Commun. Math. Phys. 255, 183–227 (2005)
Digital Object Identifier (DOI) 10.1007/s00220-004-1257-6

Communications in **Mathematical Physics**

# Sharp Regularity Results for Coulombic Many-Electron Wave Functions*

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Received: 8 March 2004 / Accepted: 1 June 2004
Published online: 11 January 2005 – © The authors 2004

**Abstract:** We show that electronic wave functions $\psi$ of atoms and molecules have a representation $\psi = \mathcal{F}\phi$, where $\mathcal{F}$ is an explicit universal factor, locally Lipschitz, and independent of the eigenvalue and the solution $\psi$ itself, and $\phi$ has second derivatives which are locally in $L^\infty$. This representation turns out to be optimal as can already be demonstrated with the help of hydrogenic wave functions. The proofs of these results are, in an essential way, based on a new elliptic regularity result which is of independent interest. Some identities that can be interpreted as cusp conditions for second order derivatives of $\psi$ are derived.

## 1. Introduction

*1.1. Motivation and results.* The non-relativistic quantum mechanical Hamiltonian of an $N$-electron molecule with L fixed nuclei is given by

$$H_{N,L}(\mathbf{X}, \mathbf{Z}) = -\Delta + V(\mathbf{X}, \mathbf{Z}) + U(\mathbf{X}, \mathbf{Z}),$$

where $V$, the Coulombic potential, is given by

$$V \equiv V(\mathbf{X}, \mathbf{Z}) = -\sum_{j=1}^{N}\sum_{k=1}^{L} \frac{Z_k}{|X_k - x_j|} + \sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|}, \tag{1.1}$$

and the internuclear repulsion $U$ by

$$U(\mathbf{X}, \mathbf{Z}) = \sum_{1\le k<\ell\le L} \frac{Z_k Z_\ell}{|X_k - X_\ell|}.$$


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The latter is merely an additive term that will be neglected in the sequel and we will henceforth consider

$$H \equiv H_{N,L}(\mathbf{X}, \mathbf{Z}) - U(\mathbf{X}, \mathbf{Z}). \tag{1.2}$$

Above, $\mathbf{x} = (x_1, x_2, \ldots, x_N) \in \mathbb{R}^{3N}$ denotes the positions of the $N$ electrons, with $x_j = (x_{j,1}, x_{j,2}, x_{j,3}) \in \mathbb{R}^3$ the position of the $j^{th}$ electron. The positions of the $L$ nuclei with the positive charges $\mathbf{Z} = (Z_1, Z_2 \ldots, Z_L) \in \mathbb{R}_+^L$ are denoted by $\mathbf{X} = (X_1, X_2, \ldots, X_L) \in \mathbb{R}^{3L}$, where $X_k = (X_{k,1}, X_{k,2}, X_{k,3}) \in \mathbb{R}^3$ is the (fixed) position of the $k^{th}$ nucleus with charge $Z_k$, and it is assumed that $X_\ell \neq X_k$ for $\ell \neq k$. The Laplacian corresponding to the $j^{th}$ electron is $\Delta_j = \sum_{i=1}^3 \frac{\partial^2}{\partial x_{j,i}{}^2}$ and so the Laplacian on $\mathbb{R}^{3N}$ is given by $\Delta = \sum_{j=1}^N \Delta_j$. We also introduce the $3N$-dimensional gradient by $\nabla = (\nabla_1, \ldots, \nabla_N)$.

The operator $H$ is selfadjoint on $L^2(\mathbb{R}^{3N})$ with operator domain $\mathcal{D}(H) = W^{2,2}(\mathbb{R}^{3N})$ [14], and it depends parametrically on $\mathbf{X}$ and $\mathbf{Z}$. In the case of an $N$-electron atom with (one) nucleus of charge $Z$ fixed at the origin $0 \in \mathbb{R}^3$, (1.2) becomes

$$\begin{aligned} H \equiv H_N(Z) &= -\Delta + V \\ &= \sum_{j=1}^N \Big( -\Delta_j - \frac{Z}{|x_j|} \Big) + \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|}. \end{aligned} \tag{1.3}$$

Generations of chemists and physicists have devoted a good part of their research to the analysis of various problems related to $H_{N,L}(\mathbf{X}, \mathbf{Z})$. Most of the present day understanding of atoms and molecules is based on the analysis of problems directly related to this operator; see any textbook in atomic and molecular quantum mechanics.

One of the central problems is the eigenvalue problem

$$H\psi = E\psi, \; E \in \mathbb{R}, \; \psi \in L^2(\mathbb{R}^{3N}). \tag{1.4}$$

Since the electrons are Fermions the $N$-electron wave function $\psi$ has to satisfy the Pauli Principle. This can be achieved in a spinless formulation by requiring that $\psi$ transforms according to certain irreducible representations of the symmetric group $\mathfrak{S}^N$. Our present work will not require any symmetry assumptions on $\psi$. More precisely, we will consider local properties of distributional solutions (locally $L^1$) in a domain $\Omega \subseteq \mathbb{R}^{3N}$ to $H\psi = E\psi$, where $E$ can be any real number.

Within mathematics and mathematical physics Schrödinger operators as (1.2) are studied mostly from an operator theoretical point of view, see the textbooks [1, 14, 18, 22] as well as the recent survey [21].

The PDE-aspects of (1.4) have been studied in relatively few works. We first note the following: Let $\Sigma(\mathbf{X})$ denote the set of points in $\mathbb{R}^{3N}$ where the potential $V$ defined in (1.1) is singular. The function $V$ is real analytic in $\mathbb{R}^{3N} \setminus \Sigma(\mathbf{X})$ and hence by classical results (see [11, Sect. 7.5, pp. 177-180]), so is $\psi$.

Therefore a basic question is how to characterize the effect of the singularities of $V$ on the local behaviour of a solution $\psi$ of (1.4).

In 1957 Kato [13] showed that a solution $\psi$ satisfying (1.4) is continuous in all of $\mathbb{R}^{3N}$ with first derivatives locally in $L^\infty$, i.e., $\psi$ is locally Lipschitz. He also analyzed how $\psi$ behaves near the so-called two-particle coalescence points, i.e., those points in $\Sigma(\mathbf{X})$ where exactly one term in the sums representing $V$ (see (1.1)) is unbounded.

