



Analyticity of the One-Particle Density Matrix

Peter Hearnshaw and Alexander V. Sobolev 

Abstract. It is proved that the one-particle density matrix $\gamma(x, y)$ for multi-particle Coulombic systems is real analytic away from the nuclei and from the diagonal $x = y$.

Mathematics Subject Classification. Primary 35B65; Secondary 35J10, 81V55.

1. Introduction

The objective of the paper is to study analytic properties of the one-particle density matrix for the molecule, consisting of N electrons and N_0 nuclei described by the following Schrödinger operator:

$$\sum_{k=1}^N \left(-\Delta_k - \sum_{l=1}^{N_0} \frac{Z_l}{|x_k - R_l|} \right) + \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|} + \sum_{1 \leq k < l \leq N_0} \frac{Z_l Z_k}{|R_l - R_k|}, \quad (1.1)$$

where $R_l \in \mathbb{R}^3$ and $Z_l > 0$, $l = 1, 2, \dots, N_0$, are the positions and the charges, respectively, of N_0 nuclei, and $x_j \in \mathbb{R}^3$, $j = 1, 2, \dots, N$ are positions of N electrons. The notation Δ_k is used for the Laplacian w.r.t. the variable x_k . The positions of the nuclei are assumed to be fixed, and as a result the very last term in (1.1) is constant. Thus, in what follows we drop this term and instead of (1.1) we study the operator

$$H = H^{(0)} + V, \quad H^{(0)} = -\Delta = -\sum_{k=1}^N \Delta_k \quad (1.2)$$

with

$$V(\mathbf{x}) = V^C(\mathbf{x}) = - \sum_{k=1}^N \sum_{l=1}^{N_0} \frac{Z_l}{|x_k - R_l|} + \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|}. \quad (1.3)$$

This operator acts on the Hilbert space $L^2(\mathbb{R}^{3N})$, and it is self-adjoint on the domain $D(H) = D(H^{(0)}) = H^2(\mathbb{R}^{3N})$, since V is infinitesimally $H^{(0)}$ -bounded, see, e.g., [20, Theorem X.16].

Let $\psi = \psi(\mathbf{x})$ be an eigenfunction of the operator H with an eigenvalue $E \in \mathbb{R}$, i.e.,

$$(H - E)\psi = 0. \quad (1.4)$$

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

$$\tilde{\gamma}(x, y) = \sum_{j=1}^N \int_{\mathbb{R}^{3N-3}} \psi(x, \hat{\mathbf{x}}_j) \overline{\psi(y, \hat{\mathbf{x}}_j)} d\hat{\mathbf{x}}_j, \quad (x, y) \in \mathbb{R}^3 \times \mathbb{R}^3, \quad (1.5)$$

see [10]. This function is one of the key objects in the multi-particle quantum mechanics, see, e.g., [5, 6, 18, 19] for details and further references. If one assumes that all N particles are fermions (resp. bosons), i.e., that the function ψ is antisymmetric (resp. symmetric) under the permutations $x_j \leftrightarrow x_k$, then the definition (1.5) simplifies:

$$\tilde{\gamma}(x, y) = N \int_{\mathbb{R}^{3N-3}} \psi(x, \hat{\mathbf{x}}) \overline{\psi(y, \hat{\mathbf{x}})} d\hat{\mathbf{x}},$$

where we have denoted $\hat{\mathbf{x}} = \hat{\mathbf{x}}_1$, so $\mathbf{x} = (x_1, \hat{\mathbf{x}})$. Our objective is to study the regularity properties of the function $\tilde{\gamma}(x, y)$ in the general form (1.5) without any symmetry assumptions.

Regularity properties of solutions of elliptic equations are a classical and widely studied subject. For instance, it immediately follows from the general theory, see, e.g., [13], that any local solution of (1.4) is real analytic away from the singularities of the potential (1.3). In his famous paper [16], T. Kato showed that a local solution is locally Lipschitz with “cusps” at the points of particle coalescence. Further regularity results include [8, 11, 12]. We cite the most recent paper [8] for further references.

As far as the one-particle density matrix (1.6) is concerned, in the analytic literature a special attention has been paid to the *one-particle density* $\tilde{\rho}(x) = \tilde{\gamma}(x, x)$. It was shown in [9] that in spite of the nonsmoothness of ψ , the density $\tilde{\rho}(x)$ remains smooth as long as $x \neq R_l, l = 1, 2, \dots, N_0$, because of the averaging in $\hat{\mathbf{x}}$. Moreover, the same authors prove in [10] that $\tilde{\rho}$ is in fact real analytic away from the nuclei, see also [14] for an alternative proof. Paper [10] also claims that the proofs therein imply the analyticity of $\tilde{\gamma}(x, y)$ for all x, y away from the nuclei. However, the methods of [10] do not suffice to substantiate this claim. The objective of the current paper is to bridge this gap

and prove the real analyticity for the one-particle density matrix $\tilde{\gamma}(x, y)$ for all $x \neq y$ away from the nuclei. We emphasize that the condition $x \neq y$ is not just an annoying technical restriction—the function $\tilde{\gamma}(x, y)$ genuinely cannot be infinitely smooth on the diagonal. We have no analytic proof of this fact, but we can present an indirect justification. As shown in [21], the eigenvalues $\lambda_k(\Gamma)$, $k = 1, 2, \dots$, of the non-negative compact operator $\Gamma : \mathcal{L}^2(\mathbb{R}^3) \rightarrow \mathcal{L}^2(\mathbb{R}^3)$ with kernel $\tilde{\gamma}(x, y)$ decay at the rate of $k^{-8/3}$ as $k \rightarrow \infty$. In general, for integral operators the rate of decay is dictated by the smoothness of the kernel: the smoother the kernel is, the faster the eigenvalues decrease, see bibliography in [21]. If the function $\tilde{\gamma}(x, y)$ were infinitely differentiable for all x and y including the diagonal $x = y$ (but excluding the nuclei), then the eigenvalues of Γ would decay faster than any negative power of their number, which is not the case. To justify the non-smoothness for $x = y$, we also mention a calculation presented in [2] (see also [3]) that suggests that $\tilde{\gamma}(x, y) - \tilde{\gamma}(x, x)$ should behave as $|x - y|^5$ for x close to y . In fact, order 5 of this homogeneous singularity is consistent with the $k^{-8/3}$ -decay of the eigenvalues, see again [21] and bibliography therein. As the anonymous referee has pointed out to the authors, the non-analyticity of the one-particle matrix on the diagonal is not only of purely theoretical interest but also has important practical consequences for the electronic structure calculations as it imposes limits upon the accuracy of electronic properties computed with finite basis sets, see, e.g., [4].

One should also say that the real analyticity of the density $\tilde{\rho}(x) = \tilde{\gamma}(x, x)$, $x \neq 0$, established in [10], means that the density matrix $\tilde{\gamma}(x, y)$ is analytic *along* the diagonal $x = y$ as a function of one variable x , which does not contradict the non-smoothness of $\tilde{\gamma}(x, y)$ *on* the diagonal as a function of the two variables x and y .

Before we state the main result note that regularity of each of the terms in (1.5) can be studied individually. Furthermore, it suffices to establish the real analyticity of the function

$$\gamma(x, y) = \int_{\mathbb{R}^{3N-3}} \psi(x, \hat{\mathbf{x}}) \overline{\psi(y, \hat{\mathbf{x}})} \, d\hat{\mathbf{x}}, \quad (x, y) \in \mathbb{R}^3 \times \mathbb{R}^3. \quad (1.6)$$

The remaining terms in the sum (1.5) are handled by relabeling the variables. Thus, from now on we use the terms *one-particle density matrix* and *one-particle density* for the functions (1.6) and $\rho(x) = \gamma(x, x)$, respectively.

The next theorem constitutes our main result.

Theorem 1.1. *Let the function $\gamma(x, y)$, $(x, y) \in \mathbb{R}^3 \times \mathbb{R}^3$, be defined by (1.6). Then, $\gamma(x, y)$ is real analytic as a function of the variables x and y on the set*

$$D_0 = \{(x, y) \in \mathbb{R}^3 \times \mathbb{R}^3 : x \neq R_l, y \neq R_l, l = 1, 2, \dots, N_0, \text{ and } x \neq y\}. \quad (1.7)$$

As mentioned above, the eigenfunction $\psi(\mathbf{x})$ loses smoothness at the particle coalescence points. Therefore, a direct differentiation of (1.6) w.r.t. x and y under the integral will not produce the required analyticity. In order to circumvent this difficulty, we use the property that the eigenfunction preserves smoothness even at the coalescence points if one replaces the standard

derivatives by cleverly chosen directional ones. For example, the function ψ is infinitely smooth in the variable $x_1 + x_2 + \cdots x_N$, as long as $x_j \neq R_l$ for each $j = 1, 2, \dots, N$, $l = 1, 2, \dots, N_0$. In other words, it is infinitely differentiable with respect to the directional derivative

$$D = \sum_{j=1}^N \nabla_{x_j}.$$

Such regularity follows from the fact that the potential (1.3) is smooth w.r.t. D on the same domain. In particular,

$$D \frac{1}{|x_j - x_k|} = 0, \quad \text{for all } j \neq k.$$

This approach was successfully used in [10] (or even in the earlier paper [9]) in the study of the electron density $\rho(x) = \gamma(x, x)$. To illustrate the use of the directional derivatives in the study of $\rho(x)$, below we give a simplified example.

Assume that $N_0 = 1$ and that $R_1 = 0$. For further simplification instead of the function $\gamma(x, x)$, we consider only a part of it. Precisely, let $\zeta \in C_0^\infty(\mathbb{R}^3)$ be a real-valued function such that $\zeta(t) = 0$ for $|t| > \varepsilon/2$ with some $\varepsilon > 0$. Let us show that the integral

$$F(x) = \int_{\mathbb{R}^{3N-3}} |\psi(x, \hat{\mathbf{x}})|^2 \prod_{j=2}^N \zeta(x - x_j) d\hat{\mathbf{x}} \quad (1.8)$$

is C^∞ for all $x \in \mathbb{R}^3$ such that $|x| > \varepsilon$. The presence of the cut-off functions in (1.8) means that all the particles are within a $\varepsilon/2$ distance from the first particle. Thus, on the domain of integration all variables are separated from 0: $|x_j| \geq |x| - |x - x_j| > \varepsilon/2$, $j = 2, 3, \dots, N$. Rewrite F making the change of variables $x_j = w_j + x$, $j = 2, 3, \dots, N$, under the integral:

$$F(x) = \int_{\mathbb{R}^{3N-3}} |\psi(x, w_2 + x, \dots, w_N + x)|^2 \prod_{j=2}^N \zeta(-w_j) d\hat{\mathbf{w}},$$

$$\hat{\mathbf{w}} = (w_2, w_3, \dots, w_N).$$

Differentiating the integral w.r.t. x , we get:

$$\begin{aligned} \nabla_x F(x) &= 2 \operatorname{Re} \int_{\mathbb{R}^{3N-3}} (D\psi)(x, w_2 + x, \dots, w_N + x) \\ &\quad \times \overline{\psi(x, w_2 + x, \dots, w_N + x)} \prod_{j=2}^N \zeta(-w_j) d\hat{\mathbf{w}} \\ &= 2 \operatorname{Re} \int_{\mathbb{R}^{3N-3}} (D\psi)(x, \hat{\mathbf{x}}) \overline{\psi(x, \hat{\mathbf{x}})} \prod_{j=2}^N \zeta(x - x_j) d\hat{\mathbf{x}}. \end{aligned}$$

Now it is clear that by virtue of smoothness of ψ w.r.t. the derivative D , this relation can be differentiated arbitrarily many times, thereby proving that $F \in C^\infty$ for all $x : |x| > \varepsilon$.

The complete proof of real analyticity of $\rho(x)$ in [10] is more involved. In particular, it requires the study of various cut-off functions that keep some of the particles “close” to each other, but separate from the rest of them (we call this group of particles *the cluster associated with the given cut-off*). Adaptation of the above argument to such cases leads to the introduction of the *cluster derivatives* (i.e., directional derivatives involving only the particles in a cluster), and it is far from straightforward.

As in [10], in the current paper our starting point is again a careful analysis of the smoothness properties of the eigenfunction ψ with respect to the cluster derivatives. However, we find the argument in [10] somewhat condensed and sketchy in places. Thus, we provide our own proofs that contain more detail and at the same time, as we believe, are sometimes simpler than in [10].

To obtain bounds for the derivatives of $\gamma(x, y)$, we use again cluster derivatives, but the method of [10] is ineffective if applied directly. It has to be reworked taking into account the presence of two variables (i.e., x, y) instead of one. At the heart of our approach is the concept of an *extended cut-off function* that depends on the variables $(x, y) \in \mathbb{R}^3 \times \mathbb{R}^3$ and $\hat{\mathbf{x}} \in \mathbb{R}^{3N-3}$. Any such function $\Phi(x, y, \hat{\mathbf{x}})$ has two clusters associated with it, whose properties are linked to each other (see Subsect. 4.2). This enables us to apply the cluster derivatives method to integrals of the form:

$$\int_{\mathbb{R}^{3N-3}} \psi(x, \hat{\mathbf{x}}) \overline{\psi(y, \hat{\mathbf{x}})} \Phi(x, y, \hat{\mathbf{x}}) d\hat{\mathbf{x}}, \quad (x, y) \in \mathbb{R}^3 \times \mathbb{R}^3. \quad (1.9)$$

At the last stage, we construct a partition of unity on \mathbb{R}^{3N+3} which consists of extended cut-offs, and split $\gamma(x, y)$ in the sum of terms of the form (1.9). Estimating each of them individually, we get the desired real analyticity.

The paper is organized as follows. In Sect. 2, we state Theorem 2.2, involving more general interactions between particles, that implies Theorem 1.1 as a special case. This step allows to include other physically meaningful potentials, such as, for example, the Yukawa potential. An important conclusion of this section is that the claimed analyticity of the function $\gamma(x, y)$ follows from appropriate L^2 -bounds on the derivatives of $\gamma(x, y)$, enunciated in Theorem 2.3. The rest of the paper is devoted to the proof of Theorem 2.3.

Section 3 is concerned with the study of the directional derivatives of the eigenfunction ψ . The main objective is to establish suitable L^2 -estimates for higher-order derivatives of ψ on the open sets, separating different clusters of variables. Here our argument follows that of [10] with some simplifications. In Sect. 4, we study in detail properties of smooth cut-off functions including the extended cut-offs $\Phi = \Phi(x, y, \hat{\mathbf{x}})$, $x, y \in \mathbb{R}^3$, $\hat{\mathbf{x}} \in \mathbb{R}^{3N-3}$, and clusters associated with them. In Sect. 5, we put together the results of Sects. 3 and 4 to estimate the derivatives of integrals of the form (1.9) with extended cut-offs Φ . These estimates are used to prove Theorem 2.3 with the help of a partition of unity that consists of extended cut-offs. This completes the proof of Theorem 2.2, and hence that of the main result, Theorem 1.1. Appendix contains some elementary combinatorial formulas that are used throughout the proof.

We conclude the introduction with some general notational conventions.

Constants. By C or c with or without indices, we denote various positive constants whose exact value is of no importance.

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

Clusters. Let $R = \{1, 2, \dots, N\}$. An index set $P \subset R$ is called *cluster*. The cluster R is called *maximal*. 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 $\mathbf{P} = \{P_1, P_2, \dots, P_M\}$, $\mathbf{P}^* = \{P_1^*, P_2^*, \dots, P_M^*\}$ and call \mathbf{P} , \mathbf{P}^* *cluster sets*. Clusters P_1, P_2, \dots, P_M in a cluster set are not assumed to be all distinct.

