, \hat{x})$ is defined in (2-13), and the density $\rho(x)$ – in (1-4)

Lemma 5.1. *Let $x, y \in \mathbb{R}^3$. Then*

$$\int f_\infty(x, \hat{\mathbf{x}}; R) f_\infty(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}} \lesssim \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}}. \quad (5-2)$$

For any $G \in L^1(\mathbb{R}^3)$ we have

$$\begin{aligned} \int [|G(x_j - x_k)| + |G(t - x_k)| + |G(x_k)|] f_\infty(x, \hat{\mathbf{x}}; R) f_\infty(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}} \\ \lesssim \|G\|_{L^1(\mathbb{R}^3)} \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}} \end{aligned} \quad (5-3)$$

for all $j, k = 2, 3, \dots, N$, $j \neq k$, and $t \in \mathbb{R}^3$. In particular,

$$\int \mathcal{M}_\varepsilon(x, y, \hat{\mathbf{x}}) f_\infty(x, \hat{\mathbf{x}}; R) f_\infty(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}} \lesssim \varepsilon^3 \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}}. \quad (5-4)$$

The implicit constants in the bounds (5-2), (5-3) and (5-4) depend on R , but are independent of $x, y, t \in \mathbb{R}^3$.

Proof. Due to the Schwarz inequality, it suffices to estimate the integrals for $x = y$. For $u \in \mathbb{R}^d$ and $R > 0$ denote by $\binom{(d)}{u, R}(x)$, $x \in \mathbb{R}^d$, the indicator function of the ball $B(u, R) \subset \mathbb{R}^d$.

Using (5-1) we get

$$\begin{aligned} \int f_\infty(x, \hat{\mathbf{x}}; R)^2 d\hat{\mathbf{x}} &\lesssim \int f_2(x, \hat{\mathbf{x}}; 2R)^2 d\hat{\mathbf{x}} \\ &= \iint |\psi(z)|^2 \binom{(3N)}{(x, \hat{\mathbf{x}}), 2R}(z) dz d\hat{\mathbf{x}} \\ &= \int |\psi(z)|^2 \int \binom{(3N)}{z, 2R}(x, \hat{\mathbf{x}}) d\hat{\mathbf{x}} dz. \end{aligned}$$

Observe that

$$\binom{(3N)}{z, 2R}(x, \hat{\mathbf{x}}) \leq \binom{(3)}{z_1, 2R}(x) \binom{(3N-3)}{\hat{\mathbf{z}}, 2R}(\hat{\mathbf{x}}) = \binom{(3)}{x, 2R}(z_1) \binom{(3N-3)}{\hat{\mathbf{z}}, 2R}(\hat{\mathbf{x}}),$$

so the integral does not exceed

$$\int |\psi(z)|^2 \binom{(3)}{x, 2R}(z_1) \left(\int \binom{(3N-3)}{\hat{\mathbf{z}}, 2R}(\hat{\mathbf{x}}) d\hat{\mathbf{x}} \right) dz \lesssim R^{3N-3} \int_{|z-x| < 2R} \rho(z) dz.$$

This proves (5-2).

Proof of (5-3). Again it suffices to estimate the integral for $x = y$:

$$\begin{aligned} \int |G(x_j - x_k)| f_\infty(x, \hat{\mathbf{x}}; R)^2 d\hat{\mathbf{x}} &\lesssim \int |G(x_j - x_k)| f_2(x, \hat{\mathbf{x}}; 2R)^2 d\hat{\mathbf{x}} \\ &= \int |\psi(z)|^2 \int |G(x_j - x_k)| \binom{(3N)}{z, 2R}(x, \hat{\mathbf{x}}) d\hat{\mathbf{x}} dz. \end{aligned}$$

Represent $\hat{\mathbf{x}} = (x_j, \tilde{\mathbf{x}}_j)$ with $\tilde{\mathbf{x}}_j \in \mathbb{R}^{3N-6}$, as defined in (1-13), and estimate:

$$\binom{(3N)}{z, 2R}(x, \hat{\mathbf{x}}) \leq \binom{(3)}{z_1, 2R}(x) \binom{(3N-6)}{\tilde{\mathbf{z}}_j, 2R}(\tilde{\mathbf{x}}_j) = \binom{(3)}{x, 2R}(z_1) \binom{(3N-6)}{\tilde{\mathbf{z}}_j, 2R}(\tilde{\mathbf{x}}_j).$$

Consequently, the integral can be estimated by

$$\begin{aligned} \int |\psi(z)|^2 \binom{3}{x, 2R}(z_1) \int_{B(\tilde{z}_j, 2R)}(\tilde{\mathbf{x}}_j) \left[\int |G(x_j - x_k)| dx_j \right] d\tilde{\mathbf{x}}_j dz \\ = \|G\|_{L^1(\mathbb{R}^3)} \int_{|z_1 - x| < 2R} |\psi(z)|^2 \int_{\tilde{z}_j, 2R}^{(3N-6)}(\tilde{\mathbf{x}}_j) d\tilde{\mathbf{x}}_j dz \\ \lesssim \|G\|_{L^1(\mathbb{R}^3)} R^{3N-6} \int_{|z - x| < 2R} \rho(z) dz, \end{aligned}$$

as claimed. The bounds with $G(t - x_k)$ and $G(x_k)$ are proved in the same way.