Generalizations with new insights for those points in $\mathbb{R}^{3N}$ where more than one term in (1.1) is singular were obtained in [10] and more recently in [9]. We mention that the present authors in [5, 6 and 4] studied the smoothness of the electron density, a question related to the present investigation; we shall not discuss this further here.

Suppose we have a solution $\psi$ to $H\psi = E\psi$, $E \in \mathbb{R}$, with $H$ as in (1.2) or (1.3). We want to find a representation for $\psi$

$$\psi(x_1, \dots, x_n) = \mathcal{F}(x_1, \dots, x_n)\,\phi(x_1, \dots, x_n)$$

such that $\phi$ is as smooth as possible and $\mathcal{F}$ is a universal (i.e., not depending on $\psi$ or $E$) positive factor reflecting the behaviour of the potential $V$ near $\Sigma(\mathbf{X})$. This means that for any two solutions $\psi_1$, $\psi_2$ of a fixed Schrödinger operator (1.2) (or (1.3)) the function $\mathcal{F}$ will be the same, i.e.,

$$\psi_1 = \mathcal{F}\phi_1, \quad \psi_2 = \mathcal{F}\phi_2.$$

Since it is already known from one-electron atoms that $\psi$ is just locally Lipschitz, $\mathcal{F}$ cannot be smoother than that. We shall see that by choosing $\mathcal{F}$ in a special way one can say a lot more. Let us first recall some of the ideas developed in [9].

Suppose $\psi$ is a solution to $(-\Delta + V)\psi = E\psi$ in $\Omega \subseteq \mathbb{R}^{3N}$. Set $\psi = e^F\phi$, then $\phi$ satisfies

$$\Delta\phi + 2\nabla F \cdot \nabla\phi + \big(\Delta F + |\nabla F|^2 + (E - V)\big)\phi = 0. \tag{1.5}$$

Now assume $H = -\Delta + V$ is given by (1.2). The specific nature of the Coulomb potential makes it possible to find an explicit $F$ such that $\Delta F = V$, namely

$$F(\mathbf{x}) \equiv F_2(\mathbf{x}) := -\frac{1}{2}\sum_{j=1}^{N}\sum_{\ell=1}^{L} Z_\ell |X_\ell - x_j| + \frac{1}{4}\sum_{1 \le i < j \le N} |x_i - x_j|.$$

We have given $F$ an index 2 to indicate that $F_2$ is a sum of functions each only depending on the coordinates of two particles. If we insert $F_2$ into (1.5) we obtain

$$\Delta\phi_2 + 2\nabla F_2 \cdot \nabla F_2 \cdot \nabla\phi_2 + \big(|\nabla F_2|^2 + E\big)\phi_2 = 0,$$

where we have also given $\phi$ an index 2 to show that it is associated with $F_2$. The regularity properties of $\phi_2$ are now determined by the regularity of $\nabla F_2$, respectively, $|\nabla F_2|^2$. Since $\nabla F_2$ is locally in $L^\infty$, standard elliptic regularity theory (see Sect. 2) gives us that

$$\phi_2 \in C^{1,\alpha}(\Omega) \quad \text{for} \quad \alpha \in (0, 1). \tag{1.6}$$

(For the definition of the Hölder-spaces $C^{k,\alpha}$, see Definition 2.1). Since $\nabla F_2$ is not continuous, one cannot in general expect anything better than (1.6). Note that since $\psi = e^{F_2}\phi_2$ we have

$$\nabla\psi - (\nabla F_2)\psi \in C^{\alpha}(\Omega) \quad \text{for} \quad \alpha \in (0, 1). \tag{1.7}$$

This is a general formulation of Kato's cusp condition [13] which plays an important role in the numerical treatment of (1.4). (Here, and in the sequel, by a 'cusp condition' we understand that condition that solution $\psi$ has to satisfy at a point in the singular set $\Sigma(\mathbf{X})$).

We are now ready to state our main result about the regularity of $\psi$.

**Theorem 1.1.** *Suppose $\psi$ is a solution to $H\psi = E\psi$ in $\Omega \subseteq \mathbb{R}^{3N}$, where $H$ is given by (1.2). Define $y_{i,\ell} = x_i - X_\ell$, $i \in \{1, \ldots, N\}$, $\ell \in \{1, \ldots, L\}$. Let*

$$\mathcal{F} = e^{F_2+F_3} \tag{1.8}$$

*with*

$$F_2(\mathbf{x}) = -\frac{1}{2}\sum_{\ell=1}^{L}\sum_{i=1}^{N} Z_\ell |y_{i,\ell}| + \frac{1}{4}\sum_{1\le i<j\le N} |x_i - x_j|, \tag{1.9}$$

$$F_3(\mathbf{x}) = C_0 \sum_{\ell=1}^{L}\sum_{1\le i<j\le N} Z_\ell\,(y_{i,\ell}\cdot y_{j,\ell})\,\ln\big(|y_{i,\ell}|^2 + |y_{j,\ell}|^2\big), \tag{1.10}$$

*where $C_0 = \frac{2-\pi}{12\pi}$.*

*Then*

$$\psi = \mathcal{F}\phi_3 \tag{1.11}$$

*with*

$$\phi_3 \in C^{1,1}(\Omega). \tag{1.12}$$

*Furthermore this representation is optimal in the following sense: There is no other function $\widetilde{\mathcal{F}}$ depending only on* $\mathbf{X}$, $\mathbf{Z}$ *and on $N$, but not on $\psi$ or $E$ itself, such that $\psi = \widetilde{\mathcal{F}}\phi$ with $\phi$ having more regularity than $C^{1,1}$.*

*Remark 1.2.*

(i) Of course one can consider more general Hamiltonians, for instance molecular Hamiltonians where the nuclei are allowed to move. Kato [13] considered this case. Our results, suitably modified, extend to this situation. We concentrate on the model with fixed nuclei since this is the 'standard model' in molecular physics.

(ii) For the proof of Theorem 1.1 a special regularity result (see Theorem 2.6) for solutions of the Poisson equation $\Delta u = g$ will be vital. Roughly speaking, if $g \in L^\infty$ has a certain multiplicative structure, we can show that $u \in C^{1,1}$, and not only $u \in C^{1,\alpha}$, $\alpha \in (0, 1)$ as in general (see Proposition 2.2). This result is of independent interest.