Derivatives. Let $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. If $x = (x', x'', x''') \in \mathbb{R}^3$ and $m = (m', m'', m''') \in \mathbb{N}_0^3$, 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

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

A central role is played by the following directional derivatives. For a cluster P and each $m = (m', m'', m''') \in \mathbb{N}_0^3$, we define the *cluster derivatives*

$$D_P^m = \left(\sum_{k \in P} \partial_{x'_k} \right)^{m'} \left(\sum_{k \in P} \partial_{x''_k} \right)^{m''} \left(\sum_{k \in P} \partial_{x'''_k} \right)^{m'''} \quad (1.10)$$

These operations can be viewed as partial derivatives w.r.t. the variable $\sum_{k \in P} x_k$. Let $\mathbf{P} = \{P_1, P_2, \dots, P_M\}$ be a cluster set, and let $\mathbf{m} = (m_1, m_2, \dots, m_M)$, $m_k \in \mathbb{N}_0^3$, $k = 1, 2, \dots, M$. Then, we denote

$$D_{\mathbf{P}}^{\mathbf{m}} = D_{P_1}^{m_1} D_{P_2}^{m_2} \dots D_{P_M}^{m_M}.$$

Supports. For any smooth function $f = f(\mathbf{x})$, we define the set $\text{supp}_0 f = \{\mathbf{x} : f(\mathbf{x}) \neq 0\}$. Note that this set is open and its closure $\overline{\text{supp}_0 f}$ gives the standard definition of the support $\text{supp } f$. For $\text{supp}_0 f$, we immediately get the useful property that

$$\text{supp}_0(fg) = \text{supp}_0 f \cap \text{supp}_0 g. \quad (1.11)$$

Furthermore, for any $\mathbf{m} \in \mathbb{N}_0^{3N}$, $|\mathbf{m}| = 1$, we have

$$\text{supp}_0 \partial^{\mathbf{m}} f \subset \text{supp}_0 f, \quad \text{if } f \geq 0. \quad (1.12)$$

2. The Main Result

2.1. Main Theorem

The main theorem 1.1 is derived from the following result that holds for more general potentials than (1.3).

Let $V_{k,l}, W_{k,j} \in C^\infty(\mathbb{R}^3 \setminus \{0\})$, $l = 1, 2, \dots, N_0$, $k, j = 1, 2, \dots, N$, be functions on \mathbb{R}^3 such that for all $v \in H^1(\mathbb{R}^3)$ we have

$$\|V_{k,l}v\|_{L^2} + \|W_{k,j}v\|_{L^2} \leq C\|v\|_{H^1}, \quad (2.1)$$

and for every $\varepsilon > 0$, we have

$$\sum_{k=1}^N \sum_{l=1}^{N_0} \max_{|x|>\varepsilon} |\partial_x^m V_{k,l}(x)| + \sum_{\substack{k,j=1 \\ k \neq j}}^N \max_{|x|>\varepsilon} |\partial_x^m W_{k,j}(x)| \leq A_0^{1+|m|} (1 + |m|)^{|m|}, \quad (2.2)$$

for all $m \in \mathbb{N}_0^3$ with some positive constant $A_0 = A_0(\varepsilon)$. The condition (2.2) implies that the functions $V_{k,l}$ and $W_{k,j}$ are real analytic on $\mathbb{R}^3 \setminus \{0\}$. Instead of the potential V^C defined in (1.3), we consider the potential

$$V(\mathbf{x}) = \sum_{k=1}^N \sum_{l=1}^{N_0} V_{k,l}(x_k - R_l) + \sum_{\substack{k,j=1 \\ k \neq j}}^N W_{k,j}(x_k - x_j). \quad (2.3)$$

The Coulomb potentials $V_{k,l}(x) = -Z_l|x|^{-1}$ and $W_{k,j}(x) = (2|x|)^{-1}$ satisfy (2.1) in view of the classical Hardy's inequality, see, e.g., [20, The Uncertainty Principle Lemma, p. 169]. Furthermore, the bounds (2.2) can be deduced from the estimates for harmonic functions, established, e.g., in [7, Theorem 7, p. 29]. Thus, the potential (1.3) is a special case of (2.3). Working with more general potentials allows one to include into consideration other physically meaningful interactions, such as, e.g., the Yukawa potential. This generalization was pointed out in [10].

We need the following elementary elliptic regularity fact, which we give with a proof, since it is quite short.

Lemma 2.1. *Suppose that V is given by (2.3). Then,*

$$\|Vv\|_{L^2} \leq C\|v\|_{H^1}, \quad (2.4)$$

for all $v \in H^1(\mathbb{R}^{3N})$.

If $v \in H^1(\mathbb{R}^{3N})$ and $Hv \in L^2(\mathbb{R}^{3N})$, then $v \in H^2(\mathbb{R}^{3N})$ and

$$\|v\|_{H^2} \leq C(\|Hv\|_{L^2} + \|v\|_{L^2}). \quad (2.5)$$

The constant C depends on N and N_0 only.

Proof. The bound (2.4) immediately follows from (2.1).

For $v \in H^1$, $Hv \in L^2$, it follows from (2.4) that

$$-\Delta v = Hv - Vv \in L^2. \quad (2.6)$$

Consequently, in view of the straightforward bound

$$\|v\|_{\mathbf{H}^2} \leq C_1(\|\Delta v\|_{\mathbf{L}^2} + \|v\|_{\mathbf{L}^2}), \quad (2.7)$$

the function v is \mathbf{H}^2 , and hence, (2.4) implies that

$$\|Vv\|_{\mathbf{L}^2} \leq \delta\|v\|_{\mathbf{H}^2} + \tilde{C}_\delta\|v\|_{\mathbf{L}^2}, \quad (2.8)$$

for all $\delta > 0$. Together with (2.6) and (2.7), this leads to the bound

$$\|v\|_{\mathbf{H}^2} \leq C_1(\|Hv\|_{\mathbf{L}^2} + \delta\|v\|_{\mathbf{H}^2} + (\tilde{C}_\delta + 1)\|v\|_{\mathbf{L}^2}).$$

Taking $\delta = (2C_1)^{-1}$, we easily derive (2.5) with a suitable constant $C > 0$. \square

Note that the estimate (2.8) shows that the potential (2.3) is infinitesimally $H^{(0)}$ -bounded, so that the operator H defined in (1.2) is self-adjoint on the domain $D(H^{(0)}) = \mathbf{H}^2(\mathbb{R}^{3N})$.

Theorem 1.1 is a consequence of the following result.

Theorem 2.2. *Let the potential V be given by (2.3), with some functions $V_{k,l}$ and $W_{k,j}$, satisfying the conditions (2.1) and (2.2). Let ψ be an eigenfunction of the operator (1.2), and let $\gamma(x, y)$ be as defined in (1.6). Then, $\gamma(x, y)$ is real analytic as a function of the variables x and y on the set (1.7).*

For the sake of simplicity, we prove this theorem only for the case of a single atom, i.e., for $N_0 = 1$. The general case requires only obvious modifications. Without loss of generality, we set $R_1 = 0$. Thus, (2.3) rewrites as:

$$V(\mathbf{x}) = \sum_{k=1}^N V_k(x_k) + \sum_{\substack{k,j=1 \\ k \neq j}}^N W_{k,j}(x_k - x_j), \quad V_k = V_{k,1}, \quad (2.9)$$

and the stated analyticity of $\gamma(x, y)$ will be proved on the set

$$\mathcal{D}_0 = \{(x, y) \in \mathbb{R}^3 \times \mathbb{R}^3 : x \neq 0, y \neq 0, x \neq y\}.$$

This result is derived from the following \mathbf{L}^2 -bound on the set

$$\mathcal{D} = \mathcal{D}_\varepsilon = \{(x, y) \in \mathbb{R}^3 \times \mathbb{R}^3 : |x| > \varepsilon, |y| > \varepsilon, |x - y| > \varepsilon\}, \quad \varepsilon > 0. \quad (2.10)$$

Theorem 2.3. *Let $\varepsilon > 0$ be arbitrary. Then, for all $k, m \in \mathbb{N}_0^3$, we have*

$$\|\partial_x^k \partial_y^m \gamma(\cdot, \cdot)\|_{L^2(\mathcal{D}_\varepsilon)} \leq A^{|k|+|m|+2}(|k| + |m| + 1)^{|k|+|m|}, \quad (2.11)$$

with some constants $A = A(\varepsilon)$, independent of k, m .

The derivation of Theorem 2.2 from Theorem 2.3 is based on the following elementary lemma.

Lemma 2.4. *Let $\Omega \subset \mathbb{R}^d$ be an open set, and let $f \in C^\infty(\Omega)$ be a function such that*

$$\|\partial_x^s f\|_{L^2(\Omega)} \leq B^{2+|s|}(1 + |s|)^{|s|}, \quad (2.12)$$

for all $s \in \mathbb{N}_0^d$, with some positive constant B . Then, f is real analytic on Ω .

Proof. Let $x_0 \in \Omega$, and let $r > 0$ be such that $B(x_0, 2r) = \{x \in \mathbb{R}^d : |x - x_0| < 2r\} \subset \Omega$. We aim to prove that

$$|\partial_x^s f(x)| \leq CR^{-|s|} s!, \quad (2.13)$$

for all $s \in \mathbb{N}_0^d$ and for each $x \in B(x_0, r)$, with some positive constants C and R , possibly depending on x_0 and r . According to [17, Proposition 2.2.10], this would imply the required analyticity.

Let $\beta \in C_0^\infty(\mathbb{R}^d)$ be a function supported on $B(x_0, 2r)$ and such that $\beta = 1$ on $B(x_0, r)$. Denote

$$g(x) = \beta(x) \partial_x^s f(x).$$

By the standard Sobolev inequalities, see, e.g., [7, Theorem 6, p. 270], for $l > d/4$ we can estimate

$$\|g\|_{L^\infty(\mathbb{R}^d)} \leq C \|(1 - \Delta)^l g\|_{L^2(\mathbb{R}^d)},$$

with a constant C depending on l . Now it follows from (2.12) that

$$\|g\|_{L^\infty(\mathbb{R}^d)} \leq C' B^{|s|+2l+2} (|s| + 2|l| + 1)^{|s|+2l}.$$

By (7.2), the right-hand side does not exceed

$$\tilde{C}(Be)^{|s|+2l+2} (|s| + 2l)! \leq \tilde{C}(Be)^{|s|+2l+2} e^{2l(|s|+2l)} |s|!$$

According to (7.5),

$$|s|! \leq d^{|s|} s!.$$

Consequently,

$$\|g\|_{L^\infty(\mathbb{R}^d)} \leq \tilde{C}(Be)^{2l+2} e^{4l^2} (Be^{1+2l} d)^{|s|} s!.$$

This bound leads to (2.13) with explicitly given constants C and R . The proof is now complete. \square

Proof of Theorem 2.2. According to Theorem 2.3 and Lemma 2.4, the function $\gamma(x, y)$ is real analytic on \mathcal{D}_ε for all $\varepsilon > 0$. Consequently, it is real analytic on

$$\mathcal{D}_0 = \bigcup_{\varepsilon > 0} \mathcal{D}_\varepsilon,$$

as required. \square

The rest of the paper is focused on the proof of Theorem 2.3.

2.2. More Notation

Here we introduce some important sets in \mathbb{R}^{3N} and \mathbb{R}^{3N-3} . For $\varepsilon \geq 0$ introduce

$$X_P(\varepsilon) = \begin{cases} \mathbb{R}^{3N} & \text{for } |P| = 0 \text{ or } N, \\ \{\mathbf{x} \in \mathbb{R}^{3N} : |x_j - x_k| > \varepsilon, \forall j \in P, k \in P^c\}, & \text{for } 0 < |P| < N, \end{cases} \quad (2.14)$$

The set $X_P(\varepsilon)$, $\varepsilon > 0$, separates the points x_k and x_j labeled by the clusters P and P^c , respectively. Note that $X_P(\varepsilon) = X_{P^c}(\varepsilon)$.

Define also the sets separating x_k 's from the origin:

$$T_{\mathbf{P}}(\varepsilon) = \begin{cases} \mathbb{R}^{3N}, & \text{for } |\mathbf{P}| = 0, \\ \{\mathbf{x} \in \mathbb{R}^{3N} : |x_j| > \varepsilon, \forall j \in \mathbf{P}\}, & \text{for } |\mathbf{P}| > 0. \end{cases} \quad (2.15)$$

It is also convenient to introduce a similar notation involving only the variable $\hat{\mathbf{x}}$:

$$\hat{T}_{\mathbf{P}^*}(\varepsilon) = \begin{cases} \mathbb{R}^{3N-3}, & \text{for } |\mathbf{P}^*| = 0, \\ \{\hat{\mathbf{x}} \in \mathbb{R}^{3N-3} : |x_j| > \varepsilon, \forall j \in \mathbf{P}^*\}, & \text{for } |\mathbf{P}^*| > 0. \end{cases} \quad (2.16)$$

For the cluster sets $\mathbf{P} = \{\mathbf{P}_1, \mathbf{P}_2, \dots, \mathbf{P}_M\}$, $\mathbf{P}^* = \{\mathbf{P}_1^*, \mathbf{P}_2^*, \dots, \mathbf{P}_M^*\}$ define

$$\begin{cases} X_{\mathbf{P}}(\varepsilon) = \bigcap_{s=1}^M X_{\mathbf{P}_s}(\varepsilon) \subset \mathbb{R}^{3N}, & T_{\mathbf{P}}(\varepsilon) = \bigcap_{s=1}^M T_{\mathbf{P}_s}(\varepsilon) \subset \mathbb{R}^{3N}, \\ U_{\mathbf{P}}(\varepsilon) = X_{\mathbf{P}}(\varepsilon) \cap T_{\mathbf{P}}(\varepsilon), \\ \hat{T}_{\mathbf{P}^*}(\varepsilon) = \bigcap_{s=1}^M \hat{T}_{\mathbf{P}_s^*}(\varepsilon) \subset \mathbb{R}^{3N-3}. \end{cases} \quad (2.17)$$

Now we introduce the standard cut-off functions with which we work. Let

$$\xi \in C^\infty(\mathbb{R}) : 0 \leq \xi(t) \leq 1, \quad \xi(t) = \begin{cases} 0, & \text{if } t \leq 0, \\ 1, & \text{if } t \geq 1. \end{cases} \quad (2.18)$$

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

$$\theta(x) = \xi\left(\frac{4N}{\varepsilon}|x| - 1\right), \quad \zeta(x) = 1 - \theta(x), \quad x \in \mathbb{R}^3, \quad (2.19)$$

so that

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

3. Regularity of the Eigenfunctions

In this section, we establish estimates for the derivatives $D_{\mathbf{P}}^{\mathbf{m}}\psi$ of the eigenfunction ψ , see (1.10) for the definition of the cluster derivatives. Our argument is an expanded version of the approach suggested in [10], which, in turn, was inspired by the proof of analyticity for solutions of elliptic equations with analytic coefficients, see, e.g., the classical monograph [13, Section 7.5].

The key point of our argument is the regularity of the functions $D_{\mathbf{P}}^{\mathbf{m}}\psi$ for all $\mathbf{m} \in \mathbb{N}_0^{3M}$ on the domain $U_{\mathbf{P}}(\varepsilon)$ with arbitrary positive ε . As before, in the estimates below we denote by C, c with or without indices positive constants whose exact value is of no importance. For constants that are important for subsequent results, we use the notation L or A with indices. The letter L (resp. A) is used when the constant is independent of (resp. dependent on) ε .

We begin the proof of the required property with studying the regularity of the potential (2.9).

3.1. Regularity of the Potential (2.9)

The next assertion is a more detailed variant of [10, Part 2 of Lemma A.3] adapted to the potential (2.9).