The bound (5-4) follows from (5-3) with $G(s) = \xi(N\varepsilon^{-1}|s|)$; see (2-1) for the definition of the function ξ .

Let us now apply the obtained bounds to integrals involving the distance function $\lambda_Q(\mathbf{x})$ with an arbitrary cluster Q . We use Lemma 5.1 with this choice of function G :

$$G(s) = \chi_{\{\varepsilon < |s| < 1\}}(s) |s|^{-a}, \quad s \in \mathbb{R}^3, \quad a \geq 0, \quad \varepsilon \in (0, 1], \quad (5-5)$$

so that $\|G\|_{L^1(\mathbb{R}^3)} \lesssim h_{a+2}(\varepsilon)$, where the function h_b is defined in (1-7). Recall that $\lambda_Q(\mathbf{x})$, $\widehat{X}_Q(t; \varepsilon)$ and $\widehat{T}_Q(\delta)$ are defined in (4-9), (2-4) and (2-5), respectively.

Lemma 5.2. *Let $a \geq 0$ and $\varepsilon > 0$. Let Q be an arbitrary cluster. Then for any $R > 0$,*

$$\begin{aligned} \int_{\widehat{X}_Q(t; \varepsilon) \cap \widehat{T}_Q(\varepsilon)} \lambda_Q(t, \hat{\mathbf{x}})^{-a} f_\infty(x, \hat{\mathbf{x}}; R) f_\infty(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}} \\ \lesssim (1 + |t|^{-a} + h_{a+2}(\varepsilon)) \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}}, \quad (5-6) \end{aligned}$$

uniformly in $x, y, t \in \mathbb{R}^3$. If $1 \notin Q$, then the term $|t|^{-a}$ is absent. The implicit constant in (5-6) may depend on R , but is independent of ε .

Proof. By the definition of λ_Q we have

$$\lambda_Q(t, \hat{\mathbf{x}})^{-a} \leq 1 + \sum_{k \in Q} |x_k|^{-a} \sum_{k \in Q} |t - x_k|^{-a} + \sum_{j \in Q, k \in (Q^c)^*} |x_j - x_k|^{-a} \quad \text{if } 1 \in Q^c, \quad (5-7)$$

and

$$\lambda_Q(t, \hat{\mathbf{x}})^{-a} \leq 1 + |t|^{-a} + \sum_{k \in Q^*} |x_k|^{-a} + \sum_{k \in Q^c} |t - x_k|^{-a} + \sum_{j \in Q^*, k \in Q^c} |x_j - x_k|^{-a} \quad \text{if } 1 \in Q. \quad (5-8)$$

Let us estimate the contributions from each of the summands. Assume first that $1 \notin Q$ (i.e., λ_Q satisfies (5-7)) and estimate the integral

$$F_{jk}(t, x, y) = \int_{\widehat{X}_Q(t; \varepsilon) \cap \widehat{T}_Q(\varepsilon)} |x_j - x_k|^{-a} f_\infty(x, \hat{\mathbf{x}}; R) f_\infty(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}} \quad (5-9)$$

for an arbitrary fixed pair $j \in Q, k \in (Q^c)^*$. Since $j, k \geq 2$, in view of the definition (2-4) of $\widehat{X}_Q(t, \varepsilon)$, we have

$$\widehat{X}_Q(t; \varepsilon) \subset \{\hat{\mathbf{x}} \in \mathbb{R}^{3N-3} : |x_j - x_k| > \varepsilon\}.$$

Therefore,

$$F_{jk}(t, x, y) \leq \int_{|x_j - x_k| > \varepsilon} |x_j - x_k|^{-a} f_{\infty}(x, \hat{\mathbf{x}}; R) f_{\infty}(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}}.$$

If $\varepsilon \geq 1$, then by (5-2) we have

$$F_{jk}(t, x, y) \lesssim \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}}. \quad (5-10)$$

If $\varepsilon < 1$, then

$$F_{jk}(t, x, y) \leq \int_{|x_j - x_k| > 1} f_{\infty}(x, \hat{\mathbf{x}}; R) f_{\infty}(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}} + \int G(x_j - x_k) f_{\infty}(x, \hat{\mathbf{x}}; R) f_{\infty}(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}},$$

where G is as in (5-5). For the first integral use (5-2) again. As mentioned before the lemma, $\|G\|_{L^1(\mathbb{R}^3)} \lesssim h_{a+2}(\varepsilon)$, so the second integral is bounded by

$$h_{a+2}(\varepsilon) \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}},$$

in view of (5-3). Thus the integral (5-9), and hence the contribution from the last term in (5-7) as well, satisfies the bound (5-6).