(iii) Note that each term in the sum $F_2$ is either a term involving the coordinates of one electron and one nucleus, or the coordinates of two electrons, whereas the terms in $F_3$ involve the coordinates of two electrons and one nucleus. In the representation (1.10) of $F_3$ no terms involving the coordinates of three electrons occur; see Sect. 3 for details.
The fact that no terms involving the coordinates of four and more particles show up in $F_3$ stems from the fact that in the summands contributing to $|\nabla F_2|^2$ only terms involving at most three particle coordinates occur (again, see Sect. 3 for details).

(iv) An immediate consequence of Theorem 1.1 is the following sharpening of (1.7):

$$\nabla\psi - \psi(\nabla F_2 + \nabla F_3) \in C^{0,1}(\Omega).$$

(v) Attempts to approximate many-particle wave functions by a product as in (1.11) are common in computational chemistry and physics. There, such an $\mathcal{F}$ is usually called a 'Jastrow factor'.

It is also interesting to consider the regularity of $\psi$ near the zero-set $\mathcal{N}(\psi) = \{\mathbf{x} \in \mathbb{R}^{3N} \mid \psi = 0\}$ of $\psi$. A simple argument shows that Theorem 1.1 actually implies that $\nabla\psi : \mathcal{N}(\psi) \mapsto \mathbb{R}^{3N}$ is locally Lipschitz, whereas $\nabla\psi$ is just locally $L^\infty$ in $\Sigma(\mathbf{X}) \setminus \mathcal{N}(\psi)$. By 'locally Lipschitz' we here mean the following: For all closed balls $K \subset \mathbb{R}^{3N}$, there is a constant $C = C(K)$ such that $|\nabla\psi(\mathbf{x}) - \nabla\psi(\mathbf{y})| \leq C(K)|\mathbf{x} - \mathbf{y}|$ for all $\mathbf{x}, \mathbf{y} \in \mathcal{N}(\psi) \cap K$. Indeed, writing $\nabla\psi = \psi\nabla(F_2 + F_3) + \exp(F_2 + F_3)\nabla\phi_3$, we get, for $\mathbf{x} \in \mathcal{N}(\psi)$, that $\nabla\psi(\mathbf{x}) = \exp(F_2(\mathbf{x}) + F_3(\mathbf{x}))\nabla\phi_3(\mathbf{x})$ since $\nabla(F_2 + F_3)$ is locally in $L^\infty$. The assertion follows, since both $\exp(F_2 + F_3)$ and $\nabla\phi_3$ are locally Lipschitz in $\mathbb{R}^{3N}$.

In [8] it was shown for a wide class of potentials that at their zero-sets real valued distributional solutions (which for these potentials are then actually continuous functions) to $(-\Delta + V)u = 0$ are, roughly speaking, by one degree smoother than away from their zero sets. So the observation above extends these results to the Coulombic case. The potentials considered in [8] were of Kato type, $K^{n,\delta}$, where $n$ is the dimension (in our case, $n = 3N$) and $\delta \in (0, 2)$; see [19] for definitions and many far-reaching results concerning these potentials. In [19] (see also [20]) it was shown that solutions are locally $C^\delta$ for $\delta < 1$ and $C^{1,\delta-1}$ for $\delta \in (1, 2)$. However, since the Coulomb potential $V$ in (1.1) is in $K^{3N,\delta}$ for all $\delta < 1$, but not in $K^{3N,1}$ these results are not sharp and actually weaker than Kato's result.

It is not surprising that logarithms occur in (1.10). Such terms have been considered in classical work by Fock [3] for the atomic case; see Morgan [16] for an analysis of these 'Fock-expansions' for two-electron atoms (see also Morgan *et al* [17]). These papers also contain many references to earlier work on such expansions.

*Proof of the optimality of the representation* (1.11). It suffices to find a simple example. Consider the one electron atom whose Hamiltonian is given on $\mathbb{R}^3$ by

$$H = -\Delta - \frac{Z}{|x|} \quad , \quad x = (x_1, x_2, x_3) \in \mathbb{R}^3.$$

With $\psi_1(x) = e^{-\frac{Z}{2}|x|}$ and $\psi_2 = x_1 e^{-\frac{Z}{4}|x|}$ we have

$$H\psi_1 = -\frac{Z^2}{4}\psi_1 \quad , \quad H\psi_2 = -\frac{Z^2}{16}\psi_2.$$

Write $\psi_1 = \mathcal{F}\phi^{(1)}$ and $\psi_2 = \mathcal{F}\phi^{(2)}$. Now $\psi_1 > 0$ and if we had an $\mathcal{F}$ which would allow more regularity of the $\phi^{(i)}$'s, then

$$\frac{\phi^{(2)}}{\phi^{(1)}} = \frac{\psi_2}{\psi_1} = x_1 e^{\frac{Z}{4}|x|} \tag{1.13}$$

would be better behaved than just $C^{1,1}$. But near the origin the right-hand side of (1.13) behaves like $x_1(1 + \frac{Z}{4}|x|)$ and this is just $C^{1,1}$, i.e., the second derivatives are bounded but not continuous. □

We point out some consequences of Theorem 1.1 which can be viewed as cusp conditions for second order derivatives of $\psi$. Indeed, we can relate the singularities of the second order derivatives of $F \equiv F_2 + F_3$ with those of the second order derivatives of $\psi$ in a precise way, thereby obtaining certain identities. Here we only explicitly state some representative cases.

**Corollary 1.3.** *Let $\psi$ be a solution to $H\psi = E\psi$ in $\mathbb{R}^{3N}$ with $H$ given by* (1.2).

(i) *Let $1 \le i < j \le N$, and fix any point $\mathbf{z}_0 = (z_1, \dots, z_N) \in \mathbb{R}^{3N}$ with $z_i = z_j \equiv z$. Then*

$$\lim_{R\to 0} \Big\| \big(|x_i - x_j|\, \nabla_i \cdot \nabla_j\, \psi\big) + \frac{1}{2}\psi(\mathbf{z}_0) \Big\|_{L^\infty(B_{3N}(\mathbf{z}_0, R))} = 0. \tag{1.14}$$

(ii) *Let $1 \le i \le N$, $1 \le \ell \le L$, and fix any point $\mathbf{z}_0 = (z_1, \dots, z_N) \in \mathbb{R}^{3N}$ with $z_i = X_\ell, z_j \neq X_\ell, j \neq i$.
Then*

$$\lim_{R\to 0} \Big\| \big(|x_i - X_\ell|\, \Delta_i \psi\big) + Z_\ell\, \psi(\mathbf{z}_0) \Big\|_{L^\infty(B_{3N}(\mathbf{z}_0, R))} = 0. \tag{1.15}$$