Lemma 3.1. *Let V be as defined in (2.9), and let $\mathbf{P} = \{P_1, P_2, \dots, P_M\}$ be an arbitrary cluster set. Then, for all $\mathbf{m} \in \mathbb{N}_0^{3M}$, $|\mathbf{m}| \geq 1$, the function $D_{\mathbf{P}}^{\mathbf{m}}V$ is C^∞ on $U_{\mathbf{P}}(\varepsilon)$, and the bound*

$$\|D_{\mathbf{P}}^{\mathbf{m}}V\|_{L^\infty(U_{\mathbf{P}}(\varepsilon))} \leq A_0^{1+|\mathbf{m}|}(|\mathbf{m}| + 1)^{|\mathbf{m}|} \quad (3.1)$$

holds, where A_0 is the constant from the condition (2.2).

Proof. Without loss of generality, we may assume that $\mathbf{m} = (m_1, m_2, \dots, m_M)$ with all $|m_j| \geq 1$. Indeed, suppose that $m_1 = 0$ and represent $\mathbf{P} = \{P_1, \tilde{\mathbf{P}}\}$ with $\tilde{\mathbf{P}} = \{P_2, P_3, \dots, P_M\}$. Then, denoting $\tilde{\mathbf{m}} = (m_2, m_3, \dots, m_M)$, we get

$$\|D_{\mathbf{P}}^{\mathbf{m}}V\|_{L^\infty(U_{\mathbf{P}}(\varepsilon))} = \|D_{\tilde{\mathbf{P}}}^{\tilde{\mathbf{m}}}V\|_{L^\infty(U_{\mathbf{P}}(\varepsilon))} \leq \|D_{\tilde{\mathbf{P}}}^{\tilde{\mathbf{m}}}V\|_{L^\infty(U_{\tilde{\mathbf{P}}}(\varepsilon))}.$$

Repeating, if necessary, this procedure we can eliminate all zero components of \mathbf{m} , and the clusters, attached to them. Thus, we assume henceforth that $|m_j| \geq 1$, $j = 1, 2, \dots, M$.

For the clusters P_1, P_2, \dots, P_M introduce two disjoint sets of index pairs:

$$\begin{aligned} \mathcal{N}_s &= \{(j, k) : j \in P_s, k \in P_s, j \neq k\} \cup \{(j, k) : j \in P_s^c, k \in P_s^c, j \neq k\}, \\ \mathcal{M}_s &= \{(j, k) : j \in P_s, k \in P_s^c \text{ or } k \in P_s, j \in P_s^c\}, \quad s = 1, 2, \dots, M. \end{aligned}$$

so that $\mathcal{N}_s \cup \mathcal{M}_s = \{(j, k) \in \mathbb{R} \times \mathbb{R} : j \neq k\}$.

If $|m| = 1$, then a direct differentiation gives the formula

$$D_{P_s}^m V_k(x_k) = \begin{cases} 0, & k \in P_s^c, \\ \partial_x^m V_k(x)|_{x=x_k}, & k \in P_s. \end{cases}$$

This function is C^∞ on $U_{P_s}(\varepsilon)$, and further differentiation gives the same formula for all $|m| \geq 1$. Similarly,

$$|D_{P_s}^m W_{k,j}(x_k - x_j)| = \begin{cases} 0, & (k, j) \in \mathcal{N}_s, \\ |\partial_x^m W_{k,j}(x)|_{x=x_k-x_j}|, & (k, j) \in \mathcal{M}_s. \end{cases}$$

Consequently,

$$D_{\mathbf{P}}^{\mathbf{m}} V_k(x_k) = \begin{cases} 0, & k \in \cup_s P_s^c, \\ \partial_x^{m_1+m_2+\dots+m_M} V_k(x)|_{x=x_k}, & k \in \cap_s P_s. \end{cases}$$

and

$$\begin{aligned} &|D_{\mathbf{P}}^{\mathbf{m}} W_{k,j}(x_k - x_j)| \\ &= \begin{cases} 0, & (k, j) \in \cup_s \mathcal{N}_s, \\ |\partial_x^{m_1+m_2+\dots+m_M} W_{k,j}(x)|_{x=x_k-x_j}|, & (k, j) \in \cap_s \mathcal{M}_s. \end{cases} \end{aligned}$$

By the definition (2.17), for $\mathbf{x} \in U_{\mathbf{P}}(\varepsilon)$ we have $|x_j| > \varepsilon$ for all $j \in \cap_s \mathbf{P}_s$, and $|x_j - x_k| > \varepsilon$ for all $(j, k) \in \cap_s \mathcal{M}_s$. Thus, the functions above are C^∞ on $U_{\mathbf{P}}(\varepsilon)$, and, by the definition (2.9), it follows from (2.2) that

$$\|\mathbf{D}_{\mathbf{P}}^{\mathbf{m}} V\|_{L^\infty(U_{\mathbf{P}}(\varepsilon))} \leq A_0^{1+|\mathbf{m}|} (1 + |\mathbf{m}|)^{|\mathbf{m}|}.$$

This bound coincides with (3.1). \square

Now we proceed to the study of the derivatives $\mathbf{D}_{\mathbf{P}}^{\mathbf{m}} \psi$.

3.2. Regularity of the Derivatives $\mathbf{D}_{\mathbf{P}}^{\mathbf{m}} \psi$

As before, let $\psi \in H^2(\mathbb{R}^{3N})$ be an eigenfunction of the operator H , with the eigenvalue $E \in \mathbb{R}$, i.e., $H_E \psi = 0$, where $H_E = H - E$. Let $\mathbf{P} = \{\mathbf{P}_1, \mathbf{P}_2, \dots, \mathbf{P}_M\}$ be a cluster set, and consider the function $u_{\mathbf{m}} = \mathbf{D}_{\mathbf{P}}^{\mathbf{m}} \psi$ with some $\mathbf{m} \in \mathbb{N}_0^{3M}$. As an eigenfunction of H , the function ψ is $H^2(\mathbb{R}^{3N})$, and, by elliptic regularity, it is smooth (even analytic) on the set $\mathcal{S} = \{x_k \neq 0, x_k \neq x_j : j, k = 1, 2, \dots, N\}$. Our objective is to show that the function ψ has derivatives $u_{\mathbf{m}}$ of all orders $|\mathbf{m}| \geq 0$ on the larger set $U_{\mathbf{P}}(0) \supset \mathcal{S}$, and that $u_{\mathbf{m}} \in H^2(U_{\mathbf{P}}(\varepsilon))$ for all $\varepsilon > 0$.

Let us begin with a formal calculation. Since $H_E \psi = 0$, by Leibniz's formula, we obtain

$$\begin{aligned} H_E u_{\mathbf{m}} &= [H_E, \mathbf{D}_{\mathbf{P}}^{\mathbf{m}}] \psi = [V, \mathbf{D}_{\mathbf{P}}^{\mathbf{m}}] \psi \\ &= - \sum_{\substack{0 \leq \mathbf{s} \leq \mathbf{m} \\ |\mathbf{s}| \geq 1}} \binom{\mathbf{m}}{\mathbf{s}} \mathbf{D}_{\mathbf{P}}^{\mathbf{s}} V u_{\mathbf{m}-\mathbf{s}} = f_{\mathbf{m}}. \end{aligned} \quad (3.2)$$

Thus, $u_{\mathbf{m}}$ is a solution of the equation $H_E u_{\mathbf{m}} = f_{\mathbf{m}}$. The next assertion gives this statement a precise meaning.

First we observe that by Lemma 3.1, $\|\mathbf{D}_{\mathbf{P}}^{\mathbf{s}} V\|_{L^\infty(U_{\mathbf{P}}(\varepsilon))} < \infty$ for every $\mathbf{s} : |\mathbf{s}| \geq 1$, and all $\varepsilon > 0$. Therefore, if $u_{\mathbf{m}} \in L^2(U_{\mathbf{P}}(\varepsilon))$ for all $\mathbf{m} : |\mathbf{m}| \leq p$, then $f_{\mathbf{m}} \in L^2(U_{\mathbf{P}}(\varepsilon))$ for all $|\mathbf{m}| \leq p + 1$.

Lemma 3.2. *Suppose that $u_{\mathbf{m}} \in L^2(U_{\mathbf{P}}(\varepsilon))$ for some $\varepsilon > 0$ and all $\mathbf{m} \in \mathbb{N}_0^{3M}$ such that $|\mathbf{m}| \leq p$ with some $p \in \mathbb{N}_0$. Then, $u_{\mathbf{m}}$ is a weak solution of the equation $H_E u_{\mathbf{m}} = f_{\mathbf{m}}$, that is, it satisfies the identity*

$$\int u_{\mathbf{m}} \overline{H_E \eta} d\mathbf{x} = \int f_{\mathbf{m}} \overline{\eta} d\mathbf{x}, \quad (3.3)$$

for all $\eta \in C_0^\infty(U_{\mathbf{P}}(\varepsilon))$ and all $\mathbf{m} : |\mathbf{m}| \leq p$.

Proof. As noted before the lemma, $f_{\mathbf{m}} \in L^2(U_{\mathbf{P}}(\varepsilon))$ for all $|\mathbf{m}| \leq p + 1$, so that both sides of (3.3) are finite. Throughout the proof we use the fact that $\mathbf{D}_{\mathbf{P}}^{\mathbf{s}} V \in C^\infty$ on $U_{\mathbf{P}}(\varepsilon)$ for all $\mathbf{s} : |\mathbf{s}| \geq 1$, see Lemma 3.1.

We prove the identity (3.3) by induction. First note that (3.3) holds for $\mathbf{m} = 0$, since ψ is an eigenfunction and $f_0 = 0$. Suppose that it holds for all $\mathbf{m} : |\mathbf{m}| \leq k$, with some $k \leq p - 1$. We need to show that this implies (3.3) for $\mathbf{m} + \mathbf{l}$, where $\mathbf{l} \in \mathbb{N}_0^{3M} : |\mathbf{l}| = 1$. As $u_{\mathbf{m}+\mathbf{l}} = \mathbf{D}_{\mathbf{P}}^{\mathbf{l}} u_{\mathbf{m}}$, we can integrate by parts,

using (3.3) for $|\mathbf{m}| \leq k$:

$$\begin{aligned}
 & \int u_{\mathbf{m}+1} \overline{H_E \eta} d\mathbf{x} \\
 &= - \int u_{\mathbf{m}} \overline{D_{\mathbf{P}}^1 H_E \eta} d\mathbf{x} = - \int u_{\mathbf{m}} \overline{H_E D_{\mathbf{P}}^1 \eta} d\mathbf{x} - \int u_{\mathbf{m}} (D_{\mathbf{P}}^1 V) \overline{\eta} d\mathbf{x} \\
 &= - \int f_{\mathbf{m}} \overline{D_{\mathbf{P}}^1 \eta} d\mathbf{x} - \int u_{\mathbf{m}} (D_{\mathbf{P}}^1 V) \overline{\eta} d\mathbf{x}.
 \end{aligned} \tag{3.4}$$

Integrating by parts and using definition of $f_{\mathbf{m}}$ (see (3.2)), we get for the first integral on the right-hand side that

$$\int f_{\mathbf{m}} \overline{D_{\mathbf{P}}^1 \eta} d\mathbf{x} = \sum_{\mathbf{s}: |\mathbf{s}| \geq 1}^{\mathbf{m}} \binom{\mathbf{m}}{\mathbf{s}} \int ((D_{\mathbf{P}}^{1+\mathbf{s}} V) u_{\mathbf{m}-\mathbf{s}} + (D_{\mathbf{P}}^{\mathbf{s}} V) u_{\mathbf{m}+1-\mathbf{s}}) \overline{\eta} d\mathbf{x}.$$

Standard calculations involving binomial coefficients show that

$$\begin{aligned}
 \int f_{\mathbf{m}} \overline{D_{\mathbf{P}}^1 \eta} d\mathbf{x} &= \sum_{\mathbf{s}: |\mathbf{s}| \geq 1}^{\mathbf{m}+1} \binom{\mathbf{m}+1}{\mathbf{s}} \int (D_{\mathbf{P}}^{\mathbf{s}} V) u_{\mathbf{m}+1-\mathbf{s}} \overline{\eta} d\mathbf{x} - \int (D_{\mathbf{P}}^1 V) u_{\mathbf{m}} \overline{\eta} d\mathbf{x} \\
 &= - \int f_{\mathbf{m}+1} \overline{\eta} d\mathbf{x} - \int (D_{\mathbf{P}}^1 V) u_{\mathbf{m}} \overline{\eta} d\mathbf{x}.
 \end{aligned}$$

Substituting this in (3.4), we obtain that

$$\int u_{\mathbf{m}+1} \overline{H_E \eta} d\mathbf{x} = \int f_{\mathbf{m}+1} \overline{\eta} d\mathbf{x},$$

which coincides with (3.3) for $\mathbf{m}+1$. Now by induction we conclude that (3.3) holds for all $\mathbf{m} : |\mathbf{m}| \leq p$, as claimed. \square

Theorem 3.3. *Let E be an eigenvalue of H and let ψ be the associated eigenfunction. For each $\varepsilon > 0$, the function $u_{\mathbf{m}} = D_{\mathbf{P}}^{\mathbf{m}} \psi$ belongs to $H^2(U_{\mathbf{P}}(\varepsilon))$ for all $\mathbf{m} \in \mathbb{N}_0^{3M}$.*

Proof. For brevity throughout the proof, we use the notation $\mathcal{H}_{\varepsilon}^{\alpha} = H^{\alpha}(U_{\mathbf{P}}(\varepsilon))$, $\alpha = 1, 2$, $\mathcal{L}_{\varepsilon}^2 = L^2(U_{\mathbf{P}}(\varepsilon))$.

The claim holds for $\mathbf{m} = 0$, since $\psi \in H^2(\mathbb{R}^{3N})$ is an eigenfunction and $f_0 = 0$. Suppose that it holds for all $\mathbf{m} : |\mathbf{m}| \leq p \in \mathbb{N}_0$. We need to show that this implies that $u_{\mathbf{m}+1} \in \mathcal{H}_{\varepsilon}^2$, for all $\varepsilon > 0$, where $\mathbf{l} \in \mathbb{N}_0^{3M} : |\mathbf{l}| = 1$ and $|\mathbf{m}| = p$.

Since $u_{\mathbf{m}} \in \mathcal{H}_{\varepsilon}^2$, we have $u_{\mathbf{m}+1} \in \mathcal{H}_{\varepsilon}^1 \subset \mathcal{L}_{\varepsilon}^2$ for all $\varepsilon > 0$. Thus, by Lemma 3.2, $u_{\mathbf{m}+1}$ satisfies (3.3) with $f_{\mathbf{m}+1} \in \mathcal{L}_{\varepsilon}^2$. In order to show that $u_{\mathbf{m}+1} \in \mathcal{H}_{\varepsilon}^2$, for all $\varepsilon > 0$, we apply Lemma 2.1. To this end let $\eta_1 \in C^{\infty}(\mathbb{R}^{3N})$ be a function such that $\eta_1(\mathbf{x}) = 0$ for $\mathbf{x} \in \mathbb{R}^{3N} \setminus U_{\mathbf{P}}(\varepsilon/2)$ and $\eta_1(\mathbf{x}) = 1$ for $\mathbf{x} \in U_{\mathbf{P}}(\varepsilon)$. Thus, by (3.3),

$$\begin{aligned}
 H_E(u_{\mathbf{m}+1} \eta_1) &= \eta_1 H_E u_{\mathbf{m}+1} - 2 \nabla \eta_1 \nabla u_{\mathbf{m}+1} - u_{\mathbf{m}+1} \Delta \eta_1 \\
 &= \eta_1 f_{\mathbf{m}+1} - 2 \nabla \eta_1 \nabla u_{\mathbf{m}+1} - u_{\mathbf{m}+1} \Delta \eta_1.
 \end{aligned}$$

Since $u_{\mathbf{m}+1} \in \mathcal{H}_{\varepsilon/2}^1$, the right-hand side belongs to $\mathbb{L}^2(\mathbb{R}^{3N})$. Therefore, $H(u_{\mathbf{m}+1}\eta) \in \mathbb{L}^2(\mathbb{R}^{3N})$, and by Lemma 2.1, $u_{\mathbf{m}+1}\eta_1 \in \mathbb{H}^2(\mathbb{R}^{3N})$. As a consequence, $u_{\mathbf{m}+1} \in \mathcal{H}_{\varepsilon}^2$, as required. Now, by induction, $u_{\mathbf{m}} \in \mathcal{H}_{\varepsilon}^2$ for all $\mathbf{m} \in \mathbb{N}_0^{3M}$. \square

3.3. Eigenfunction Estimates

Apart from the qualitative fact of smoothness of $u_{\mathbf{m}} = \mathbf{D}_{\mathbf{P}}^{\mathbf{m}}\psi$, now we need to establish explicit estimates for $u_{\mathbf{m}}$. As before, we denote $H_E = H - E$ with an arbitrary $E \in \mathbb{R}$.