In the same way, using (5-3) we derive the bound (5-6) for the integrals containing the remaining terms in (5-7). Let us estimate, for example, the integral

$$F_k(t, x, y) = \int_{\widehat{X}_Q(t; \varepsilon) \cap \widehat{T}_Q(\varepsilon)} |x_k|^{-a} f_{\infty}(x, \hat{\mathbf{x}}; R) f_{\infty}(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}}$$

for an arbitrary fixed $k \in Q$. By the definition (2-5),

$$\widehat{T}_Q(\varepsilon) \subset \{\hat{\mathbf{x}} \in \mathbb{R}^{3N-3} : |x_k| > \varepsilon\},$$

so that

$$F_k(t, x, y) \leq \int_{|x_k| > \varepsilon} |x_k|^{-a} f_{\infty}(x, \hat{\mathbf{x}}; R) f_{\infty}(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}}.$$

As in the case of the integral (5-9), if $\varepsilon \geq 1$, then F_k satisfies the bound (5-10). If $\varepsilon < 1$, then

$$F_k(t, x, y) \leq \int_{|x_k| > 1} f_{\infty}(x, \hat{\mathbf{x}}; R) f_{\infty}(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}} + \int G(x_k) f_{\infty}(x, \hat{\mathbf{x}}; R) f_{\infty}(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}},$$

where G is again given by (5-5). Arguing as for F_{jk} above, we conclude that F_k satisfies (5-6) as well. This proves (5-6) for the case $1 \notin Q$.

Suppose now that $1 \in Q$ so that λ_Q satisfies (5-8). The sums on the right-hand side of (5-8) are similar to those in (5-7) and are treated as in the first part of the proof, and hence they lead to the estimate (5-6). The only term which is new compared to (5-7) is $|t|^{-a}$. Using (5-2) we estimate its contribution by

$$|t|^{-a} \int f_{\infty}(x, \hat{\mathbf{x}}; R) f_{\infty}(y, \hat{\mathbf{x}}; R) d\hat{\mathbf{x}} \lesssim |t|^{-a} \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}}.$$

This completes the proof of (5-6).

Lemma 5.2 has a useful corollary that will be crucial in the proof of **Theorem 1.1**. Let $\Phi = \Phi(x, y, \hat{x}; \varepsilon)$ be an extended cut-off as defined in (2-6), and let $P = P(\varepsilon)$ and $S = S(\varepsilon)$ be the clusters for the admissible cut-offs associated with Φ . For all $a \geq 0$ define

$$\begin{cases} \mathcal{J}_a^{(1)}(x, y; \varepsilon, R) = \int_{\text{supp}_0 \Phi(x, y, \cdot; \varepsilon)} \lambda_{\{S^*, \cdot\}}(x, \hat{x})^{-a} f_\infty(x, \hat{x}; R) f_\infty(y, \hat{x}; R) d\hat{x}, \\ \mathcal{J}_a^{(2)}(x, y; \varepsilon, R) = \int_{\text{supp}_0 \Phi(x, y, \cdot; \varepsilon)} \lambda_{\{S, \cdot\}}(y, \hat{x})^{-a} f_\infty(x, \hat{x}; R) f_\infty(y, \hat{x}; R) d\hat{x}, \\ \mathcal{J}_a^{(3)}(x, y; \varepsilon, R) = \varepsilon^{-a} \int \mathcal{M}_\varepsilon(x, y; \hat{x}) f_\infty(x, \hat{x}; R) f_\infty(y, \hat{x}; R) d\hat{x}. \end{cases} \quad (5-11)$$

Lemma 5.3. For any $\varepsilon, R > 0$, we have

$$\begin{aligned} \mathcal{J}_a^{(1)}(x, y; \varepsilon, R) + \mathcal{J}_a^{(2)}(x, y; \varepsilon, R) + \mathcal{J}_a^{(3)}(x, y; \varepsilon, R) \\ \lesssim (1 + |x|^{-a} + |y|^{-a} + h_{a+2}(\varepsilon)) \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}} \end{aligned} \quad (5-12)$$

for all $|x| > \varepsilon$, $|y| > \varepsilon$ and $|x - y| > \varepsilon$. The implicit constant in (5-12) may depend on R , but is independent of ε .

Proof. Since $|x - y| > \varepsilon$, by **Proposition 2.3** we may assume that $P^* \subset S^c$.

We first estimate $\mathcal{J}_a^{(1)}(x, y; \varepsilon, R)$. By the definition (4-10), we have

$$\lambda_{\{S^*, \cdot\}}(x, \hat{x})^{-1} = \max\{\lambda_{S^*}(x, \hat{x})^{-1}, \lambda_{\{S^*, \cdot\}}(x, \hat{x})^{-1}\} \leq \lambda_{S^*}(x, \hat{x})^{-1} + \lambda_{\{S^*, \cdot\}}(x, \hat{x})^{-1}.$$

Furthermore, since $P^* \subset S^c$ and $|x| > \varepsilon$, $|y| > \varepsilon$, we can use (2-9) and (2-10):

$$\begin{aligned} \text{supp}_0 \Phi(x, y; \cdot; \varepsilon) &\subset \widehat{X}(x; \varepsilon(4N)^{-1}) \cap \widehat{T}^*(\varepsilon/2), \\ \text{supp}_0 \Phi(x, y, \cdot; \varepsilon) &\subset \widehat{X}_{S^*}(x; \varepsilon(4N)^{-1}) \cap \widehat{T}_{S^*}(\varepsilon/2). \end{aligned}$$