*Proof.* We first note that (1.12) implies that (with $F = F_2 + F_3$),

$$\psi \nabla_i \cdot \nabla_j F - \nabla_i \cdot \nabla_j \psi \in L^\infty_{\rm loc}(\mathbb{R}^{3N}). \tag{1.16}$$

In order to show (1.14) we first show that

$$\lim_{\mathbf{x}\to\mathbf{z}_0} |x_i - x_j|\, \nabla_i \cdot \nabla_j\, F(\mathbf{x}) = -\frac{1}{2}. \tag{1.17}$$

An easy calculation shows that

$$\lim_{\mathbf{x}\to\mathbf{z}_0} |x_i - x_j| \nabla_i \cdot \nabla_j\, F_2(\mathbf{x}) = -\frac{1}{2}.$$

If $z \neq X_\ell$ for all $\ell$ then $\nabla_i \cdot \nabla_j\;\, F_3$ is smooth near $\mathbf{z}_0$. We therefore only need to consider the case $z = X_\ell$. We have

$$\begin{aligned} &\nabla_i \cdot \nabla_j F_3 = \\ &\quad C_0 Z_\ell \nabla_i \cdot \nabla_j \big\{\big((x_i - X_\ell)\cdot(x_j - X_\ell)\big) \ln\big(|x_i - X_\ell|^2 + |x_j - X_\ell|^2\big)\big\} \\ &\quad = 3C_0 Z_\ell\, \ln\big(|x_i - X_\ell|^2 + |x_j - X_\ell|^2\big) + \eta, \end{aligned}$$

where $\eta$ is bounded in a neighbourhood of $\mathbf{z}_0$. Noting that

$$|x_i - x_j| \le \sqrt{2}\,\big(|x_i - X_\ell|^2 + |x_j - X_\ell|^2\big)^{1/2},$$

we see that

$$\lim_{\mathbf{x}\to\mathbf{z}_0} |x_i - x_j|\, \nabla_i \cdot \nabla_j F_3(\mathbf{x}) = 0.$$

Using the triangle inequality we obtain

$$\begin{aligned} &\Big\|\, |x_i - x_j|\, (\nabla_i \cdot \nabla_j \psi) + \frac{1}{2}\psi(\mathbf{z}_0)\Big\|_{L^\infty(B_{3N}(\mathbf{z}_0,R))} \\ &\le \Big\| |x_i - x_j|\, \big((\nabla_i \cdot \nabla_j \psi) - (\nabla_i \cdot \nabla_j F)\psi\big)\Big\|_{L^\infty(B_{3N}(\mathbf{z}_0,R))} \\ &\qquad + \Big\| |x_i - x_j|\, (\nabla_i \cdot \nabla_j\, F)\psi + \frac{1}{2}\psi(\mathbf{z}_0)\Big\|_{L^\infty(B_{3N}(\mathbf{z}_0,R))}. \end{aligned}$$

This, (1.16), and (1.17) imply (1.14).

The proof of (1.15) is similar. Just note that

$$|x_i - X_\ell|\, \Delta_i F_2 = -Z_\ell + |x_i - X_\ell| \Big( \sum_{j \neq i} \frac{1}{2|x_j - x_i|} - \sum_{k \neq \ell}^{L} \frac{Z_k}{|x_i - X_k|} \Big).$$

□

The results in Theorem 1.1 are not well suited for obtaining *a priori* estimates. In particular neither $F_2$ nor $F_3$ stay bounded as $|\mathbf{x}|$ tends to infinity so that if, say, $\psi \in L^2(\mathbb{R}^{3N})$ then $\phi_3$ is not necessarily in $L^2(\mathbb{R}^{3N})$. These shortcomings will be dealt with below in a similar way as in [9].

**Definition 1.4.** *Let* $\chi \in C_0^\infty(\mathbb{R})$, $0 \leq \chi \leq 1$, *with*

$$\chi(x) = \begin{cases} 1 & \text{for } |x| \leq 1 \\ 0 & \text{for } |x| \geq 2. \end{cases} \tag{1.18}$$

*We define*

$$F_{\mathrm{cut}} = F_{2,\mathrm{cut}} + F_{3,\mathrm{cut}}, \tag{1.19}$$

*where*

$$F_{2,\mathrm{cut}}(\mathbf{x}) = -\frac{1}{2} \sum_{\ell=1}^{L} \sum_{i=1}^{N} Z_\ell\, \chi(|y_{i,\ell}|)\, |y_{i,\ell}| + \frac{1}{4} \sum_{1 \leq i < j \leq N} \chi(|x_i - x_j|)\, |x_i - x_j|, \tag{1.20}$$

$$F_{3,\mathrm{cut}}(\mathbf{x}) = C_0 \sum_{\ell=1}^{L} \sum_{1 \leq i < j \leq N} Z_\ell\, \chi(|y_{i,\ell}|)\chi(|y_{j,\ell}|)(y_{i,\ell} \cdot y_{j,\ell})\, \ln\big(|y_{i,\ell}|^2 + |y_{j,\ell}|^2\big), \tag{1.21}$$

*and where* $C_0$ *is the constant from* (1.10)*. We also introduce* $\phi_{3,\mathrm{cut}}$ *by*

$$\psi = e^{F_{\mathrm{cut}}} \phi_{3,\mathrm{cut}}. \tag{1.22}$$

**Theorem 1.5.** *Suppose* $\psi$ *is a solution to* $H\psi = E\psi$ *in* $\mathbb{R}^{3N}$*. Then for all* $0 < R < R'$ *there exists a constant* $C(R, R')$*, not depending on* $\psi$ *nor* $\mathbf{x}_0 \in \mathbb{R}^{3N}$*, such that for any second order derivative,*

$$\partial^2 = \frac{\partial^2}{\partial x_{i,k} \partial x_{j,\ell}}, \quad i, j = 1, 2, \ldots, N, \quad k, \ell = 1, 2, 3,$$

*the following estimate holds:*

$$\|\partial^2 \psi - \psi\, \partial^2 F_{\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0, R))} \leq C(R, R') \|\psi\|_{L^\infty(B_{3N}(\mathbf{x}_0, R'))}. \tag{1.23}$$

*Remark 1.6.* Theorem 1.5 strengthens results obtained in [9]. More precisely, to prove Theorem 1.5 we will show that

$$\|\phi_{3,\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,R))} \le C(R,R')\|\phi_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,R'))}. \tag{1.24}$$

The estimate (1.23) is then a trivial consequence of (1.24). (On the other hand, (1.23) and (1.25) imply (1.24)).