Lemma 3.4. *Let $v \in \mathbb{H}^2(U_{\mathbf{P}}(\varepsilon))$ and let $\mathbf{m} \in \mathbb{N}_0^{3N}$, $|\mathbf{m}| \leq 2$. Then, for any $\varepsilon > 0$, $\delta \in (0, 1)$ we have*

$$\delta^{|\mathbf{m}|} \|\partial^{\mathbf{m}} v\|_{\mathbb{L}^2(U_{\mathbf{P}}(\varepsilon+\delta))} \leq C_0 \left(\delta^2 \|Hv\|_{\mathbb{L}^2(U_{\mathbf{P}}(\varepsilon))} + \max_{\substack{\mathbf{j} \in \mathbb{N}_0^{3N} \\ |\mathbf{j}| \leq 1}} \delta^{|\mathbf{j}|} \|\partial^{\mathbf{j}} v\|_{\mathbb{L}^2(U_{\mathbf{P}}(\varepsilon))} \right),$$

with a constant C_0 independent of the function v , constants ε , δ and of the cluster set \mathbf{P} .

Proof. Let $|\mathbf{m}| \leq 1$. Since $U_{\mathbf{P}}(\varepsilon + \delta) \subset U_{\mathbf{P}}(\varepsilon)$, we have

$$\delta^{|\mathbf{m}|} \|\partial^{\mathbf{m}} v\|_{\mathbb{L}^2(U_{\mathbf{P}}(\varepsilon+\delta))} \leq \max_{\substack{\mathbf{j} \in \mathbb{N}_0^{3N} \\ |\mathbf{j}| \leq 1}} \delta^{|\mathbf{j}|} \|\partial^{\mathbf{j}} v\|_{\mathbb{L}^2(U_{\mathbf{P}}(\varepsilon))},$$

so that the required bound holds.

Assume now that $|\mathbf{m}| = 2$. Without loss of generality assume that all clusters $\mathbf{P}_s \in \mathbf{P}$, $s = 1, 2, \dots, M$, are distinct. Let ξ be the smooth function defined in (2.18). For arbitrary $\varepsilon, \delta > 0$ define the cut-off

$$\eta(\mathbf{x}) = \eta_{\mathbf{P}}(\mathbf{x}) = \prod_{s=1}^M \prod_{\substack{k \in \mathbf{P}_s \\ j \in \mathbf{P}_s^c}} \xi\left(\frac{|x_k| - \varepsilon}{\delta}\right) \xi\left(\frac{|x_k - x_j| - \varepsilon}{\delta}\right).$$

Then, $\text{supp}_0 \eta \subset U_{\mathbf{P}}(\varepsilon)$ and $\eta = 1$ on $U_{\mathbf{P}}(\varepsilon + \delta)$. It is also clear that

$$\max_{\mathbf{P}} \|\partial^{\mathbf{k}} \eta\| \leq C_{\mathbf{k}} |\delta|^{-|\mathbf{k}|}, \quad \forall \mathbf{k} \in \mathbb{N}_0^{3N},$$

with some positive constants $C_{\mathbf{k}}$ independent of ε and δ , where the maximum is taken over all sets \mathbf{P} of distinct clusters. Estimate, using the bound (2.5):

$$\begin{aligned} \|\partial^{\mathbf{m}} v\|_{\mathbb{L}^2(U_{\mathbf{P}}(\varepsilon+\delta))} &\leq \|\partial^{\mathbf{m}}(v\eta)\|_{\mathbb{L}^2} \leq C(\|H(v\eta)\|_{\mathbb{L}^2} + \|v\eta\|_{\mathbb{L}^2}) \\ &\leq C(\|\eta H v\|_{\mathbb{L}^2} + \|v \Delta \eta\|_{\mathbb{L}^2} + 2\|(\nabla \eta) \nabla v\|_{\mathbb{L}^2} + \|v\eta\|_{\mathbb{L}^2}) \\ &\leq \tilde{C}(\|Hv\|_{\mathbb{L}^2(U_{\mathbf{P}}(\varepsilon))} + (\delta^{-2} + 1)\|v\|_{\mathbb{L}^2(U_{\mathbf{P}}(\varepsilon))} \\ &\quad + \delta^{-1}\|\nabla v\|_{\mathbb{L}^2(U_{\mathbf{P}}(\varepsilon))}), \end{aligned}$$

with constants independent of ε, δ . Multiplying by δ^2 , we get the required estimate. \square

Let E be an eigenvalue of H and ψ be the associated eigenfunction. Now we use Lemma 3.4 for the function $v = u_{\mathbf{m}} = \mathbf{D}_{\mathbf{P}}^{\mathbf{m}}\psi \in \mathbb{H}^2(U_{\mathbf{P}}(\varepsilon))$, $\varepsilon > 0$.

Corollary 3.5. *There exists a constant $L_2 > 0$ independent of the cluster set \mathbf{P} and of the parameters $\varepsilon > 0, \delta \in (0, 1)$, such that for all $\mathbf{m} \in \mathbb{N}_0^{3M}$, $\mathbf{k}, \mathbf{l} \in \mathbb{N}_0^{3N}$, $|\mathbf{k}| + |\mathbf{l}| \leq 2$, we have*

$$\begin{aligned} & \delta^{|\mathbf{k}|+|\mathbf{l}|} \|\partial^{\mathbf{k}} \mathbf{D}_{\mathbf{P}}^{\mathbf{m}+1} \psi\|_{L^2(U_{\mathbf{P}}(\varepsilon+\delta))} \\ & \leq L_2 \left(\delta^2 \|f_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon))} + \max_{\substack{\mathbf{j} \in \mathbb{N}_0^{3N} \\ |\mathbf{j}| \leq 1}} \delta^{|\mathbf{j}|} \|\partial^{\mathbf{j}} \mathbf{D}_{\mathbf{P}}^{\mathbf{m}} \psi\|_{L^2(U_{\mathbf{P}}(\varepsilon))} \right). \end{aligned} \quad (3.5)$$

Proof. Apply Lemma 3.4 to the function $v = u_{\mathbf{m}}$ and estimate

$$\begin{aligned} \|Hu_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon))} & \leq \|H_E u_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon))} + |E| \|u_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon))} \\ & = \|f_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon))} + |E| \|u_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon))}. \end{aligned}$$

□

Now we use the bound (3.5) to obtain estimates for the function $u_{\mathbf{m}}$ with arbitrary $\mathbf{m} \in \mathbb{N}_0^{3M}$. Let A_0 , L_2 and L_3 be the constants featuring in (3.1), (3.5) and (7.3), respectively. Define

$$A_1 = 2A_0 + L_2(L_3A_0 + 1) + \max_{\mathbf{j}: |\mathbf{j}| \leq 1} \|\partial^{\mathbf{j}} \psi\|_{L^2(\mathbb{R}^{3N})}. \quad (3.6)$$

Thus, defined constant depends on the eigenvalue E and $\varepsilon > 0$, but is independent of the cluster set \mathbf{P} and of $\delta \in (0, 1]$.

Lemma 3.6. *Let the constant A_1 be as defined in (3.6). Then, for all $\mathbf{m} \in \mathbb{N}_0^{3M}$, all $\mathbf{k} \in \mathbb{N}_0^{3N}$, $|\mathbf{k}| \leq 1$, and all $\varepsilon > 0$ and $\delta > 0$ such that $\delta(|\mathbf{m}| + 1) \leq 1$, we have*

$$\|\partial^{\mathbf{k}} \mathbf{D}_{\mathbf{P}}^{\mathbf{m}} \psi\|_{L^2(U_{\mathbf{P}}(\varepsilon+(|\mathbf{m}|+1)\delta))} \leq A_1^{|\mathbf{m}|+1} \delta^{-|\mathbf{m}|-|\mathbf{k}|}. \quad (3.7)$$

Proof. The formula (3.7) holds for $\mathbf{m} = \mathbf{0}$. Indeed, since $\delta \leq 1$, we get

$$\delta^{|\mathbf{k}|} \|\partial^{\mathbf{k}} \psi\|_{L^2(U_{\mathbf{P}}(\varepsilon+\delta))} \leq \max_{\mathbf{j}: |\mathbf{j}| \leq 1} \delta^{|\mathbf{j}|} \|\partial^{\mathbf{j}} \psi\|_{L^2(\mathbb{R}^{3N})} \leq A_1.$$

Further proof is by induction. As before, we use the notation $u_{\mathbf{m}} = \mathbf{D}_{\mathbf{P}}^{\mathbf{m}} \psi$. Suppose that (3.7) holds for all $\mathbf{m} \in \mathbb{N}_0^{3M}$ such that $|\mathbf{m}| \leq p$ with some p . Our task is to deduce from this that (3.7) holds for all \mathbf{m} , such that $|\mathbf{m}| = p + 1$. Precisely, we need to show that if $|\mathbf{m}| = p$ and $\mathbf{l} \in \mathbb{N}_0^{3M}$ is such that $|\mathbf{l}| = 1$, then

$$\|\partial^{\mathbf{k}} u_{\mathbf{m}+\mathbf{l}}\|_{L^2(U_{\mathbf{P}}(\varepsilon+(p+2)\delta))} \leq A_1^{p+2} \delta^{-p-|\mathbf{k}|-1}, \quad (3.8)$$

for all $\delta > 0$ such that $(p+2)\delta \leq 1$.

Since $|\mathbf{l}| + |\mathbf{k}| = 1 + |\mathbf{k}| \leq 2$, it follows from (3.5) that

$$\begin{aligned} \delta^{|\mathbf{k}|+1} \|\partial^{\mathbf{k}} u_{\mathbf{m}+\mathbf{l}}\|_{L^2(U_{\mathbf{P}}(\varepsilon+(p+2)\delta))} & \leq L_2 \left(\delta^2 \|f_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon+(p+1)\delta))} \right. \\ & \quad \left. + \max_{\substack{\mathbf{j} \in \mathbb{N}_0^{3N} \\ |\mathbf{j}| \leq 1}} \delta^{|\mathbf{j}|} \|\partial^{\mathbf{j}} u_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon+(p+1)\delta))} \right). \end{aligned} \quad (3.9)$$

By the induction hypothesis, the second term in the brackets on the right-hand side satisfies the bound

$$\max_{\substack{\mathbf{j} \in \mathbb{N}_0^{3N} \\ |\mathbf{j}| \leq 1}} \delta^{|\mathbf{j}|} \|\partial^{\mathbf{j}} u_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon + (p+1)\delta))} \leq \delta^{-p} A_1^{p+1}. \quad (3.10)$$

Let us estimate the first term on the right-hand side of (3.9). First we find suitable bounds for the norms of the functions $u_{\mathbf{m}-\mathbf{s}}$, $0 \leq \mathbf{s} \leq \mathbf{m}$, $|\mathbf{s}| \geq 1$, featuring in the definition of the function $f_{\mathbf{m}}$, see (3.2). Denote $q = |\mathbf{s}|$. Since $|\mathbf{m} - \mathbf{s}| \leq p$, we can use the induction assumption to obtain

$$\|u_{\mathbf{m}-\mathbf{s}}\|_{L^2(U_{\mathbf{P}}(\varepsilon + (p-q+1)\tilde{\delta}))} \leq A_1^{p-q+1} \tilde{\delta}^{-p+q},$$

for all $\tilde{\delta}$ such that $(p-q+1)\tilde{\delta} \leq 1$. In particular, the value $\tilde{\delta} = (p+1)(p-q+1)^{-1}\delta$ satisfies the latter requirement, because $(p+1)\delta \leq 1$. Thus,

$$\|u_{\mathbf{m}-\mathbf{s}}\|_{L^2(U_{\mathbf{P}}(\varepsilon + (p+1)\delta))} \leq A_1^{p-q+1} (p+1)^{-p+q} (p-q+1)^{p-q} \delta^{-p+q}.$$

For the derivatives of V , we use (3.1), so that

$$\|\mathbf{D}_{\mathbf{P}}^{\mathbf{s}} V\|_{L^\infty(U_{\mathbf{P}}(\varepsilon + (p+1)\delta))} \leq \|\mathbf{D}_{\mathbf{P}}^{\mathbf{s}} V\|_{L^\infty(U_{\mathbf{P}}(\varepsilon))} \leq A_0^{q+1} (q+1)^q.$$

Using the definition of $f_{\mathbf{m}}$, see (3.2), and putting together the two previous estimates, we obtain

$$\begin{aligned} & \|f_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon + (p+1)\delta))} \\ & \leq \sum_{q=1}^p \sum_{|\mathbf{s}|=q} \binom{\mathbf{m}}{\mathbf{s}} A_0^{q+1} (q+1)^q A_1^{p-q+1} (p+1)^{-p+q} (p-q+1)^{p-q} \delta^{-p+q}. \end{aligned}$$

In view of (7.4), the right-hand side coincides with

$$A_0 A_1^{p+1} \sum_{q=1}^p \binom{p}{q} (A_0 A_1^{-1})^q (q+1)^q (p+1)^{-p+q} (p-q+1)^{p-q} \delta^{-p+q}.$$

Estimate the coefficient $\binom{p}{q}$, using (7.3):

$$\begin{aligned} & \|f_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon + (p+1)\delta))} \\ & \leq L_3 A_0 A_1^{p+1} \delta^{-p} \sum_{q=1}^p (A_0 A_1^{-1})^q ((1+p)\delta)^q \leq L_3 A_0 A_1^{p+1} \delta^{-p} \sum_{q=1}^p (A_0 A_1^{-1})^q, \end{aligned}$$

where we have taken into account that $(p+1)\delta \leq 1$. By (3.6), we have $A_0 A_1^{-1} \leq 1/2$, so that the sum on the right-hand side does not exceed 1. Since $\delta \leq 1$, we can now conclude that

$$\delta^2 \|f_{\mathbf{m}}\|_{L^2(U_{\mathbf{P}}(\varepsilon + (p+1)\delta))} \leq L_3 A_0 A_1^{p+1} \delta^{-p+2} \leq L_3 A_0 A_1^{p+1} \delta^{-p}.$$

Substituting this bound together with (3.10) in (3.9), we arrive at the estimate

$$\|\partial^{\mathbf{k}} u_{\mathbf{m}+\mathbf{l}}\|_{L^2(U_{\mathbf{P}}(\varepsilon + (p+2)\delta))} \leq \delta^{-p-1-|\mathbf{k}|} A_1^{p+1} L_2 (1 + L_3 A_0).$$

By the definition (3.6), the factor $L_2(1 + L_3 A_0)$ does not exceed A_1 . This leads to the bound (3.8), and hence proves the lemma. \square

Corollary 3.7. *For any $\varepsilon \in (0, 1]$, there is a constant $A_2 = A_2(\varepsilon)$, such that for all cluster sets $\mathbf{P} = \{P_1, P_2, \dots, P_M\}$ and all $\mathbf{m} \in \mathbb{N}_0^{3M}$, we have*

$$\|D_{\mathbf{P}}^{\mathbf{m}}\psi\|_{L^2(U_{\mathbf{P}}(2\varepsilon))} \leq A_2^{|\mathbf{m}|+1}(1 + |\mathbf{m}|)^{|\mathbf{m}|}.$$