These lead to the bound

$$\begin{aligned} \mathcal{J}_a^{(1)}(x, y; \varepsilon, R) &\lesssim \int_{\widehat{X}(x; \varepsilon(4N)^{-1}) \cap \widehat{T}(\varepsilon/2)} \lambda_{\{S^*, \cdot\}}(x, \hat{x})^{-a} f_\infty(x, \hat{x}; R) f_\infty(y, \hat{x}; R) d\hat{x} \\ &\quad + \int_{\widehat{X}_{S^*}(x; \varepsilon(4N)^{-1}) \cap \widehat{T}_{S^*}(\varepsilon/2)} \lambda_{S^*}(x, \hat{x})^{-a} f_\infty(x, \hat{x}; R) f_\infty(y, \hat{x}; R) d\hat{x}. \end{aligned}$$

By (5-6) with $t = x$, each of these integrals is bounded by

$$(1 + |x|^{-a} + h_{a+2}(\varepsilon)) \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}},$$

which implies (5-12). The integral $\mathcal{J}_a^{(2)}(x, y; \varepsilon, R)$ is estimated in the same way.

The integral $\mathcal{J}_a^{(3)}(x, y; \varepsilon, R)$ is estimated with the help of (5-4):

$$\begin{aligned} \mathcal{J}_a^{(3)}(x, y; \varepsilon, R) &\lesssim \varepsilon^{3-a} \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}} \\ &\lesssim h_{a+2}(\varepsilon) \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}}. \end{aligned}$$

Combining the obtained bounds we complete the proof of (5-12).

Now we are in a position to prove **Theorem 1.1**.

6. Estimates for the density matrix: proof of Theorem 1.1

Denote for convenience of notation

$$\gamma_{r,p}(x, y) := \partial_x^r \partial_y^p \gamma(x, y) = \int \partial_x^r \psi(x, \hat{x}) \overline{\partial_y^p \psi(y, \hat{x})} d\hat{x}, \quad (6-1)$$

where $r, p \in \mathbb{Z}_0^3$. If $|r| \leq 1$, $|p| \leq 1$, then by Corollary 4.6 the integrand in (6-1) does not exceed $f_\infty(x, \hat{x}; R) f_\infty(y, \hat{x}; R)$, see (4-19) for the definition of $f_\infty(x; R)$. Therefore, the estimate (5-2) entails the bound

$$|\gamma_{r,p}(x, y)| \lesssim \|\rho\|_{L^1(B(x, 2R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, 2R))}^{\frac{1}{2}}, \quad |r| \leq 1, \quad |p| \leq 1. \quad (6-2)$$

For further derivatives, the direct differentiation under the integral is not effective because of the singularities of ψ at the coalescence points. Instead, we study local quantities inserting under the integral the extended cut-off functions as follows. For a fixed $\varepsilon > 0$, let $\Phi = \Phi(x, y, \hat{x}; \varepsilon)$ be an extended cut-off as defined in (2-6). Define

$$\gamma_{r,p}(x, y; \Phi, \varepsilon) = \int \Phi(x, y, \hat{x}; \varepsilon) \partial_x^r \psi(x, \hat{x}) \overline{\partial_y^p \psi(y, \hat{x})} d\hat{x}. \quad (6-3)$$

To estimate this integral we can use the cluster derivatives associated with the cut-off Φ , as described in the introduction.

The first step towards Theorem 1.1 is the following lemma.

Lemma 6.1. *Let $\varepsilon > 0$, $R > 0$, and $|r| \leq 1$, $|p| \leq 1$. Then for all $\beta \in \mathbb{Z}_0^3$, the bound*

$$|\partial_x^\beta \partial_y^\beta \gamma_{r,p}(x, y; \Phi; \varepsilon)| \lesssim (1 + |x| + |\beta| + |y| + |\beta| + h_{|\beta|+2}(\varepsilon)) \|\rho\|_{L^1(B(x, R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, R))}^{\frac{1}{2}} \quad (6-4)$$

holds for all $|x| > \varepsilon$, $|y| > \varepsilon$ and $|x - y| > \varepsilon$. The implicit constant is independent of ψ , ε , but dependent on R .

Proof. Throughout the proof for the brevity of notation we often omit the dependence on ε . Let P and S be the clusters for the admissible cut-offs ϕ and μ associated with Φ . In particular, $1 \in P \cap S$. By Proposition 2.3 we may assume that $S^* \subset P^c$, which is equivalent to $P^* \subset S^c$.