The estimate (1.24) is a strengthening of Proposition 1.7 below to $\alpha = 1$. We state and prove the proposition here, since we need it in the proof of (1.24). It essentially follows from ideas in [9].

**Proposition 1.7.** *Suppose $\psi$ is a solution to $H\psi = E\psi$ in $\mathbb{R}^{3N}$. Then for all $0 < R < R'$ and all $\alpha \in (0,1)$ there exists a constant $C(\alpha,R,R')$, not depending on $\psi$ nor $\mathbf{x}_0 \in \mathbb{R}^{3N}$, such that, with $\phi_{3,\mathrm{cut}}$ defined as above,*

$$\|\phi_{3,\mathrm{cut}}\|_{C^{1,\alpha}(B_{3N}(\mathbf{x}_0,R))} \le C\|\phi_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,R'))}. \tag{1.25}$$

*Proof of Proposition 1.7.* Note first that with $\psi = e^{F_{2,\mathrm{cut}}}\phi_{2,\mathrm{cut}}$, (1.5) and $\Delta F_2 = V$ gives

$$\begin{aligned}&\Delta\phi_{2,\mathrm{cut}} + 2\nabla F_{2,\mathrm{cut}}\cdot\nabla\phi_{2,\mathrm{cut}}\\&\quad + \big(\Delta(F_{2,\mathrm{cut}}-F_2) + |\nabla F_{2,\mathrm{cut}}|^2 + E\big)\phi_{2,\mathrm{cut}} = 0.\end{aligned} \tag{1.26}$$

It follows from the form of $F_{2,\mathrm{cut}}$ and $F_2$ (see (1.20), (1.18), and (1.9)) that the coefficients in (1.26) above are uniformly bounded in $\mathbb{R}^{3N}$. Therefore, (1.25), with $\phi_{2,\mathrm{cut}}$ instead of $\phi_{3,\mathrm{cut}}$, follows from standard elliptic regularity results (see Proposition 2.2). To get (1.25) with $\phi_{3,\mathrm{cut}}$, note that $\phi_{3,\mathrm{cut}} = e^{-F_{3,\mathrm{cut}}}\phi_{2,\mathrm{cut}}$, and that $F_{3,\mathrm{cut}} \in C^{1,\alpha}(\mathbb{R}^{3N})$ and has compact support (see (1.21) and (1.18)). □

*1.2. Organisation of the paper.* For simplicity we shall only give the proofs of Theorems 1.1 and 1.5 for the atomic case (i.e., $\ell = 1$, $X_1 = 0$ and $Z_1 = Z$, see (1.3)). Indeed, no additional complications arise for molecules. Also, we only give the proof of Theorem 1.1 in the case $\Omega = \mathbb{R}^{3N}$.

In Subsect. 1.3 we define some notation to be used in the entire paper. Sect. 2 contains standard elliptic regularity results in Subsect. 2.1. Subsect. 2.2 contains in particular the elliptic regularity result Theorem 2.6, which is proved in Subsect. 2.3. Theorem 2.6 is the essential new mathematical input necessary for the proofs of Theorems 1.1 and 1.5. These proofs are given in Sect. 3—the proof of Theorem 1.1 in Subsect. 3.1 and that of Theorem 1.5 in Subsect. 3.2. The Appendices A, B, and C contain the construction of solutions to certain Poisson equations. These solutions are another important ingredient for the proofs of the main theorems.

*1.3. Notation.* Throughout the paper, constants occurring in inequalities will be denoted by the symbol $C$, although their actual value might change from line to line.

For $x \in \mathbb{R}^n$ ($n \ge 2$) we write $x = r\omega$, with $r = |x|$, $\omega = x/|x| \in \mathbb{S}^{n-1}$, the unit sphere in $\mathbb{R}^n$. Denote by $B_n(x,r)$ the open ball of radius $r > 0$ around $x$.

We denote by $Y_{l,m}(\omega)$ the normalised (in $L^2(\mathbb{S}^{n-1})$) real valued spherical harmonics of degree $l$, $l \in \mathbb{N}_0$, with $m = 0, 1, \dots, h(l)-1$, where

$$h(l) = \frac{(2l+n-2)(l+n-3)!}{(n-2)!\,l\,!}. \tag{1.27}$$

Then $\{Y_{l,m}\}_{l,m}$ constitutes an orthonormal basis in $L^2(\mathbb{S}^{n-1})$.

The $Y_{l,m}$'s are the eigenfunctions for $\mathcal{L}^2$, the Laplace-Beltrami operator on $\mathbb{S}^{n-1}$:

$$\mathcal{L}^2 Y_{l,m} = l(l+n-2)Y_{l,m},$$

where $-\frac{\mathcal{L}^2}{r^2}$ is the angular part of the Laplacian in $\mathbb{R}^n$, so

$$-\Delta = -\frac{\partial^2}{\partial r^2} - \frac{n-1}{r}\frac{\partial}{\partial r} + \frac{\mathcal{L}^2}{r^2}.$$

We define $\mathcal{P}^{(n)}_{l,m}$ to be the orthogonal projection in $L^2(\mathbb{S}^{n-1})$ on $Y_{l,m}$:

$$\big(\mathcal{P}^{(n)}_{l,m} f\big)(\omega) = Y_{l,m}(\omega)\int_{\mathbb{S}^{n-1}} Y_{l,m}(\omega) f(\omega)\, d\omega \quad , \quad f \in L^2(\mathbb{S}^{n-1}),$$

and

$$\mathcal{P}^{(n)}_{l} = \sum_{m=0}^{h(l)-1} \mathcal{P}^{(n)}_{l,m}. \tag{1.28}$$

We denote $\mathfrak{h}^{(n)}_l = \mathrm{Ran}(\mathcal{P}^{(n)}_l)$.