Proof. Use (3.7) with $\mathbf{k} = \mathbf{0}$ and $\delta = (|\mathbf{m}| + 1)^{-1}\varepsilon$:

$$\|D_{\mathbf{P}}^{\mathbf{m}}\psi\|_{L^2(U_{\mathbf{P}}(2\varepsilon))} \leq \varepsilon^{-|\mathbf{m}|} A_1^{|\mathbf{m}|+1}(1 + |\mathbf{m}|)^{|\mathbf{m}|} \leq A_2^{|\mathbf{m}|+1}(1 + |\mathbf{m}|)^{|\mathbf{m}|},$$

with $A_2 = \varepsilon^{-1}A_1$, where we have taken into account that $\varepsilon \leq 1$. \square

4. Cut-Off Functions and Associated Clusters

4.1. Admissible Cut-Off Functions

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 , θ or $\partial_x^l \theta$, $l \in \mathbb{N}_0^3$, $|l| = 1$, and $f_{jk} = f_{kj}$. We work with the smooth functions of the form:

$$\phi(\mathbf{x}) = \prod_{1 \leq j < k \leq N} f_{jk}(x_j - x_k). \quad (4.1)$$

We call such functions *admissible cut-off functions* or simply *admissible cut-offs*. For any such function ϕ we also introduce the following “partial” products. For an arbitrary cluster $\mathbf{P} \subset \mathbf{R} = \{1, 2, \dots, N\}$ define

$$\phi(\mathbf{x}; \mathbf{P}) = \begin{cases} \prod_{\substack{j < k \\ j, k \in \mathbf{P}}} f_{jk}(x_j - x_k), & \text{if } |\mathbf{P}| \geq 2; \\ 1, & \text{if } |\mathbf{P}| \leq 1. \end{cases}$$

Furthermore, for any two clusters $\mathbf{P}, \mathbf{S} \subset \mathbf{R}$, such that $\mathbf{S} \cap \mathbf{P} = \emptyset$, we define

$$\phi(\mathbf{x}; \mathbf{P}, \mathbf{S}) = \begin{cases} \prod_{j \in \mathbf{P}, k \in \mathbf{S}} f_{jk}(x_j - x_k), & \text{if } \mathbf{P} \neq \emptyset \text{ and } \mathbf{S} \neq \emptyset; \\ 1, & \text{if } \mathbf{P} = \emptyset \text{ or } \mathbf{S} = \emptyset. \end{cases} \quad (4.2)$$

Note that

$$D_{\mathbf{P}}^l \phi(\mathbf{x}; \mathbf{P}) = D_{\mathbf{P}}^l \phi(\mathbf{x}; \mathbf{P}^c) = 0, \quad \text{for all } l \in \mathbb{N}_0^3, |l| \geq 1. \quad (4.3)$$

It is straightforward to see that for any cluster \mathbf{P} the function $\phi(\mathbf{x})$ can be represented as follows:

$$\phi(\mathbf{x}) = \phi(\mathbf{x}; \mathbf{P})\phi(\mathbf{x}; \mathbf{P}^c)\phi(\mathbf{x}; \mathbf{P}, \mathbf{P}^c). \quad (4.4)$$

Following [10], we associate with the function ϕ a cluster $\mathbf{Q}(\phi)$ defined next.

Definition 4.1. For an admissible cut-off ϕ , let $I(\phi) \subset \{(j, k) \in \mathbf{R} \times \mathbf{R} : j \neq k\}$ be the set such that $(j, k) \in I(\phi)$, iff $f_{jk} \neq \theta$. We say that two indices $j, k \in \mathbf{R}$, 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 $\mathbf{Q}(\phi)$ 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 index 1. Note also that the notion of being linked defines an equivalence relation on R , and the cluster $Q(\phi)$ is nothing but the equivalence class of index 1.

For example, if $N = 4$ and

$$\phi(\mathbf{x}) = \zeta(x_1 - x_2)\theta(x_1 - x_3)\theta(x_1 - x_4)\partial_x^l\theta(x_2 - x_3)\theta(x_2 - x_4)\theta(x_3 - x_4),$$

with some $l \in \mathbb{N}_0^3$, $|l| = 1$, then $Q(\phi) = \{1, 2, 3\}$.

Let $P = Q(\phi)$. If P^c is not empty, i.e., $P \neq R$, then by the definition of P , we always have $f_{jk}(x) = \theta(x)$ for all $j \in P$ and $k \in P^c$, and hence the representation (4.4) holds with

$$\phi(\mathbf{x}; P, P^c) = \prod_{j \in P, k \in P^c} \theta(x_j - x_k). \quad (4.5)$$

The notion of associated cluster is useful because of its connection with the support of the cut-off ϕ . This is clear from the next two lemmata. Recall that the sets X_P, \widehat{T}_P are defined in (2.14) and (2.16), respectively.

Lemma 4.2. *For $P = Q(\phi)$ the inclusion*

$$\text{supp}_0 \phi \subset X_P(\varepsilon(4N)^{-1}) \quad (4.6)$$

holds.

Proof. If $P^c = \emptyset$, then, by definition, $X_P = \mathbb{R}^{3N}$, and hence (4.6) is trivial.

Suppose that P^c is non-empty. The inclusion (4.6) immediately follows from the representation (4.4), formula (4.5) and the definition of the function θ . \square

Lemma 4.3. *If $j \in Q(\phi)$, then $|x_1 - x_j| < \varepsilon/2$ for all $\mathbf{x} \in \text{supp}_0 \phi$. Moreover,*

$$\text{supp}_0 \phi(x_1, \cdot) \subset \widehat{T}_{P^*}(\varepsilon/2), \quad (4.7)$$

for all $x_1 : |x_1| > \varepsilon$.

Proof. Let $\mathbf{x} \in \text{supp}_0 \phi$. By the definition of ζ and θ , if $(j, k) \in I(\phi)$, then $|x_j - x_k| < \varepsilon(2N)^{-1}$. Thus, if j and k are ϕ -linked to each other, then

$$\begin{aligned} |x_j - x_k| &\leq |x_j - x_{j_1}| + \sum_{p=1}^{s-1} |x_{j_p} - x_{j_{p+1}}| + |x_{j_s} - x_k| \\ &\leq \frac{\varepsilon}{2N}(s+1) < \frac{\varepsilon}{2}. \end{aligned}$$

In particular, for $j \in Q(\phi)$ we have $|x_1 - x_j| < \varepsilon/2$, as claimed.

Proof of (4.7). Suppose that $\mathbf{x} \in \text{supp}_0 \phi$ and $|x_1| > \varepsilon$. By Lemma 4.3, for each $j \in P^*$ we have $|x_1 - x_j| < \varepsilon/2$, so that

$$|x_j| \geq |x_1| - |x_1 - x_j| > \frac{\varepsilon}{2},$$

as claimed. \square

To summarize in words, on the support of the admissible cut-off ϕ the variables x_j , indexed by $j \in P = Q(\phi)$, are “close” to each other and “far” from the remaining variables.

Let ϕ be of the form (4.1), and let $P = Q(\phi)$. For each $l \in \mathbb{N}_0^3$, the function $D_P^l \phi$ has the form:

$$D_P^l \phi(\mathbf{x}) = \phi(\mathbf{x}; P) \phi(\mathbf{x}; P^c) D_P^l \phi(\mathbf{x}; P, P^c), \quad P = Q(\phi), \quad (4.8)$$

where we have used the factorization (4.4) and property (4.3). By the definition (4.2), $D_P^l \phi = 0$ if $P^c = \emptyset$.

Lemma 4.4. *Let $P = Q(\phi)$ and $l \in \mathbb{N}_0^3, |l| = 1$. If $P^c \neq \emptyset$, then the function (4.8) is represented in the form:*

$$D_P^l \phi(\mathbf{x}) = \sum_{s \in P, r \in P^c} \phi_{s,r}^{(l)}, \quad (4.9)$$

where each $\phi_{s,r}^{(l)}$ is an admissible cut-off of the form:

$$\phi_{s,r}^{(l)}(\mathbf{x}) = \phi(\mathbf{x}; P) \phi(\mathbf{x}; P^c) \partial_x^l \theta(x_s - x_r) \prod_{\substack{j \in P, k \in P^c \\ (j,k) \neq (s,r)}} \theta(x_j - x_k). \quad (4.10)$$

Moreover, $P \subset Q(\phi_{s,r}^{(l)})$ and $|Q(\phi_{s,r}^{(l)})| \geq |P| + 1$.

Proof. The representation (4.9) immediately follows from the definition (4.5). It is clear from (4.10) that $\phi_{s,r}^{(l)}$ has the form (4.1), and hence, it is admissible.

Due to the presence of the derivative $\partial_x^l \theta$, in addition to all indices linked to index 1 by the function ϕ , the new function $\phi_{s,r}^{(l)}$ links the indices r and s as well, and hence its associated cluster $Q(\phi_{s,r}^{(l)})$ contains P and $|Q(\phi_{s,r}^{(l)})| \geq |P| + 1$, as claimed. \square

In what follows a special role is played by the factorization (4.4) with $P = \{1\}$, so that

$$\phi(x_1, \hat{\mathbf{x}}) = \omega(x_1, \hat{\mathbf{x}}) \varkappa(\hat{\mathbf{x}}) \quad \text{with} \quad \omega(x_1, \hat{\mathbf{x}}) = \phi(x_1, \hat{\mathbf{x}}; \{1\}, R^*), \quad \varkappa(\hat{\mathbf{x}}) = \phi(\mathbf{x}; R^*). \quad (4.11)$$

We call the functions ω and \varkappa the *canonical factors* of ϕ . In the next corollary, we find the canonical factors for the cut-offs $\phi_{s,r}^{(l)}$ defined in (4.10).

Corollary 4.5. *Let ω, \varkappa be the canonical factors of ϕ , and let $P^c \neq \emptyset$. Then, the functions $\phi_{s,r}^{(l)}$ can be represented as follows:*

$$\phi_{s,r}^{(l)}(x_1, \hat{\mathbf{x}}) = \omega_{r,s}^{(l)}(x_1, \hat{\mathbf{x}}) \varkappa_{s,r}^{(l)}(\hat{\mathbf{x}}), \quad s \in P, r \in P^c,$$

with

$$\begin{aligned} \omega_{1,r}^{(l)}(x_1, \hat{\mathbf{x}}) &= \phi(x_1, \hat{\mathbf{x}}; \{1\}, P^*) \partial_x^l \theta(x_1 - x_r) \prod_{k \in P^c, k \neq r} \theta(x_1 - x_k), \\ \varkappa_{1,r}^{(l)}(\hat{\mathbf{x}}) &= \varkappa(\hat{\mathbf{x}}), \end{aligned} \quad (4.12)$$

and

$$\begin{aligned}\omega_{s,r}^{(l)}(x_1, \hat{\mathbf{x}}) &= \omega(x_1, \hat{\mathbf{x}}), \\ \kappa_{s,r}^{(l)}(\hat{\mathbf{x}}) &= \phi(\hat{\mathbf{x}}; \mathbf{P}^*)\phi(\hat{\mathbf{x}}; \mathbf{P}^c)\partial_x^l \theta(x_s - x_r) \prod_{\substack{j \in \mathbf{P}^*, k \in \mathbf{P}^c \\ (j,k) \neq (s,r)}} \theta(x_j - x_k),\end{aligned}\quad (4.13)$$

for all $s \in \mathbf{P}^*$.

Proof. The claim is an immediate consequence of (4.10). \square

4.2. Extended Cut-Offs

Now we are ready to introduce the cut-off functions with which we work when estimating the derivatives of the one-particle density matrix $\gamma(x, y)$. These cut-offs are functions of $3N + 3$ variables and they are defined as follows. We say that two admissible cut-offs $\phi = \phi(x_1, \hat{\mathbf{x}})$ and $\mu = \mu(x_1, \hat{\mathbf{x}})$ are *coupled to each other* if they share the same canonical factor $\kappa = \kappa(\hat{\mathbf{x}}) = \phi(\mathbf{x}; \mathbf{R}^*) = \mu(\mathbf{x}; \mathbf{R}^*)$, i.e.,

$$\phi(x_1, \hat{\mathbf{x}}) = \omega(x_1, \hat{\mathbf{x}})\kappa(\hat{\mathbf{x}}), \quad \mu(x_1, \hat{\mathbf{x}}) = \tau(x_1, \hat{\mathbf{x}})\kappa(\hat{\mathbf{x}}),$$

where ω is defined as in (4.11) and $\tau(x_1, \hat{\mathbf{x}}) = \mu(x_1, \hat{\mathbf{x}}; \{1\}, \mathbf{R}^*)$. Out of two coupled cut-offs ϕ, μ we construct a new function of $3N + 3$ variables:

$$\begin{aligned}\Phi(x, y, \hat{\mathbf{x}}) &= \omega(x, \hat{\mathbf{x}})\tau(y, \hat{\mathbf{x}})\kappa(\hat{\mathbf{x}}) \\ &= \phi(x, \hat{\mathbf{x}})\tau(y, \hat{\mathbf{x}}) = \omega(x, \hat{\mathbf{x}})\mu(y, \hat{\mathbf{x}}), \quad (x, y) \in \mathbb{R}^3 \times \mathbb{R}^3, \hat{\mathbf{x}} \in \mathbb{R}^{3N-3}.\end{aligned}\quad (4.14)$$

We call such Φ an *extended* cut-off. It is clear that every extended cut-off defines a pair of coupled admissible ϕ and μ uniquely. We say that the pair ϕ, μ and the extended cut-off Φ are associated with each other. The representations (4.14) and identity (1.11) give the equality

$$\text{supp}_0 \Phi(x, y, \cdot) = \text{supp}_0 \phi(x, \cdot) \cap \text{supp}_0 \mu(y, \cdot), \quad \forall (x, y) \in \mathbb{R}^3 \times \mathbb{R}^3. \quad (4.15)$$

From now on we denote $\mathbf{P} = \mathbf{Q}(\phi)$ and $\mathbf{S} = \mathbf{Q}(\mu)$.

Below we list some useful properties of the extended cut-offs Φ and associated admissible ϕ, μ . Due to the nature of the definition (4.14), in all statements involving the functions ϕ, μ and Φ , the pairs $\{\phi, \mathbf{P}\}$ and $\{\mu, \mathbf{S}\}$ can be interchanged.

Lemma 4.6. *If $\mathbf{P}^* \cap \mathbf{S}$ is non-empty, then $\Phi(x, y, \hat{\mathbf{x}}) = 0$ for all $\hat{\mathbf{x}} \in \mathbb{R}^{3N-3}$ if $(x, y) \in \mathcal{D}_\varepsilon$.*

Proof. Suppose that $\mathbf{P}^* \cap \mathbf{S}$ is non-empty and that $(x, \hat{\mathbf{x}}) \in \text{supp}_0 \phi$, $(y, \hat{\mathbf{x}}) \in \text{supp}_0 \mu$. By Lemma 4.3, for each $j \in \mathbf{P}^* \cap \mathbf{S}$ we have $|x - x_j| < \varepsilon/2$ and $|y - x_j| < \varepsilon/2$. Hence, $|x - y| < \varepsilon$, and so

$$\text{supp}_0 \phi(x, \cdot) \cap \text{supp}_0 \mu(y, \cdot) = \emptyset, \quad \text{if } (x, y) \in \mathcal{D}_\varepsilon.$$

By (4.15), $\Phi(x, y, \hat{\mathbf{x}}) = 0$ for all $\hat{\mathbf{x}} \in \mathbb{R}^{3N-3}$ if $(x, y) \in \mathcal{D}_\varepsilon$, as claimed. \square

Due to Lemma 4.6 from now on we may assume that $\mathbf{P}^* \subset \mathbf{S}^c$.