If $\beta = 0$, then (6-4) holds because of (6-2). Thus we may assume that $|\beta| + |\beta| \geq 1$. Let us make the following change of variables under the integral $\gamma_{r,p}(x, y; \Phi)$. Define $\hat{z} = (z_2, z_3, \dots, z_N) \in \mathbb{R}^{3N-3}$ by

$$z_j = \begin{cases} x, & j \in P^*, \\ y, & j \in S^*, \\ 0, & j \in P^c \cap S^c. \end{cases}$$

Change the variable in (6-3): $\hat{x} = \hat{w} + \hat{z}$, so that (6-3) rewrites as

$$\gamma_{r,p}(x, y; \Phi) = \int \Phi(x, y, \hat{w} + \hat{z}) \partial_x^r \psi(x, \hat{w} + \hat{z}) \overline{\partial_y^p \psi(y, \hat{w} + \hat{z})} d\hat{w}.$$

For any function $g = g(x, \hat{\mathbf{x}})$ and all $l, m_1, m_2 \in \mathbb{Z}_0^3$, we have

$$\partial_x^l g(x, \hat{\mathbf{w}} + \hat{\mathbf{z}}) = (\partial_x^l g)(x, \hat{\mathbf{w}} + \hat{\mathbf{z}}), \quad \partial_x^l g(y, \hat{\mathbf{w}} + \hat{\mathbf{z}}) = (\partial_x^l g)(y, \hat{\mathbf{w}} + \hat{\mathbf{z}})$$

and

$$\partial_x^{m_1} \partial_y^{m_2} \Phi(x, y, \hat{\mathbf{w}} + \hat{\mathbf{z}}) = (\partial_x^{m_1} \partial_y^{m_2} \Phi)(x, y, \hat{\mathbf{w}} + \hat{\mathbf{z}}),$$

where we have used the notation (2-11) for the cluster derivatives of the function Φ . Denote

$$Z(x, y) = \text{supp}_0 \Phi(x, y, \cdot).$$

Thus we conclude that $\partial_x \partial_y^\beta \gamma_{r,p}(x, y; \Phi)$, $\beta \in \mathbb{Z}_0^3$, is a linear combination of terms of the form

$$\mathcal{J}_{\mathbf{m}, \mathbf{n}, \mathbf{k}}(x, y; \varepsilon) = \int_{Z(x, y)} \partial_x^{m_1} \partial_y^{m_2} \Phi(x, y, \hat{\mathbf{x}}) \partial_x^{\mathbf{n}} \psi(x, \hat{\mathbf{x}}) \overline{\partial_y^{\mathbf{k}} \psi(y, \hat{\mathbf{x}})} d\hat{\mathbf{x}} \quad (6-5)$$

with

$$\mathbf{m} = (m_1, m_2), \quad \mathbf{n} = (n_1, n_2), \quad \mathbf{k} = (k_1, k_2),$$

where

$$|m_1| + |n_1| + |k_1| = |\alpha|, \quad |m_2| + |n_2| + |k_2| = |\beta|.$$

The cluster derivatives of Φ are defined in (2-11). For these derivatives we use the bound (2-12):

$$|\partial_x^{m_1} \partial_y^{m_2} \Phi(x, y, \hat{\mathbf{x}})| \lesssim \begin{cases} 1 & \text{if } |\mathbf{m}| = 0, \\ \varepsilon^{-|\mathbf{m}|} \mathcal{M}_\varepsilon(x, y, \hat{\mathbf{x}}) & \text{if } |\mathbf{m}| \geq 1, \end{cases} \quad (6-6)$$

For the derivatives of ψ we use Corollary 4.6:

$$\begin{cases} |\partial_x^{\mathbf{n}} \psi(x, \hat{\mathbf{x}})| \lesssim \lambda_{\{S^*, \cdot\}}(x, \hat{\mathbf{x}}) |\mathbf{n}| f_\infty(x, \hat{\mathbf{x}}; R/2), \\ |\partial_y^{\mathbf{k}} \psi(y, \hat{\mathbf{x}})| \lesssim \lambda_{\{S, \cdot\}}(y, \hat{\mathbf{x}}) |\mathbf{k}| f_\infty(y, \hat{\mathbf{x}}; R/2). \end{cases} \quad (6-7)$$

In order to avoid cumbersome expressions, in the following calculations we use the notation

$$\mu(x, \hat{\mathbf{x}}) = \lambda_{\{S^*, \cdot\}}(x, \hat{\mathbf{x}}), \quad \tilde{\mu}(y, \hat{\mathbf{x}}) = \lambda_{\{S, \cdot\}}(y, \hat{\mathbf{x}}).$$

Assume first that $\mathbf{m} = \mathbf{0}$. In this case, by virtue of (6-6) and (6-7), the integral (6-5) satisfies the estimate

$$|\mathcal{J}_{\mathbf{0}, \mathbf{n}, \mathbf{k}}(x, y; \varepsilon)| \lesssim \int_{Z(x, y)} \mu(x, \hat{\mathbf{x}}) |\mathbf{n}| \tilde{\mu}(y, \hat{\mathbf{x}}) |\mathbf{k}| f_\infty(x, \hat{\mathbf{x}}; R/2) f_\infty(y, \hat{\mathbf{x}}; R/2) d\hat{\mathbf{x}}.$$

By Young's inequality, for all $\mathbf{n}, \mathbf{k}$ such that $|\mathbf{n}| + |\mathbf{k}| = |\alpha| + |\beta| \geq 1$, we have

$$\mu(x, \hat{\mathbf{x}}) |\mathbf{n}| \tilde{\mu}(y, \hat{\mathbf{x}}) |\mathbf{k}| \leq \frac{|\mathbf{n}|}{|\alpha| + |\beta|} \mu(x, \hat{\mathbf{x}})^{|\alpha| + |\beta|} + \frac{|\mathbf{k}|}{|\alpha| + |\beta|} \tilde{\mu}(y, \hat{\mathbf{x}})^{|\alpha| + |\beta|}.$$

Consequently, using the notation (5-11) we can estimate,

$$|\mathcal{J}_{\mathbf{0}, \mathbf{n}, \mathbf{k}}(x, y; \varepsilon)| \lesssim \mathcal{J}_{|\alpha| + |\beta|}^{(1)}(x, y; \varepsilon, R/2) + \mathcal{J}_{|\alpha| + |\beta|}^{(2)}(x, y; \varepsilon, R/2),$$

with a constant independent of ε . By (5-12), the right-hand side satisfies (6-4), as required.