By abuse of notation, for a function $f : \mathbb{R}^n \to \mathbb{C}$ we write $f(r\omega) = f(x)$, and, whenever $f(r_0\,\cdot) : \mathbb{S}^{n-1} \to \mathbb{C}$ is in $L^2(\mathbb{S}^{n-1})$ for some $r_0 \in (0,\infty)$, we write

$$\big(\mathcal{P}^{(n)}_{l,m} f\big)(r_0\omega) = Y_{l,m}(\omega)\int_{\mathbb{S}^{n-1}} Y_{l,m}(\omega) f(r_0\omega)\, d\omega \equiv f_{l,m}(r_0)Y_{l,m}(\omega).$$

## 2. Elliptic Regularity

In this section we collect results on the regularity of solutions to second order elliptic equations needed for the proof of Theorems 1.1. and 1.5. The results fall in two parts, known ones (in Subsect. 2.1) and new ones, developed for our purpose, and of interest in themselves. The latter are in Subsect. 2.2. The result of main interest is Theorem 2.6, which is proved in Subsect. 2.3.

*2.1. Known results.* We start by recalling the definition of Hölder continuity:

**Definition 2.1.** *Let $\Omega$ be a domain in $\mathbb{R}^n$, $k \in \mathbb{N}$, and $\alpha \in (0,1]$. We say that a function $u$ belongs to $C^{k,\alpha}(\Omega)$ whenever $u \in C^k(\Omega)$, and for all $\beta \in \mathbb{N}^n$ with $|\beta| = k$, and all open balls $B_n(x_0,r)$ with $\overline{B_n(x_0,r)} \subset \Omega$, we have*

$$\sup_{x,y\in B_n(x_0,r),\, x\neq y} \frac{|D^\beta u(x) - D^\beta u(y)|}{|x-y|^\alpha} \le C(x_0,r).$$

*For any domain $\Omega'$, with $\Omega' \subset\subset \Omega$, we define the following norms:*

$$\|u\|_{C^{k,\alpha}(\Omega')} = \sum_{|\beta|\le k} \|D^\beta u\|_{L^\infty(\Omega')} + [u]_{k,\alpha,\Omega'},$$

$$[u]_{k,\alpha,\Omega'} = \sum_{|\beta|=k} \sup_{x,y\in\Omega',\, x\neq y} \frac{|D^\beta u(x) - D^\beta u(y)|}{|x-y|^\alpha}.$$

*For* $k = 0$ *we use the notation* $C^{\alpha}(\Omega) \equiv C^{0,\alpha}(\Omega)$ *and* $[u]_{\alpha,\Omega'} \equiv [u]_{0,\alpha,\Omega'}$.

Furthermore, for a function $u \in C^{\alpha}(\mathbb{R}^n \setminus \{0\})$ we define

$$\|u\|_{C^{\alpha}(\mathbb{S}^{n-1})} = \sup_{\mathbb{S}^{n-1}} |u| + [u]_{\alpha,\mathbb{S}^{n-1}}, \tag{2.1}$$
$$[u]_{\alpha,\mathbb{S}^{n-1}} = \sup_{x,y\in\mathbb{S}^{n-1},\, x\neq y} \frac{|u(x)-u(y)|}{|x-y|^{\alpha}}.$$

We will need the following result on elliptic regularity in order to conclude that the solutions of elliptic second order equations with bounded coefficients are $C^{1,\alpha}$. The proposition is a reformulation of Corollary 8.36 in Gilbarg and Trudinger [7], adapted for our purposes:

**Proposition 2.2.** *Let* $\Omega_0$ *be a bounded domain in* $\mathbb{R}^n$ *and suppose* $u \in W^{1,2}(\Omega_0)$ *is a weak solution of* $\Delta u + \sum_{j=1}^{n} b_j D_j u + Wu = g$ *in* $\Omega_0$, *where* $b_j, W, g \in L^{\infty}(\Omega_0)$. *Then* $u \in C^{1,\alpha}(\Omega_0)$ *for all* $\alpha \in (0,1)$ *and for any domains* $\Omega', \Omega$, $\overline{\Omega'} \subset \Omega$, $\overline{\Omega} \subset \Omega_0$ *we have*

$$\|u\|_{C^{1,\alpha}(\Omega')} \leq C\big(\sup_{\Omega} |u| + \sup_{\Omega} |g|\big)$$

*for* $C = C(\alpha, n, M, \mathrm{dist}(\Omega', \partial\Omega))$, *with*

$$\max\{1, \max_{j=1,\dots,n} \|b_j\|_{L^{\infty}(\Omega)}, \|W\|_{L^{\infty}(\Omega)}, \|g\|_{L^{\infty}(\Omega)}\} \leq M.$$

We further need results concerning the regularity of solutions of the Poisson equation. These regularity properties are based on the regularity properties of the Newton potential of the inhomogeneity. For our further considerations we recall here the properties of this function.

Let $g \in L^{\infty}(\Omega)$ for $\Omega$ a bounded domain in $\mathbb{R}^n$, $n \geq 2$. The Newton potential of $g$ is the function $w$ defined on $\mathbb{R}^n$ by

$$w(x) = \int_{\Omega} \Gamma(x-y) g(y) dy \tag{2.2}$$

with

$$\Gamma(x) = \begin{cases} \frac{1}{2\pi} \ln(|x|), & n = 2, \\ \frac{1}{(2-n)\,|\mathbb{S}^{n-1}|}\, |x|^{2-n}, & n \geq 3. \end{cases}$$

From [15, Theorem 10.2 and 10.3] we have

**Proposition 2.3.** *Let* $\Omega \subset \mathbb{R}^n$, $n \geq 2$, *be a bounded domain, then:*

(i) *If* $g \in L^{\infty}(\Omega)$, *then* $w \in C^{1,\alpha}(\Omega)$ *for all* $\alpha \in (0,1)$, *and* $\Delta w = g$ *in* $\Omega$ *holds in the distributional sense.*
(ii) *If* $g \in C^{k,\alpha}(\Omega)$ *for some* $k \in \mathbb{N}$ *and some* $\alpha \in (0,1)$, *then* $w \in C^{k+2,\alpha}(\Omega)$.

Since every solution to the Poisson equation can be written as a sum of the Newton potential of the inhomogeneity and a harmonic function, the above implies in particular the following well-known result:

**Proposition 2.4.** *Let $g \in C^{k,\alpha}(\Omega_0)$ for some $k \in \mathbb{N}$ and some $\alpha \in (0,1)$, and assume $u$ is a weak solution to $\Delta u = g$ in $\Omega_0$.*

*Then $u \in C^{k+2,\alpha}(\Omega_0)$. Furthermore, for any domains $\Omega', \Omega$ with $\overline{\Omega'} \subset \Omega$, $\overline{\Omega} \subset \Omega_0$, we have*

$$\|u\|_{C^{k+2,\alpha}(\Omega')} \leq C\big(\sup_{\Omega} |u| + \|g\|_{C^{k,\alpha}(\Omega)}\big), \tag{2.3}$$

*with $C = C(n, k, \alpha, \mathrm{dist}(\Omega', \partial\Omega))$.*

The next lemma, which is taken from Gilbarg and Trudinger [7, Lemma 4.2], is essential for the proof of the main regularity result in Subsect. 2.2.