Lemma 4.7. *Let ϕ and μ be coupled admissible cut-offs, and let $P^* \subset S^c$. Then,*

$$\tau(x_1, \hat{\mathbf{x}}) = \mu(x_1, \hat{\mathbf{x}}; \{1\}, P^c) \prod_{j \in P^*} \theta(x_1 - x_j), \quad (4.16)$$

and

$$\text{supp}_0 \mu \subset X_{P^*}(\varepsilon(4N)^{-1}). \quad (4.17)$$

Furthermore,

$$\tau(y, \hat{\mathbf{x}}) = \mu(y, \hat{\mathbf{x}}; \{1\}, P^c), \quad \text{if } (x, y) \in \mathcal{D}_\varepsilon \quad \text{and } (x, \hat{\mathbf{x}}) \in \text{supp}_0 \phi. \quad (4.18)$$

Proof. Since $R^* = P^* \cup P^c$, the function $\tau(x_1, \hat{\mathbf{x}}) = \mu(x_1, \hat{\mathbf{x}}; \{1\}, R^*)$ factorizes as follows:

$$\tau(x_1, \hat{\mathbf{x}}) = \mu(x_1, \hat{\mathbf{x}}; \{1\}, P^c) \mu(x_1, \hat{\mathbf{x}}; \{1\}, P^*).$$

As $P^* \subset S^c$, we have

$$\mu(x_1, \hat{\mathbf{x}}; \{1\}, P^*) = \prod_{j \in P^*} \theta(x_1 - x_j),$$

which leads to (4.16).

If $P^c = \emptyset$, i.e., $P = R$, then the inclusion $P^* \subset S^c$ implies that $S^c = P^*$. By Lemma 4.2,

$$\text{supp}_0 \mu \subset X_S(\varepsilon(4N)^{-1}).$$

As $X_S = X_{S^c}$, the claimed result follows.

Assume now that $P^c \neq \emptyset$. Consider separately the factors in the representation $\mu(\mathbf{x}) = \tau(x_1, \hat{\mathbf{x}}) \varkappa(\hat{\mathbf{x}})$. Since

$$\varkappa(\hat{\mathbf{x}}) = \phi(\hat{\mathbf{x}}; P^*) \phi(\hat{\mathbf{x}}; P^c) \phi(\hat{\mathbf{x}}; P^*, P^c),$$

in view of (4.5) and definition (2.19) we have

$$\begin{aligned} \text{supp}_0 \varkappa &\subset \text{supp}_0 \phi(\cdot; P^*, P^c) \\ &\subset \{ \hat{\mathbf{x}} : |x_j - x_k| > \varepsilon(4N)^{-1}, j \in P^*, k \in P^c \}. \end{aligned} \quad (4.19)$$

In view of (4.16), by the definition (2.19) again,

$$\text{supp}_0 \tau \subset \{ \mathbf{x} : |x_1 - x_j| > \varepsilon(4N)^{-1}, j \in P^* \}.$$

Since $P^c \cup \{1\} = (P^*)^c$, together with (4.19), this gives the inclusion

$$\begin{aligned} \text{supp}_0 \mu &= \text{supp}_0 \varkappa \tau \subset \{ \mathbf{x} : |x_j - x_k| > \varepsilon(4N)^{-1}, j \in P^*, k \in (P^*)^c \} \\ &= X_{P^*}(\varepsilon(4N)^{-1}), \end{aligned}$$

as required.

Proof of (4.18). Since $(x, \hat{\mathbf{x}}) \in \text{supp}_0 \phi$, by Lemma 4.3 we have $|x - x_j| < \varepsilon/2$, $j \in P^*$. As $(x, y) \in \mathcal{D}_\varepsilon$, this implies that $|y - x_j| > \varepsilon/2$ for all $j \in P^*$. By definition (2.19), $\theta(y - x_j) = 1$ if $|y - x_j| > \varepsilon(2N)^{-1}$. Therefore, $\theta(y - x_j) = 1$ for all $j \in P^*$. Hence, the product on the right-hand side of (4.16) equals one, which implies (4.18). \square

In the next lemma, we collect all the information on the supports of the coupled ϕ, μ and associated extended cut-off Φ that we need in the next section.

Lemma 4.8. *If $P^* \subset S^c$, then*

$$\begin{cases} \text{supp}_0 \phi \subset X_P(\varepsilon(4N)^{-1}) \cap X_{S^*}(\varepsilon(4N)^{-1}), \\ \text{supp}_0 \mu \subset X_S(\varepsilon(4N)^{-1}) \cap X_{P^*}(\varepsilon(4N)^{-1}). \end{cases} \quad (4.20)$$

If $(x, y) \in \mathcal{D}_\varepsilon$, then

$$\text{supp}_0 \Phi(x, y, \cdot) = \text{supp}_0 \phi(x, \cdot) \cap \text{supp}_0 \mu(y, \cdot) \subset \widehat{T}_{P^*}(\varepsilon/2) \cap \widehat{T}_{S^*}(\varepsilon/2). \quad (4.21)$$

Proof. The second inclusion in (4.20) follows from the inclusion (4.6) applied to function μ and from the relation (4.17). The condition $P^* \subset S^c$ is equivalent to $S^* \subset P^c$. Thus, the first inclusion in (4.20) follows from the inclusion (4.6) and the relation (4.17) applied to the function ϕ .

Since $|x| > \varepsilon$ and $|y| > \varepsilon$ for $(x, y) \in \mathcal{D}_\varepsilon$, the inclusion (4.21) follows from (4.7) applied to ϕ and μ . \square

Similarly to the cluster derivatives (4.8) of the admissible cut-offs, now we need to investigate the cluster derivatives of the extended cut-offs. As before, let $\Phi(x, y, \hat{\mathbf{x}})$ be an extended cut-off associated with the coupled admissible cut-offs ϕ, μ , and let $P = Q(\phi)$, $S = Q(\mu)$. It will be sufficient to confine our attention to the derivatives D_P^l w.r.t. the variable \mathbf{x} for the cluster P .

Assume that $P^c \neq \emptyset$. Let $\phi_{s,r}^{(l)}$, $s \in P, r \in P^c$, be the admissible cut-offs defined in (4.10), and let $\omega_{s,r}^{(l)}$ and $\varkappa_{s,r}^{(l)}$ be their canonical factors detailed in (4.12) and (4.13), respectively. Using the factor τ from the canonical factorization $\mu(\hat{\mathbf{x}}) = \tau(x_1, \hat{\mathbf{x}})\varkappa(\hat{\mathbf{x}})$ we define a new admissible cut-off

$$\mu_{s,r}^{(l)}(x_1, \hat{\mathbf{x}}) = \tau(x_1, \hat{\mathbf{x}})\varkappa_{s,r}^{(l)}(\hat{\mathbf{x}}).$$

It is clear that $\phi_{s,r}^{(l)}$ and $\mu_{s,r}^{(l)}$ are coupled to each other. Introduce the associated extended cut-off:

$$\Phi_{s,r}^{(l)}(x, y, \hat{\mathbf{x}}) = \phi_{s,r}^{(l)}(x, \hat{\mathbf{x}})\tau(y, \hat{\mathbf{x}}) = \omega_{s,r}^{(l)}(x, \hat{\mathbf{x}})\mu_{s,r}^{(l)}(y, \hat{\mathbf{x}}). \quad (4.22)$$

It follows from (4.10), (4.13) and (1.11), (1.12) that

$$\text{supp}_0 \phi_{s,r}^{(l)} \subset \text{supp}_0 \phi, \quad \text{supp}_0 \mu_{s,r}^{(l)} \subset \text{supp}_0 \mu. \quad (4.23)$$

Now we can describe the cluster derivatives of Φ . The notation $D_P^l \Phi(x, y, \hat{\mathbf{x}})$ means taking the l th P -cluster derivative w.r.t. the variable $\mathbf{x} = (x, \hat{\mathbf{x}})$.

Lemma 4.9. *Let $\Phi = \Phi(x, y, \hat{\mathbf{x}})$ be an extended cutoff associated with the coupled admissible ϕ and μ and assume that $P^* \subset S^c$. Let $l \in \mathbb{N}_0^3$ be an arbitrary multi-index such that $|l| = 1$.*

If $P^c = \emptyset$, i.e., $P = R$, then $D_P^l \Phi(x, y, \hat{\mathbf{x}}) = 0$ for all $(x, y) \in \mathcal{D}_\varepsilon$.

If $P^c \neq \emptyset$, then

$$D_P^l \Phi(x, y, \hat{\mathbf{x}}) = \sum_{s \in P, r \in P^c} \Phi_{s,r}^{(l)}(x, y, \hat{\mathbf{x}}), \quad \text{for all } (x, y) \in \mathcal{D}_\varepsilon, \quad (4.24)$$

where the extended cut-offs $\Phi_{s,r}^{(l)}(x, y, \hat{\mathbf{x}})$ are defined in (4.22).

Proof. According to (4.18),

$$\Phi(x, y, \hat{\mathbf{x}}) = \phi(x, \hat{\mathbf{x}}) \mu(y, \hat{\mathbf{x}}; \{1\}, \mathbf{P}^c), \quad (x, y) \in \mathcal{D}_\varepsilon.$$

Therefore, if $\mathbf{P}^c = \emptyset$, then $\Phi(x, y, \hat{\mathbf{x}}) = \phi(x, \hat{\mathbf{x}})$. As $D_{\mathbf{P}}^l \phi(\mathbf{x}) = 0$, we also have $D_{\mathbf{P}}^l \Phi(x, y, \hat{\mathbf{x}}) = 0$, as claimed.

Assume that $\mathbf{P}^c \neq \emptyset$. By (4.23) and (4.18),

$$\Phi_{s,r}^{(l)}(x, y, \hat{\mathbf{x}}) = \phi_{s,r}^{(l)}(x, \hat{\mathbf{x}}) \mu(y, \hat{\mathbf{x}}; \{1\}, \mathbf{P}^c), \quad s \in \mathbf{P}, r \in \mathbf{P}^c, \quad (4.25)$$

for all $(x, y) \in \mathcal{D}_\varepsilon$. Since the factor $\mu(y, \hat{\mathbf{x}}; \{1\}, \mathbf{P}^c)$ does not depend on x_j with $j \in \mathbf{P}^*$, we have

$$\begin{aligned} D_{\mathbf{P}}^l \Phi(x, y, \hat{\mathbf{x}}) &= D_{\mathbf{P}}^l \phi(x, \hat{\mathbf{x}}) \mu(y, \hat{\mathbf{x}}; \{1\}, \mathbf{P}^c) + \phi(x, \hat{\mathbf{x}}) D_{\mathbf{P}^*}^l \mu(y, \hat{\mathbf{x}}; \{1\}, \mathbf{P}^c) \\ &= D_{\mathbf{P}}^l \phi(x, \hat{\mathbf{x}}) \mu(y, \hat{\mathbf{x}}; \{1\}, \mathbf{P}^c). \end{aligned}$$

Using (4.9) and (4.25) we get

$$D_{\mathbf{P}}^l \Phi(x, y, \hat{\mathbf{x}}) = \sum_{s \in \mathbf{P}, r \in \mathbf{P}^c} \phi_{s,r}^{(l)}(x, \hat{\mathbf{x}}) \mu(y, \hat{\mathbf{x}}; \{1\}, \mathbf{P}^c) = \sum_{s \in \mathbf{P}, r \in \mathbf{P}^c} \Phi_{s,r}^{(l)}(x, y, \hat{\mathbf{x}}),$$

as required. \square

5. Estimating the Density Matrix

The proof of Theorem 2.3 which is given in Sect. 6, uses a partition of unity that consists of extended cut-off functions, i.e., functions of the form (4.14). Thus, the objective of this section is to estimate the derivatives of the function

$$\gamma(x, y; \Phi) = \int_{\mathbb{R}^{3(N-1)}} \psi(x, \hat{\mathbf{x}}) \overline{\psi(y, \hat{\mathbf{x}})} \Phi(x, y, \hat{\mathbf{x}}) d\hat{\mathbf{x}}, \quad (5.1)$$

with an extended cut-off Φ on the set \mathcal{D}_ε :

Theorem 5.1. *Let Φ be an extended cut-off. Then, for all $m, k \in \mathbb{N}_0^3$ we have*

$$\|\partial_x^k \partial_y^m \gamma(\cdot, \cdot; \Phi)\|_{L^2(\mathcal{D}_\varepsilon)} \leq A^{|k|+|m|+2} (|k| + |m| + 1)^{|k|+|m|}.$$

The constant A depends on $\varepsilon > 0$, but does not depend on Φ .

The proof of Theorem 5.1 is conducted by induction, and hence, we have to involve a more general object than (5.1). Precisely, for cluster sets $\mathbf{P} = \{\mathbf{P}_1, \mathbf{P}_2, \dots, \mathbf{P}_M\}$, $\mathbf{S} = \{\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_K\}$, and multi-indices $\mathbf{k} \in \mathbb{N}_0^{3M}$, $\mathbf{m} \in \mathbb{N}_0^{3K}$, introduce the function

$$\gamma_{\mathbf{k}, \mathbf{m}}(x, y; \mathbf{P}, \mathbf{S}; \Phi) = \int_{\mathbb{R}^{3(N-1)}} D_{\mathbf{P}}^{\mathbf{k}} \psi(x, \hat{\mathbf{x}}) \overline{D_{\mathbf{S}}^{\mathbf{m}} \psi(y, \hat{\mathbf{x}})} \Phi(x, y, \hat{\mathbf{x}}) d\hat{\mathbf{x}}. \quad (5.2)$$

If $\mathbf{m} = \mathbf{0}$ (and/or $\mathbf{k} = \mathbf{0}$), then this integral is independent of \mathbf{P} (and/or \mathbf{S}), and in this case we set $\mathbf{P} = \emptyset$ (and/or $\mathbf{S} = \emptyset$). Thus, $\gamma_{\mathbf{0}, \mathbf{0}}(x, y; \emptyset, \emptyset; \Phi)$ coincides with the function in (5.1). Note the symmetry of $\gamma_{\mathbf{k}, \mathbf{m}}$:

$$\gamma_{\mathbf{k}, \mathbf{m}}(x, y; \mathbf{P}, \mathbf{S}; \Phi) = \overline{\gamma_{\mathbf{m}, \mathbf{k}}(y, x; \mathbf{S}, \mathbf{P}; \tilde{\Phi})}, \quad \tilde{\Phi}(y, x; \hat{\mathbf{x}}) = \Phi(x, y; \hat{\mathbf{x}}). \quad (5.3)$$

We estimate the function $\gamma_{\mathbf{k},\mathbf{m}}$ and its derivatives on the set $\mathcal{D}_\varepsilon, \varepsilon > 0$, defined in (2.10) with the help of Corollary 3.7 by reducing the estimates to the integrals $\|\mathbf{D}_{\mathbf{P}}^{\mathbf{k}}\psi\|_{L^2(U_{\mathbf{P}}(\varepsilon))}$ and $\|\mathbf{D}_{\mathbf{S}}^{\mathbf{m}}\psi\|_{L^2(U_{\mathbf{S}}(\varepsilon))}$. To this end we assume that the admissible cut-offs ϕ and μ associated with Φ satisfy the following support conditions:

$$\text{supp}_0 \phi \subset X_{\mathbf{P}}(\varepsilon(4N)^{-1}), \quad \text{supp}_0 \mu \subset X_{\mathbf{S}}(\varepsilon(4N)^{-1}), \quad (5.4)$$

and

$$\text{supp}_0 \phi(x, \cdot) \cap \text{supp}_0 \mu(y, \cdot) \subset \widehat{T}_{\mathbf{P}^*}(\varepsilon/2) \cap \widehat{T}_{\mathbf{S}^*}(\varepsilon/2), \quad \text{for all } (x, y) \in \mathcal{D}_\varepsilon. \quad (5.5)$$

Note that conditions (5.4) and (5.5) are automatically satisfied for $\mathbf{P} = \{\mathbf{P}\}$, $\mathbf{S} = \{\mathbf{S}\}$, where as usual $\mathbf{P} = \mathbf{Q}(\phi)$, $\mathbf{S} = \mathbf{Q}(\mu)$. Indeed, (5.4) follows from (4.6), and (5.5) follows from (4.21).