Now assume that $|\mathbf{m}| \geq 1$. Using again (6-6) and (6-7) we get the estimate

$$|\mathcal{J}_{\mathbf{m},\mathbf{n},\mathbf{k}}(x, y; \varepsilon)| \lesssim \varepsilon^{|\mathbf{m}|} \int_{Z(x,y)} \mathcal{M}_\varepsilon(x, y, \hat{\mathbf{x}}) \mu(x, \hat{\mathbf{x}})^{|\mathbf{n}|} \tilde{\mu}(y, \hat{\mathbf{x}})^{|\mathbf{k}|} f_\infty(x, \hat{\mathbf{x}}; R/2) f_\infty(y, \hat{\mathbf{x}}; R/2) d\hat{\mathbf{x}}.$$

By Young's inequality again, for all $\mathbf{m}, \mathbf{n}, \mathbf{k}$ such that $|\mathbf{m}| + |\mathbf{n}| + |\mathbf{k}| = |\alpha| + |\beta| \geq 1$, we have

$$\begin{aligned} & \varepsilon^{|\mathbf{m}|} \mu(x, \hat{\mathbf{x}})^{|\mathbf{n}|} \tilde{\mu}(y, \hat{\mathbf{x}})^{|\mathbf{k}|} \\ & \leq \frac{|\mathbf{m}|}{|\alpha| + |\beta|} \varepsilon^{|\alpha| + |\beta|} + \frac{|\mathbf{n}|}{|\alpha| + |\beta|} \mu(x, \hat{\mathbf{x}})^{|\alpha| + |\beta|} + \frac{|\mathbf{k}|}{|\alpha| + |\beta|} \tilde{\mu}(y, \hat{\mathbf{x}})^{|\alpha| + |\beta|}. \end{aligned}$$

Therefore,

$$\begin{aligned} |\mathcal{J}_{\mathbf{m},\mathbf{n},\mathbf{k}}(x, y; \varepsilon)| & \lesssim \varepsilon^{|\alpha| + |\beta|} \int_{Z(x,y)} \mathcal{M}_\varepsilon(x, y, \hat{\mathbf{x}}) f_\infty(x, \hat{\mathbf{x}}; R/2) f_\infty(y, \hat{\mathbf{x}}; R/2) d\hat{\mathbf{x}} \\ & + \int_{Z(x,y)} \mu(x, \hat{\mathbf{x}})^{|\alpha| + |\beta|} \mathcal{M}_\varepsilon(x, y, \hat{\mathbf{x}}) f_\infty(x, \hat{\mathbf{x}}; R/2) f_\infty(y, \hat{\mathbf{x}}; R/2) d\hat{\mathbf{x}} \\ & + \int_{Z(x,y)} \tilde{\mu}(y, \hat{\mathbf{x}})^{|\alpha| + |\beta|} \mathcal{M}_\varepsilon(x, y, \hat{\mathbf{x}}) f_\infty(x, \hat{\mathbf{x}}; R/2) f_\infty(y, \hat{\mathbf{x}}; R/2) d\hat{\mathbf{x}}. \end{aligned}$$

In the second and in the third integral estimate $|\mathcal{M}_\varepsilon(x, y, \hat{\mathbf{x}})| \lesssim 1$ and use the notation (5-11):

$$|\mathcal{J}_{\mathbf{m},\mathbf{n},\mathbf{k}}(x, y; \varepsilon)| \lesssim \mathcal{J}_{|\alpha|+|\beta|}^{(1)}(x, y; \varepsilon, R/2) + \mathcal{J}_{|\alpha|+|\beta|}^{(2)}(x, y; \varepsilon, R/2) + \mathcal{J}_{|\alpha|+|\beta|}^{(3)}(x, y; \varepsilon, R/2),$$

with a constant independent of ε . By (5-12), the right-hand side satisfies (6-4).

Putting the estimates for $|\mathbf{m}| = 0$ and $|\mathbf{m}| \geq 1$ together, and summing over $\mathbf{m}, \mathbf{n}, \mathbf{k}$, we arrive at (6-4), thereby completing the proof.

Corollary 6.2. *Let $\varepsilon > 0$, $R > 0$, and $|p| \leq 1$, $|r| \leq 1$. Then for all $\beta \in \mathbb{R}^3$ the bound*

$$|\partial_x \partial_y^\beta \gamma_{r,p}(x, y)| \lesssim (1 + |x|^{|\alpha| + |\beta|} + |y|^{|\alpha| + |\beta|} + h_{|\alpha|+|\beta|+2}(\varepsilon)) \|\rho\|_{L^1(B(x,R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y,R))}^{\frac{1}{2}} \quad (6-8)$$

holds for all $|x| > \varepsilon$, $|y| > \varepsilon$ and $|x - y| > \varepsilon$. The implicit constant is independent of x, y and ε but may depend on R .