**Lemma 2.5.** *Let $\Omega$ be a bounded domain in $\mathbb{R}^n$, $n \geq 2$ and let $g \in C^\alpha(\Omega) \cap L^\infty(\Omega)$ for some $\alpha \in (0,1]$.*

*Then the Newton potential $w$ of $g$ (given in (2.2)) satisfies, for $x \in \Omega$ and $i, j = 1, 2, \ldots, n$,*

$$D_{ij}w(x) = \int_{\Omega_0} D_{ij}\Gamma(x-y)\big(g(y) - g(x)\big)\,dy \\ - g(x)\int_{\partial\Omega_0} D_i\Gamma(x-y)\nu_j(y)\,d\sigma(y). \tag{2.4}$$

*Here, $\Omega_0$ is any bounded domain containing $\Omega$ for which the divergence theorem holds, and $g$ is extended to vanish outside $\Omega$. In the last integral, $d\sigma$ denotes the surface measure of $\partial\Omega_0$, and $\nu_j$ the $j^{th}$ coordinate of its (outward directed) unit normal vector.*

*2.2. New results.* We here collect a number of more explicit regularity results needed in the proof of Theorems 1.1 and 1.5.

The following result shows that one can push the $C^{1,\alpha}$, $\alpha \in (0,1)$, in Proposition 2.2 to $C^{1,1}$ in certain cases.

**Theorem 2.6.** *Let $g \in L^\infty(\mathbb{R}^k)$, $k \geq 2$, be a homogeneous function of degree 0 which has the properties $g \in C^\alpha(\mathbb{R}^k \setminus \{0\})$ and $g|_{\mathbb{S}^{k-1}}$ is orthogonal to $\mathfrak{h}_2^{(k)}$ (the subspace of $L^2(\mathbb{S}^{k-1})$ spanned by the spherical harmonics of degree 2). Let $f \in C^\alpha(\mathbb{R}^d)$ for some $d \geq 0$ and let $u \in C^{1,\alpha}(\mathbb{R}^{k+d})$ be a weak solution of the equation*

$$\Delta u(x', x'') = g(x')f(x''), \tag{2.5}$$

*where $x' \in \mathbb{R}^k$, $x'' \in \mathbb{R}^d$, $\Delta = \Delta_{x'} + \Delta_{x''}$.*

*Then $u \in W^{2,\infty}_{\mathrm{loc}}(\mathbb{R}^n)$, $n = k + d$, and the following* a priori *estimate holds: For all balls $B_n(z, R)$ and $B_n(z, R_1)$ in $\mathbb{R}^n$ where $0 < R < R_1$, $z \in \mathbb{R}^n$,*

$$\sup_{B_n(z,R)} |D_{ij}u| \leq C\Big(\sup_{B_n(z,R_1)} |u| + \big(\sup_{\mathbb{S}^{k-1}} |g|\big)\, \|f\|_{C^\alpha(\pi_d B_n(z,R_1))} \\ + \big(\sup_{\pi_d B_n(z,R_1)} |f|\big)\, \|g\|_{C^\alpha(\mathbb{S}^{k-1})}\Big) \tag{2.6}$$

*with $C = C(n, \alpha, R, R_1)$. Here $\pi_d(x', x'') = x''$ for $x' \in \mathbb{R}^k$, $x'' \in \mathbb{R}^d$ for $d > 0$; for $d = 0$, $\pi_d(x') = 0$.*

*Remark 2.7.*

(i) The case $d = 0$ means that $f$ is a constant and the terms in (2.6) with $f$ then equal this constant.
(ii) The reason for the condition $k \geq 2$ will become clear in the proof of the theorem, when Lemma 2.5 is applied.
(iii) Note that if $k = 0$, $d \geq 2$, one has stronger conclusions: Eq. (2.5) becomes $\Delta u(y) = f(y)$ with $f \in C^\alpha(\mathbb{R}^d)$, so by Proposition 2.4, $u \in C^{2,\alpha}(\mathbb{R}^d)$. The *a priori* estimate analogous to (2.6) is then a consequence of Hölder-estimates for $u$ (see e. g., [7, Corollary 6.3]).
(iv) Using the standard fact ([2, Theorem 4 in 5.8]) that $W^{2,\infty}_{\mathrm{loc}}(\mathbb{R}^n) = C^{1,1}_{\mathrm{loc}}(\mathbb{R}^n)$ (with equivalent norms) we may replace the term $\sup_{B_n(z,R)} |D_{ij}u|$ by $[u]_{1,1,B_n(z,R)}$ on the left-hand side in (2.6).
(v) For the special solution to (2.5) given by the Newton potential of $gf$, the estimate (2.6) holds without the term $\sup_{B_n(z,R_1)} |u|$ on the right-hand side (see (2.16)).

Since the proof of Theorem 2.6 is a bit lengthy we present it separately in Subsect. 2.3.

The following proposition, on solutions to Poisson's equation, when the inhomogeneity $f$ in $\Delta u = f$ is a homogeneous function, is needed often in the paper.

**Proposition 2.8.** *Assume that the function g satisfies* $g(r\omega) = r^k G(\omega)$ *with* $G \in L^\infty(\mathbb{S}^{n-1})$ *and* $\mathcal{P}^{(n)}_{k+2} G = 0$.

*Then there exists a solution u to*

$$\Delta u = g \quad on \quad B_n(0, R) \subset \mathbb{R}^n, \tag{2.7}$$

*satisfying* $u(r\omega) = r^{k+2} U(\omega)$ *with* $U \in C^{1,\alpha}(\mathbb{S}^{n-1})$ *for all* $\alpha \in (0, 1)$.