Recall that the sets X, T, \widehat{T} with various subscripts are defined in (2.14), (2.15), (2.16), (2.17). For brevity, throughout the proofs below for an arbitrary cluster set \mathbf{Q} we use the notation $T_{\mathbf{Q}} = T_{\mathbf{Q}}(\varepsilon/2)$, $\widehat{T}_{\mathbf{Q}} = \widehat{T}_{\mathbf{Q}}(\varepsilon/2)$ and $X_{\mathbf{Q}} = X_{\mathbf{Q}}(\varepsilon(4N)^{-1})$.

Lemma 5.2. *Suppose that Φ is of the form (4.14) and that (5.4) and (5.5) hold. Then, there exists a constant A_3 , independent of the cluster sets \mathbf{P}, \mathbf{S} , and of the cut-off Φ , such that*

$$\|\gamma_{\mathbf{k},\mathbf{m}}(\cdot, \cdot, \cdot; \mathbf{P}, \mathbf{S}; \Phi)\|_{L^2(\mathcal{D}_\varepsilon)} \leq A_3^{|\mathbf{k}|+|\mathbf{m}|+2} (|\mathbf{k}| + |\mathbf{m}| + 1)^{|\mathbf{k}|+|\mathbf{m}|},$$

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

Proof. Let

$$C_a = \max \left\{ 1, \max_{l: |l|=1} \|\partial^l \theta\|^{N^2} \right\},$$

so that $|\omega|, |\tau|, |\varkappa|, |\phi|, |\mu| \leq C_a$. Therefore,

$$\begin{aligned} |\Phi(x, y, \hat{\mathbf{x}})| &= |\omega(x, \hat{\mathbf{x}})| |\tau(y, \hat{\mathbf{x}})| |\varkappa(\hat{\mathbf{x}})| \\ &= |\omega(x, \hat{\mathbf{x}})|^{\frac{1}{2}} |\tau(y, \hat{\mathbf{x}})|^{\frac{1}{2}} |\omega(x, \hat{\mathbf{x}}) \varkappa(\hat{\mathbf{x}})|^{\frac{1}{2}} |\tau(y, \hat{\mathbf{x}}) \varkappa(\hat{\mathbf{x}})|^{\frac{1}{2}} \\ &\leq C_a |\phi(x, \hat{\mathbf{x}})|^{\frac{1}{2}} |\mu(y, \hat{\mathbf{x}})|^{\frac{1}{2}}. \end{aligned}$$

Now, using (5.5), we can estimate:

$$\begin{aligned} &\|\gamma_{\mathbf{k},\mathbf{m}}(\cdot, \cdot, \cdot; \mathbf{P}, \mathbf{S}; \Phi)\|_{L^2(\mathcal{D})}^2 \\ &\leq C_a^2 \int \int_{|x|>\varepsilon, |y|>\varepsilon} \left[\int_{\widehat{T}_{\mathbf{P}^*} \cap \widehat{T}_{\mathbf{S}^*}} |\mathbf{D}_{\mathbf{P}}^{\mathbf{k}}\psi(x, \hat{\mathbf{x}})| |\mathbf{D}_{\mathbf{S}}^{\mathbf{m}}\psi(y, \hat{\mathbf{x}})| |\phi(x, \hat{\mathbf{x}})|^{\frac{1}{2}} |\mu(y, \hat{\mathbf{x}})|^{\frac{1}{2}} \right. \\ &\quad \left. \times d\hat{\mathbf{x}} \right]^2 dy dx. \end{aligned}$$

By Hölder's inequality and by (5.4), the right-hand side does not exceed

$$\begin{aligned} & C_a^2 \int_{|x|>\varepsilon} \int_{\hat{T}_{\mathbf{P}^*}} |\mathbf{D}_{\mathbf{P}}^{\mathbf{k}} \psi(x, \hat{\mathbf{x}})|^2 |\phi(x, \hat{\mathbf{x}})| d\hat{\mathbf{x}} dx \int_{|y|>\varepsilon} \int_{\hat{T}_{\mathbf{S}^*}} |\mathbf{D}_{\mathbf{S}}^{\mathbf{m}} \psi(y, \hat{\mathbf{x}})|^2 |\mu(y, \hat{\mathbf{x}})| d\hat{\mathbf{x}} dy \\ & \leq C_a^4 \iint_{X_{\mathbf{P}} \cap T_{\mathbf{P}}} |\mathbf{D}_{\mathbf{P}}^{\mathbf{k}} \psi(x, \hat{\mathbf{x}})|^2 d\hat{\mathbf{x}} dx \iint_{X_{\mathbf{S}} \cap T_{\mathbf{S}}} |\mathbf{D}_{\mathbf{S}}^{\mathbf{m}} \psi(y, \hat{\mathbf{x}})|^2 d\hat{\mathbf{x}} dy. \end{aligned}$$

Since $X_{\mathbf{P}} \cap T_{\mathbf{P}} \subset U_{\mathbf{P}}(\varepsilon(4N)^{-1})$ (see the definition (2.17)), and a similar inclusion holds for the cluster set \mathbf{S} , by Corollary 3.7, the right-hand side does not exceed

$$\begin{aligned} & C_a^4 A_2^{2(|\mathbf{k}|+|\mathbf{m}|+2)} (|\mathbf{k}|+1)^{2|\mathbf{k}|} (|\mathbf{m}|+1)^{2|\mathbf{m}|} \\ & \leq A_3^{2(|\mathbf{k}|+|\mathbf{m}|+2)} (|\mathbf{k}|+|\mathbf{m}|+1)^{2(|\mathbf{k}|+|\mathbf{m}|)}, \end{aligned}$$

with $A_3 = C_a^2 A_2$. This implies the required bound. \square

Let the functions $\phi_{s,r}^{(l)}$ and $\mu_{s,r}^{(l)}, \Phi_{s,r}^{(l)}$ be as defined in (4.10) and (4.22), respectively. As in the previous section, we use the notation $\mathbf{P} = \mathbf{Q}(\phi)$ and $\mathbf{S} = \mathbf{Q}(\mu)$. In the next lemma, we show how the derivatives of $\gamma_{\mathbf{k},\mathbf{m}}$ w.r.t. the variable x transform into directional derivatives under the integral (5.2).

Lemma 5.3. *Suppose that (5.4) and (5.5) hold. Assume that $\mathbf{P}^* \subset \mathbf{S}^c$. Then,*

$$\text{supp}_0 \phi \subset X_{\{\mathbf{P}, \mathbf{P}^*\}}, \quad \text{supp}_0 \mu \subset X_{\{\mathbf{P}^*, \mathbf{S}\}}. \quad (5.6)$$

Furthermore,

$$\text{supp}_0 \phi(x, \cdot) \cap \text{supp}_0 \mu(y, \cdot) \subset \hat{T}_{\{\mathbf{P}^*, \mathbf{P}^*\}} \cap \hat{T}_{\{\mathbf{P}^*, \mathbf{S}^*\}}, \quad \text{for all } (x, y) \in \mathcal{D}_\varepsilon. \quad (5.7)$$

Let $l \in \mathbb{N}_0^3$ be such that $|l| = 1$. If $\mathbf{P}^c = \emptyset$, then

$$\begin{aligned} \partial_x^l \gamma_{\mathbf{k},\mathbf{m}}(x, y; \mathbf{P}, \mathbf{S}; \Phi) &= \gamma_{(l,\mathbf{k}),\mathbf{m}}(x, y; \{\mathbf{P}, \mathbf{P}\}, \mathbf{S}; \Phi) \\ &+ \gamma_{\mathbf{k},(l,\mathbf{m})}(x, y; \mathbf{P}, \{\mathbf{P}^*, \mathbf{S}\}; \Phi), \end{aligned} \quad (5.8)$$

and both sides are square-integrable in $(x, y) \in \mathcal{D}_\varepsilon$.

If $\mathbf{P}^c \neq \emptyset$, then for all $s \in \mathbf{P}, r \in \mathbf{P}^c$ we have

$$\text{supp}_0 \phi_{s,r}^{(l)} \subset X_{\mathbf{P}}, \quad \text{supp}_0 \mu_{s,r}^{(l)} \subset X_{\mathbf{S}}, \quad (5.9)$$

and

$$\text{supp}_0 \phi_{s,r}^{(l)}(x, \cdot) \cap \text{supp}_0 \mu_{s,r}^{(l)}(y, \cdot) \subset \hat{T}_{\mathbf{P}^*} \cap \hat{T}_{\mathbf{S}^*}, \quad (5.10)$$

for every $(x, y) \in \mathcal{D}_\varepsilon$. Furthermore, the formula holds:

$$\begin{aligned} & \partial_x^l \gamma_{\mathbf{k},\mathbf{m}}(x, y; \mathbf{P}, \mathbf{S}; \Phi) \\ &= \gamma_{(l,\mathbf{k}),\mathbf{m}}(x, y; \{\mathbf{P}, \mathbf{P}\}, \mathbf{S}; \Phi) + \gamma_{\mathbf{k},(l,\mathbf{m})}(x, y; \mathbf{P}, \{\mathbf{P}^*, \mathbf{S}\}; \Phi) \\ &+ \sum_{s \in \mathbf{P}, r \in \mathbf{P}^c} \gamma_{\mathbf{k},\mathbf{m}}(x, y; \mathbf{P}, \mathbf{S}; \Phi_{s,r}^{(l)}), \end{aligned} \quad (5.11)$$

and both sides are square-integrable in $(x, y) \in \mathcal{D}_\varepsilon$.

Proof. According to (4.20) and the assumption (5.4), we have

$$\text{supp}_0 \phi \subset X_{\mathbf{P}} \cap X_{\mathbf{P}} = X_{\{\mathbf{P}, \mathbf{P}\}}, \quad \text{supp}_0 \mu \subset X_{\mathbf{P}^*} \cap X_{\mathbf{S}} = X_{\{\mathbf{P}^*, \mathbf{S}\}},$$

which coincides with (5.6). Moreover, by (4.21) and (5.5),

$$\text{supp}_0 \phi(x, \cdot) \cap \text{supp}_0 \mu(y, \cdot) \subset \widehat{T}_{\mathbf{P}^*} \cap \widehat{T}_{\mathbf{P}} \cap \widehat{T}_{\mathbf{S}^*},$$

which implies (5.7) for all $(x, y) \in \mathcal{D}_\varepsilon$. Thus, by Lemma 5.2 the terms on the right-hand side of (5.8) and two first terms on the right-hand side of (5.11) are square-integrable in $(x, y) \in \mathcal{D}_\varepsilon$.

Let $\mathbf{P}^c \neq \emptyset$. Then, the inclusions (5.9) and (5.10) are consequences of (4.23) and (5.4), (5.5). Again by Lemma 5.2, the third term on the right-hand side of (5.11) is square-integrable in $(x, y) \in \mathcal{D}_\varepsilon$, as claimed.

It remains to prove (5.8) and (5.11). We assume throughout that $(x, y) \in \mathcal{D}_\varepsilon$. Introduce the vector $\hat{\mathbf{z}} = (z_2, z_3, \dots, z_N)$ such that

$$z_j = \begin{cases} x, & j \in \mathbf{P}^*, \\ 0, & j \in \mathbf{P}^c, \end{cases}$$

and make the following change of variables under the integral (5.2): $\hat{\mathbf{x}} = \hat{\mathbf{w}} + \hat{\mathbf{z}}$, so

$$\gamma_{\mathbf{k}, \mathbf{m}}(x, y; \mathbf{P}, \mathbf{S}; \Phi) = \int_{\mathbb{R}^{3(N-1)}} D_{\mathbf{P}}^{\mathbf{k}} \psi(x, \hat{\mathbf{w}} + \hat{\mathbf{z}}) \overline{D_{\mathbf{S}}^{\mathbf{m}} \psi(y, \hat{\mathbf{w}} + \hat{\mathbf{z}})} \Phi(x, y, \hat{\mathbf{w}} + \hat{\mathbf{z}}) d\hat{\mathbf{w}}.$$

Before differentiating this integral w.r.t. x , we make the following useful observation. For each $l \in \mathbb{N}_0^3$ and for arbitrary functions $g = g(\mathbf{x})$ and $h = h(x, y, \hat{\mathbf{x}})$, due to the definition of $\hat{\mathbf{z}} = \hat{\mathbf{z}}(x)$, we have

$$\begin{aligned} \partial_x^l (g(x, \hat{\mathbf{w}} + \hat{\mathbf{z}})) &= (D_{\mathbf{P}}^l g)(x, \hat{\mathbf{w}} + \hat{\mathbf{z}}), & \partial_x^l (g(y, \hat{\mathbf{w}} + \hat{\mathbf{z}})) &= (D_{\mathbf{P}^*}^l g)(y, \hat{\mathbf{w}} + \hat{\mathbf{z}}) \\ \text{and} \quad \partial_x^l (h(x, y, \hat{\mathbf{w}} + \hat{\mathbf{z}})) &= (D_{\mathbf{P}}^l h)(x, y, \hat{\mathbf{w}} + \hat{\mathbf{z}}). \end{aligned}$$

Therefore, for $|l| = 1$ we have

$$\begin{aligned} \partial_x^l \gamma_{\mathbf{k}, \mathbf{m}}(x, y; \mathbf{P}, \mathbf{S}; \Phi) &= \int_{\mathbb{R}^{3(N-1)}} D_{\mathbf{P}}^l D_{\mathbf{P}}^{\mathbf{k}} \psi(x, \hat{\mathbf{w}} + \hat{\mathbf{z}}) \overline{D_{\mathbf{S}}^{\mathbf{m}} \psi(y, \hat{\mathbf{w}} + \hat{\mathbf{z}})} \Phi(x, y, \hat{\mathbf{w}} + \hat{\mathbf{z}}) d\hat{\mathbf{w}} \\ &+ \int_{\mathbb{R}^{3(N-1)}} D_{\mathbf{P}}^{\mathbf{k}} \psi(x, \hat{\mathbf{w}} + \hat{\mathbf{z}}) \overline{D_{\mathbf{P}^*}^l D_{\mathbf{S}}^{\mathbf{m}} \psi(y, \hat{\mathbf{w}} + \hat{\mathbf{z}})} \Phi(x, y, \hat{\mathbf{w}} + \hat{\mathbf{z}}) d\hat{\mathbf{w}} \\ &+ \int_{\mathbb{R}^{3(N-1)}} D_{\mathbf{P}}^{\mathbf{k}} \psi(x, \hat{\mathbf{w}} + \hat{\mathbf{z}}) \overline{D_{\mathbf{S}}^{\mathbf{m}} \psi(y, \hat{\mathbf{w}} + \hat{\mathbf{z}})} D_{\mathbf{P}}^l \Phi(x, y, \hat{\mathbf{w}} + \hat{\mathbf{z}}) d\hat{\mathbf{w}}. \end{aligned}$$

Changing the variables back to $\hat{\mathbf{x}}$, we rewrite the right-hand side as:

$$\begin{aligned} &\int_{\mathbb{R}^{3(N-1)}} D_{\mathbf{P}}^l D_{\mathbf{P}}^{\mathbf{k}} \psi(x, \hat{\mathbf{x}}) \overline{D_{\mathbf{S}}^{\mathbf{m}} \psi(y, \hat{\mathbf{x}})} \Phi(x, y, \hat{\mathbf{x}}) d\hat{\mathbf{x}} \\ &+ \int_{\mathbb{R}^{3(N-1)}} D_{\mathbf{P}}^{\mathbf{k}} \psi(x, \hat{\mathbf{x}}) \overline{D_{\mathbf{P}^*}^l D_{\mathbf{S}}^{\mathbf{m}} \psi(y, \hat{\mathbf{x}})} \Phi(x, y, \hat{\mathbf{x}}) d\hat{\mathbf{x}} \\ &+ \int_{\mathbb{R}^{3(N-1)}} D_{\mathbf{P}}^{\mathbf{k}} \psi(x, \hat{\mathbf{x}}) \overline{D_{\mathbf{S}}^{\mathbf{m}} \psi(y, \hat{\mathbf{x}})} D_{\mathbf{P}}^l \Phi(x, y, \hat{\mathbf{x}}) d\hat{\mathbf{x}}. \end{aligned} \tag{5.12}$$

In the case $P^c = \emptyset$, we have $D_P^l \Phi(x, y, \hat{x}) = 0$ by Lemma 4.9, so the sum coincides with the right-hand side of (5.8).