Proof. In order to use Lemma 6.1 we build a partition of unity consisting of extended cut-offs. Recall the notation $R = \{1, 2, \dots, N\}$. Let $\Xi = \{(j, k) \in R \times R : j < k\}$. For each subset $\Upsilon \subset \Xi$ introduce the admissible cut-off (see (2-3) for the definition of admissible cut-offs)

$$\phi_\Upsilon(\mathbf{x}; \varepsilon) = \prod_{(j,k) \in \Upsilon} \zeta_\varepsilon(x_j - x_k) \prod_{(j,k) \in \Upsilon^c} \theta_\varepsilon(x_j - x_k).$$

It is clear that

$$\sum_{\Upsilon \subset \Xi} \phi_\Upsilon(\mathbf{x}; \varepsilon) = \prod_{(j,k) \in \Xi} (\zeta_\varepsilon(x_j - x_k) + \theta_\varepsilon(x_j - x_k)) = 1.$$

Furthermore, for every cluster $S \subset R^*$ define

$$\tau_S(y, \hat{\mathbf{x}}; \varepsilon) = \prod_{j \in S} \zeta_\varepsilon(y - x_j) \prod_{j \in (S^c)^*} \theta_\varepsilon(y - x_j).$$

It is clear that

$$\sum_{S \subset \mathbb{R}^*} \tau_S(y, \hat{x}; \varepsilon) = \prod_{j \in \mathbb{R}^*} (\zeta_\varepsilon(x_1 - x_j) + \theta_\varepsilon(x_1 - x_j)) = 1.$$

Define

$$\Phi_{\Upsilon, S}(x, y, \hat{x}; \varepsilon) = \phi_\Upsilon(x, \hat{x}; \varepsilon) \tau_S(y, \hat{x}; \varepsilon), \quad (x, y) \in \mathbb{R}^3 \times \mathbb{R}^3, \hat{x} \in \mathbb{R}^{3N-3},$$

so that

$$\sum_{\Upsilon \subset \Xi, S \subset \mathbb{R}^*} \Phi_{\Upsilon, S}(x, y, \hat{x}; \varepsilon) = 1.$$

Each function $\Phi_{\Upsilon, S}$ is an extended cut-off function, as defined in [Section 2B](#). Using the definition (6-3), the function (6-1) can be represented as

$$\gamma_{r, p}(x, y) = \sum_{\Upsilon \subset \Xi, S \subset \mathbb{R}^*} \gamma_{r, p}(x, y; \Phi_{\Upsilon, S}, \varepsilon).$$

Applying [Lemma 6.1](#) to each summand we arrive at (6-8).

Proof of the bound (1-8). Assume that $x \neq 0$, $y \neq 0$, $x \neq y$ and that $|l| \geq 1$, $|m| \geq 1$. Represent $l = - + r$, $m = \beta + p$ with $|r| = |p| = 1$, so that $|l| = | - | + 1$, $|m| = |\beta| + 1$. Furthermore, denote

$$\varepsilon = \frac{1}{2} \min\{|x|, |y|, |x - y|\},$$

so that $|x - y| > \varepsilon$ and $|x| > \varepsilon$, $|y| > \varepsilon$. Thus it follows from (6-8) that

$$\begin{aligned} |\partial_x^l \partial_y^m \gamma(x, y)| &= |\partial_x^l \partial_y^\beta \gamma_{r, p}(x, y)| \\ &\lesssim (1 + |x|^{2-|l|} + |y|^{2-|l|-|m|} + h_{|l|+|m|}(\varepsilon)) \|\rho\|_{L^1(B(x, R))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, R))}^{\frac{1}{2}}. \end{aligned} \quad (6-9)$$

Since for all $a \geq 0$ we have

$$\begin{aligned} h_a(\varepsilon) &\lesssim h_a(|x - y|) + h_a(|x|) + h_a(|y|) \\ &\lesssim 1 + |x|^{2-a} + |y|^{2-a} + h_a(|x - y|), \end{aligned}$$

the bound (6-9) implies (1-8).

Proof of (1-9). We prove this estimate for the derivative $\partial_x^l \gamma(x, y)$ only, as the proof for the derivative with respect to y is the same up to obvious modifications. For convenience denote

$$A(x, y; R_1, R_2) = \|\rho\|_{L^1(B(x, R_1))}^{\frac{1}{2}} \|\rho\|_{L^1(B(y, R_2))}^{\frac{1}{2}}.$$

Assume that $|l| \geq 1$. Representing $l = - + r$, with some $r : |r| = 1$, and taking $\beta = p = 0$, we obtain from (6-8) that

$$\begin{aligned} |\partial_x^l \gamma(x, y)| &= |\partial_x^l \gamma_{r, 0}(x, y)| \\ &\lesssim (1 + |x|^{1-|l|} + |y|^{1-|l|} + h_{|l|+1}(|x - y|)) A(x, y; R/2, R/2). \end{aligned} \quad (6-10)$$