If $P^c \neq \emptyset$, then by (4.24) the sum (5.12) coincides with the right-hand side of (5.11) again. This completes the proof. \square

Proposition 5.4. *Let Φ be an extended cut-off, and let \mathbf{P}, \mathbf{S} be a pair of cluster sets such that (5.4) and (5.5) hold. Then, for all $m, k \in \mathbb{N}_0^3$ we have*

$$\begin{aligned} & \|\partial_x^k \partial_y^m \gamma_{\mathbf{k}, \mathbf{m}}(\cdot, \cdot; \mathbf{P}, \mathbf{S}; \Phi)\|_{L^2(\mathcal{D}_\varepsilon)} \\ & \leq A^{|k|+|m|} A_3^{|\mathbf{k}|+|\mathbf{m}|+2} (|\mathbf{k}| + |\mathbf{m}| + |k| + |m| + 1)^{|\mathbf{k}|+|\mathbf{m}|+|k|+|m|}, \end{aligned} \quad (5.13)$$

where the constant A_3 is as in Lemma 5.2 and $A = 2A_3 + N^2$.

The proof of this proposition is by induction. Lemma 5.2 provides the base step. Now we need to establish the induction step:

Lemma 5.5. *Suppose that for every extended cut-off Φ and every pair $\mathbf{P} = \{P_1, P_2, \dots, P_M\}$ and $\mathbf{S} = \{S_1, S_2, \dots, S_K\}$ of cluster sets such that Φ satisfies (5.4) and (5.5), the bound (5.13) holds for all multi-indices $\mathbf{k} \in \mathbb{N}_0^{3M}$, $\mathbf{m} \in \mathbb{N}_0^{3K}$, and all $k, m \in \mathbb{N}_0^3$, such that $|k| \leq p$, $|m| \leq n$ with some $p, n \in \mathbb{N}_0$. Then, for such extended cut-offs Φ and cluster sets \mathbf{P}, \mathbf{S} the bound (5.13) holds for all k, m , such that $|k| \leq p+1$, $|m| \leq n$.*

Proof. Let $|m| \leq n$, $k = k_0 + l$ with $l \in \mathbb{N}_0^3$, $|l| = 1$, and arbitrary $k_0 \in \mathbb{N}_0^3$, such that $|k_0| = p$. In view of Lemma 4.6, we may assume that $P^* \subset S^c$, since otherwise the integrand in (5.2) equals zero. Thus, we can apply Lemma 5.3. Assume first that $P^c \neq \emptyset$. It follows from (5.11) that

$$\begin{aligned} & \partial_x^{k_0+l} \partial_y^m \gamma_{\mathbf{k}, \mathbf{m}}(x, y; \mathbf{P}, \mathbf{S}; \Phi) \\ & = \partial_x^{k_0} \partial_y^m \gamma_{(l, \mathbf{k}), \mathbf{m}}(x, y; \{\mathbf{P}, \mathbf{P}\}, \mathbf{S}; \Phi) + \partial_x^{k_0} \partial_y^m \gamma_{\mathbf{k}, (l, \mathbf{m})}(x, y; \mathbf{P}, \{\mathbf{P}^*, \mathbf{S}\}; \Phi) \\ & \quad + \sum_{s \in \mathbf{P}, r \in \mathbf{P}^c} \partial_x^{k_0} \partial_y^m \gamma_{\mathbf{k}, \mathbf{m}}(x, y; \mathbf{P}, \mathbf{S}; \Phi_{s,r}^{(l)}). \end{aligned} \quad (5.14)$$

According to (5.6), (5.7), the function Φ satisfies the conditions (5.4) and (5.5) for the pair of cluster sets $\{\mathbf{P}, \mathbf{P}\}, \mathbf{S}$ and also for the pair $\mathbf{P}, \{\mathbf{P}^*, \mathbf{S}\}$. Similarly, due to (5.9) and (5.10), the extended cut-off function $\Phi_{s,r}^{(l)}$ satisfies (5.4), (5.5) for the pair of cluster sets \mathbf{P}, \mathbf{S} . Since $|m| \leq n$ and $|k_0| = p$, by the assumptions of the lemma, each term on the right-hand side of (5.14) satisfies the bound of the form (5.13). With the notation $q = |m|$, this gives the following estimate:

$$\begin{aligned} & \|\partial_x^{k_0+l} \partial_y^m \gamma_{\mathbf{k}, \mathbf{m}}(\cdot, \cdot; \mathbf{P}, \mathbf{S}; \Phi)\|_{L^2(\mathcal{D}_\varepsilon)} \\ & \leq 2A^{p+q} A_3^{|\mathbf{k}|+|\mathbf{m}|+3} (|\mathbf{k}| + |\mathbf{m}| + p + q + 2)^{|\mathbf{k}|+|\mathbf{m}|+p+q+1} \\ & \quad + N^2 A^{p+q} A_3^{|\mathbf{k}|+|\mathbf{m}|+2} (|\mathbf{k}| + |\mathbf{m}| + p + q + 1)^{|\mathbf{k}|+|\mathbf{m}|+p+q} \\ & \leq A^{p+q} A_3^{|\mathbf{k}|+|\mathbf{m}|+2} (2A_3 + N^2) (|\mathbf{k}| + |\mathbf{m}| + p + q + 2)^{|\mathbf{k}|+|\mathbf{m}|+p+q+1}. \end{aligned}$$

Setting $A = 2A_3 + N^2$, we get (5.13) with $k = k_0 + l$, as required.

If $P^c = \emptyset$, then the only difference in the proof is that instead of (5.11) we use (5.8). \square

Proof of Proposition 5.4. Step 1. Proof of (5.13) for all k and $m = 0$. According to Lemma 5.2, the required bound holds for $k = m = 0$. Thus, using Lemma 5.5, by induction we conclude that (5.13) holds for all $k \in \mathbb{N}_0^3$ and $m = 0$, as claimed.

Step 2. Proof of (5.13) for $k = 0$ and all m . Using the symmetry property (5.3) and Step 1, we conclude that (5.13) holds for all $m \in \mathbb{N}_0^3$ and $k = 0$.

Step 3. Using Step 2 and Lemma 5.5, by induction we conclude that (5.13) holds for all $k, m \in \mathbb{N}_0^3$, as required. \square

Proof of Theorem 5.1. Recall that in the case $\mathbf{m} = \mathbf{0}, \mathbf{k} = \mathbf{0}$ we take $\mathbf{P} = \mathbf{S} = \emptyset$, so that the conditions (5.4) and (5.5) are automatically satisfied. Thus, the required bound follows directly from (5.13). \square

6. Proof of Theorem 2.3

First, we build a suitable partition of unity, using the functions ζ and θ , defined in (2.19). Recall the notation $\mathbf{R} = \{1, 2, \dots, N\}$.

Let $\Xi = \{(j, k) \in \mathbf{R} \times \mathbf{R} : j < k\}$. For each subset $\Upsilon \subset \Xi$ introduce the admissible cut-off

$$\phi_{\Upsilon}(\mathbf{x}) = \prod_{(j,k) \in \Upsilon} \zeta(x_j - x_k) \prod_{(j,k) \in \Upsilon^c} \theta(x_j - x_k).$$

It is clear that

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

For every cluster $\mathbf{S} \subset \mathbf{R}^*$ define

$$\tau_{\mathbf{S}}(x_1, \hat{\mathbf{x}}) = \prod_{j \in \mathbf{S}} \zeta(x_1 - x_j) \prod_{j \in (\mathbf{S}^c)^*} \theta(x_1 - x_j).$$

It is clear that

$$\sum_{\mathbf{S} \subset \mathbf{R}^*} \tau_{\mathbf{S}}(x_1, \hat{\mathbf{x}}) = \prod_{j \in \mathbf{R}^*} (\zeta(x_1 - x_j) + \theta(x_1 - x_j)) = 1.$$

Define

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

so that

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

Note that each function $\Phi_{\Upsilon, \mathbf{S}}$ is an extended cut-off function, as defined in Subsect. 4.2. Using the definition (5.1), the function (1.6) can be represented as:

$$\gamma(x, y) = \sum_{\Upsilon \subset \Xi, \mathbf{S} \subset \mathbf{R}^*} \gamma(x, y; \Phi_{\Upsilon, \mathbf{S}}).$$

Since each function $\Phi_{\Upsilon, S}$ is an extended cut-off, we can use Theorem 5.1 for each term, which leads to (2.11), as required.

As explained in Sect. 2, Theorem 2.3 implies Theorem 2.2, and hence Theorem 1.1.

7. Appendix: Elementary Combinatorial Formulas

Here, we collect some elementary formulas.

7.1. Stirling's Formula

It follows from Stirling's formula

$$\lim_{p \rightarrow \infty} \frac{p! e^p}{p^{p + \frac{1}{2}}} = \sqrt{2\pi}$$

that

$$C^{-1}(p+1)^{p+\frac{1}{2}}e^{-p} \leq p! \leq C(p+1)^{p+\frac{1}{2}}e^{-p}, \quad (7.1)$$

for all $p = 0, 1, 2, \dots$. Therefore,

$$(p+1)^p \leq C e^p p!, \quad \forall p \in \mathbb{N}_0. \quad (7.2)$$

The bounds (7.1) also imply for any $p = 0, 1, \dots$ and $q = 0, 1, \dots, p$, that

$$\binom{p}{q} = \frac{p!}{q!(p-q)!} \leq L_3 \frac{(p+1)^p}{(q+1)^q(p-q+1)^{p-q}}, \quad (7.3)$$

with some constant $L_3 > 0$, independent of p and q .

7.2. Multiindices and Factorials

For $k = (k_1, k_2, \dots, k_d) \in \mathbb{N}_0^d$, we use the standard notation

$$k! = k_1! k_2! \cdots k_d!, \quad |k| = |k_1| + |k_2| + \cdots + |k_d|.$$

We say that $k \leq s$ for $k, s \in \mathbb{N}_0^d$ if $k_j \leq s_j$, $j = 1, 2, \dots, d$. In this case we define

$$\binom{k}{s} = \frac{k!}{s!(k-s)!}.$$

Note the useful identity

$$\sum_{\substack{l \leq k \\ |l|=p}} \binom{k}{l} = \binom{|k|}{p}, \quad \forall p \leq |k|. \quad (7.4)$$

It follows by comparing the coefficients of the term t^p in the expansions of both sides of the equality

$$(1+t)^{k_1} (1+t)^{k_2} \cdots (1+t)^{k_d} = (1+t)^{|k|}, \quad t \in \mathbb{R}.$$

This simple argument is found in [15, Proposition 2.1].

And to conclude, the multinomial formula (see, e.g., [1, §24.1.2])

$$d^p = \left(\sum_{l=1}^d 1 \right)^p = \sum_{\substack{k \in \mathbb{N}_0^d \\ |k|=p}} \frac{|k|!}{k!}$$

implies that

$$|k|! \leq d^{|k|} k!, \quad \forall k \in \mathbb{N}_0^d. \quad (7.5)$$

Acknowledgements

The authors are grateful to S. Fournais, T. Hoffman-Ostenhof, M. Lewin and T. Ø. Sørensen for stimulating discussions and advice. Thanks also go to the anonymous referees for their constructive comments and for pointing out papers [3, 4] and the book [6]. The second author was supported by the EPSRC grant EP/P024793/1.

Open Access. This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

References

- [1] Abramowitz, M., Stegun, I.A.: Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables. National Bureau of Standards Applied Mathematics Series, vol. 55. U.S. Government Printing Office, Washington, DC, For sale by the Superintendent of Documents (1964)
- [2] Cioslowski, J.: Off-diagonal derivative discontinuities in the reduced density matrices of electronic systems. *J. Chem. Phys.* **153**(15), 154108 (2020)
- [3] Cioslowski, J.: Reverse engineering in quantum chemistry: how to reveal the fifth-order off-diagonal cusp in the one-electron reduced density matrix without actually calculating it. *Int. J. Quantum Chem.* e26651 (2021)
- [4] Cioslowski, J., Strasburger, K.: Angular-Momentum Extrapolations to the Complete Basis Set Limit: Why and When They Work. *J. Chem. Theory Comput.* **17**(6), 3403–3413 (2021)
- [5] Coleman, A., Yukalov, V.: Reduced Density Matrices. Lecture Notes in Chemistry, vol. 72. Springer, Berlin (2000)

- [6] Davidson, E.: Reduced Density Matrices in Quantum Chemistry. Academic Press (1976)
- [7] Evans, L.C.: Partial Differential Equations, Graduate Studies in Mathematics, vol. 19. American Mathematical Society, Providence (1998)
- [8] Fournais, S., Sørensen, T.Ø.: Pointwise estimates on derivatives of Coulombic wave functions and their electron densities. [arXiv:1803.03495](https://arxiv.org/abs/1803.03495) [math.AP] (2018)
- [9] Fournais, S., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., Sørensen, T.Ø.: The electron density is smooth away from the nuclei. *Comm. Math. Phys.* **228**(3), 401–415 (2002)
- [10] Fournais, S., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., Sørensen, T.Ø.: Analyticity of the density of electronic wavefunctions. *Ark. Mat.* **42**(1), 87–106 (2004)
- [11] Fournais, S., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., Sørensen, T.Ø.: Sharp regularity results for Coulombic many-electron wave functions. *Comm. Math. Phys.* **255**(1), 183–227 (2005)
- [12] Fournais, S., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., Sørensen, T.Ø.: Analytic structure of many-body Coulombic wave functions. *Comm. Math. Phys.* **289**(1), 291–310 (2009)
- [13] Hörmander, L.: Linear partial differential operators. Springer Verlag, Berlin-New York (1976)
- [14] Jecko, T.: A new proof of the analyticity of the electronic density of molecules. *Lett. Math. Phys.* **93**(1), 73–83 (2010)
- [15] Kato, K.: New idea for proof of analyticity of solutions to analytic nonlinear elliptic equations. *SUT J. Math.* **32**(2), 157–161 (1996)
- [16] Kato, T.: On the eigenfunctions of many-particle systems in quantum mechanics. *Comm. Pure Appl. Math.* **10**, 151–177 (1957)
- [17] Krantz, S.G., Parks, H.R.: A Primer of Real Analytic Functions. Birkhäuser Advanced Texts: Basler Lehrbücher. [Birkhäuser Advanced Texts: Basel Textbooks], second edn. Birkhäuser, Boston (2002)
- [18] Lieb, E.H., Seiringer, R.: The stability of matter in quantum mechanics. Cambridge University Press, Cambridge (2010)
- [19] Lewin, M., Lieb, E.H., Seiringer, R.: Universal Functionals in Density Functional Theory (2019)
- [20] Reed, M., Simon, B.: Methods of Modern Mathematical Physics. II. Fourier Analysis, Self-Adjointness. Academic Press [Harcourt Brace Jovanovich, Publishers], New York (1975)
- [21] Sobolev, A.V.: Eigenvalue asymptotics for the one-particle density matrix. [arXiv:2103.11896](https://arxiv.org/abs/2103.11896)

Peter Hearnshaw and Alexander V. Sobolev

Department of Mathematics

University College London

Gower Street

London WC1E 6BT

UK

e-mail: peter.hearnshaw.18@ucl.ac.uk;

a.sobolev@ucl.ac.uk

Communicated by Jan Dereziński.

Received: May 11, 2021.

Accepted: September 30, 2021.