To “upgrade” this bound to (1-9) we use the fundamental theorem of calculus. Let $z \in \mathbb{R}^3$, $z \neq x$, be such that the segment

$$\{y_s = y + s(z - y), s \in [0, 1]\},$$

does not contain the point x . Then

$$\partial_x^l \gamma(x, y) - \partial_x^l \gamma(x, z) = \int_0^1 (z - y) \cdot \nabla_y (\partial_x^l \gamma)(x, y_s) ds. \quad (6-11)$$

A similar formula holds for the derivative $\partial_y^l \gamma(x, y)$, but we omit this part of the argument and complete the proof for the derivative $\partial_x^l \gamma(x, y)$ only. Since the integrand in (6-11) contains derivatives both with respect to x and y , we can use the bound (1-8) proved previously. First we make a convenient choice of z . Denote

$$|x - y| = d, \quad \delta = \frac{1}{4} \min\{|x|, |y|\}, \quad \delta_1 = \min\{1, \delta, R/2\}, \quad e = \frac{x - y}{|x - y|},$$

so

$$x = y + |x - y|e = y + de.$$

Take $z = y - \delta_1 e$, so that

$$|y - y_s| = s\delta_1, \quad |z - y| = \delta_1, \quad |z - x| = \delta_1 + d, \quad |z| \geq |y| - \delta_1 \geq \frac{3}{4}|y|,$$

and

$$|y_s| \geq |y| - s\delta_1 \geq \frac{3}{4}|y|, \quad |x - y_s| = d + s\delta_1, \quad s \in [0, 1].$$

Now apply (1-8) with the radius $R/2$ to estimate the integrand in (6-11):

$$\begin{aligned} |(z - y) \cdot \nabla_y (\partial_x^l \gamma)(x, y_s)| &\lesssim |z - y| (1 + |y_s|^{1-|l|} + |x|^{1-|l|} + h_{|l|+1}(|x - y_s|)) A(x, y_s; R/2, R/2) \\ &\lesssim \delta_1 (1 + |y|^{1-|l|} + |x|^{1-|l|} + h_{|l|+1}(d + s\delta_1)) A(x, y; R/2, R). \end{aligned} \quad (6-12)$$

An elementary calculation shows that for all $a \geq 0$ the bound

$$\delta_1 \int_0^1 h_{a+1}(d + s\delta_1) ds \lesssim h_a(d).$$

holds. Consequently, integrating the bound (6-12) in $s \in [0, 1]$ we obtain from (6-11) that

$$|\partial_x^l \gamma(x, y)| \lesssim |\partial_x^l \gamma(x, z)| + (1 + |y|^{1-|l|} + |x|^{1-|l|} + h_{|l|}(|x - y|)) A(x, y; R, R). \quad (6-13)$$

To estimate $|\partial_x^l \gamma(x, z)|$ we use (6-10):

$$|\partial_x^l \gamma(x, z)| \lesssim (1 + |x|^{1-|l|} + |z|^{1-|l|} + h_{|l|+1}(|x - z|)) A(x, z; R/2, R/2).$$

As $|z - x| = d + \delta_1 \geq \delta_1$ we can estimate:

$$h_{|l|+1}(|x - z|) \leq h_{|l|+1}(\delta_1) \lesssim 1 + |x|^{1-|l|} + |y|^{1-|l|}.$$

Furthermore, as $|y - z| = \delta_1 \leq R/2$, we have $A(x, z; R/2, R/2) \leq A(x, y; R/2, R)$. Consequently,

$$|\partial_x^l \gamma(x, z)| \lesssim (1 + |x|^{1-|l|} + |y|^{1-|l|}) A(x, y; R/2, R).$$

Together with (6-13) this bound entails (1-9).

This completes the proof of Theorem 1.1.

Appendix

Here we provide an elementary fact concerning extensions of Sobolev spaces. The proof can be found in the appendix to [27].

Consider spaces of functions that depend either on one variable $x \in \mathbb{R}^d$ or on two variables $(t, x) \in \mathbb{R}^l \times \mathbb{R}^d$. Denote $K = \{t \in \mathbb{R}^l : |t| < 1\}$, $B = \{x \in \mathbb{R}^d : |x| < 1\}$ and $B_0 = B \setminus \{0\}$.

Proposition A.1. *Let the dimension l be arbitrary, let $d \geq 2$, $m \geq 1$, and $p \in [d(d-1)^{-1}, \infty]$. Then $W^{m,p}(B_0) = W^{m,p}(B)$ and $W^{m,p}(K \times B_0) = W^{m,p}(K \times B)$.*

We use this fact in Remark 1.2 to describe smoothness properties of the one-particle density matrix $\gamma(x, y)$.

Acknowledgments

The authors are grateful to A. Nazarov for his help regarding Proposition 3.1, and to D. Edmunds, V. Kozlov, V. Maz'ya, G. Rozenblum and D. Vassiliev for their advice on Sobolev spaces. Thanks also go to the referees for their suggestions.

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Received 5 Oct 2022. Revised 16 Jun 2023. Accepted 18 Aug 2023.

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