*Proof.* Let

$$g_{l,m}(r) = \int_{\mathbb{S}^{n-1}} g(r\omega) Y_{l,m}(\omega)\, d\omega = r^k \int_{\mathbb{S}^{n-1}} G(\omega) Y_{l,m}(\omega)\, d\omega = r^k g_{l,m}.$$

Then (see (1.27) for $h(l)$)

$$g(r\omega) = r^k \sum_{l=0, l\neq k+2}^{\infty} \sum_{m=0}^{h(l)-1} g_{l,m} Y_{l,m}(\omega),$$

since $g_{k+2,m} = 0$ for all $m$.

Now define

$$U(\omega) = \sum_{l=0, l\neq k+2}^{\infty} \sum_{m=0}^{h(l)-1} \frac{g_{l,m}}{b_l(n,k)} Y_{l,m}(\omega) \tag{2.8}$$

with $b_l(n, k) \equiv (k+2)((k+2) + n - 2) - l(l + n - 2)$. Note that $b_l(n, k)) \neq 0$ for $l \neq k + 2$. Since $\sum_{l,m} g_{l,m} Y_{l,m} \in L^2(\mathbb{S}^{n-1})$ (since $G \in L^\infty(\mathbb{S}^{n-1})$) the sum (2.8) therefore converges in $L^2(\mathbb{S}^{n-1})$.

Make the Ansatz $u(r\omega) = r^{k+2}U(\omega)$, and denote for $N \in \mathbb{N}$,

$$g_N(r\omega) = \sum_{l=0,l\neq k+2}^{N} \sum_{m=0}^{h(l)-1} g_{l,m} r^k \, Y_{l,m}(\omega),$$
$$u_N(r\omega) = r^{k+2} \sum_{l=0,l\neq k+2}^{N} \sum_{m=0}^{h(l)-1} \frac{g_{l,m}}{b_l(n,k)} Y_{l,m}(\omega).$$

Now let $\phi \in C_0^\infty\big(B_n(0,R)\big)$, then, using that $\mathcal{L}^2 Y_{l,m} = l(l+n-2)Y_{l,m}$,

$$\int_{B_n(0,R)} \phi(\Delta u - g)\,dx = \int_{B_n(0,R)} (\Delta\phi)(u-u_N)\,dx + \int_{B_n(0,R)} \phi(g_N - g)\,dx. \tag{2.9}$$

Since $u - u_N \to 0$, $g - g_N \to 0$ (in $L^2$ - sense) for $N \to \infty$, the RHS of 2.9 tends to zero for $N \to \infty$. Hence $u = r^{k+2}U(\omega)$ solves 2.7 in the distributional sense. With $w$ the Newton potential corresponding to $g$ (see 2.2), we have $w \in C^{1,\alpha}(B_n(0,R))$ due to Proposition 2.3, and $u - w$ is harmonic, so $u \in C^{1,\alpha}(B_n(0,R))$. This implies that $U \in C^{1,\alpha}(\mathbb{S}^{n-1})$. $\square$

We prove the following useful lemma:

**Lemma 2.9.** *Let* $G : U \to \mathbb{R}^n$ *for* $U \subset \mathbb{R}^{n+m}$ *a neighbourhood of a point* $(0, y_0) \in \mathbb{R}^n \times \mathbb{R}^m$. *Assume* $G(0,y) = 0$ *for all* $y$ *such that* $(0,y) \in U$. *Let*

$$f(x,y) = \begin{cases} \frac{x}{|x|}\cdot G(x,y), & x \neq 0,\\ 0, & x = 0.\end{cases}$$

*Then, for* $\alpha \in (0,1]$,

$$G \in C^{0,\alpha}(U;\mathbb{R}^n) \Rightarrow f \in C^{0,\alpha}(U). \tag{2.10}$$

*Furthermore,* $\|f\|_{C^\alpha(U)} \leq 2\|G\|_{C^\alpha(U)}$.

*Proof.* Let $\alpha \in (0,1]$. We need to estimate $\frac{f(x_1,y_1)-f(x_2,y_2)}{|(x_1,y_1)-(x_2,y_2)|^\alpha}$.

Suppose first that $x_2 = 0$. Then $f(x_2,y_2) = 0$ and we get

$$\frac{|f(x_1,y_1) - f(0,y_2)|}{|(x_1,y_1)-(0,y_2)|^\alpha} \leq \frac{\left|\frac{x_1}{|x_1|}\cdot G(x_1,y_1)\right|}{|x_1|^\alpha} \leq \left|\frac{x_1}{|x_1|}\right| \cdot \frac{|G(x_1,y_1)|}{|x_1|^\alpha}$$
$$\leq \|G\|_{C^\alpha(U)},$$

since $G \in C^\alpha(U;\mathbb{R}^n)$ and $G(0,y_1) = 0$.

Next, suppose $0 < |x_2| \leq |x_1|$. By the triangle inequality:

$$\big|f(x_1,y_1) - f(x_2,y_2)\big| \leq \left|\frac{x_1}{|x_1|}\cdot\big(G(x_1,y_1) - G(x_2,y_2)\big)\right|$$
$$+ \left|\Big(\frac{x_1}{|x_1|} - \frac{x_2}{|x_2|}\Big)\cdot G(x_2,y_2)\right|.$$

Using that $G$ is $C^\alpha$ and that $G(0, y_2) = 0$, we get

$$\begin{aligned}&\big|f(x_1, y_1) - f(x_2, y_2)\big|\\ &\quad\leq \|G\|_{C^\alpha(U)}\left(\big|(x_1, y_1) - (x_2, y_2)\big|^\alpha + \Big|\Big(\frac{x_1}{|x_1|} - \frac{x_2}{|x_2|}\Big)\Big|\,|x_2|^\alpha\right).\end{aligned}$$

To control the last term—divided by $\big|(x_1, y_1)-(x_2, y_2)\big|^\alpha$—we first derive a lower bound on $\big|(x_1, y_1) - (x_2, y_2)\big|^\alpha$:

$$\begin{aligned}&\big|(x_1, y_1) - (x_2, y_2)\big|^2 \geq |x_1 - x_2|^2\\ &= \big(|x_1| - |x_2|\big)^2 + |x_1|\,|x_2|\Big(\frac{x_1}{|x_1|} - \frac{x_2}{|x_2|}\Big)^2 \geq |x_1|\,|x_2|\Big(\frac{x_1}{|x_1|} - \frac{x_2}{|x_2|}\Big)^2.\end{aligned}$$

Therefore, using the assumption $0 < |x_2| \leq |x_1|$,

$$\big|(x_1, y_1) - (x_2, y_2)\big|^\alpha \geq |x_2|^\alpha \left|\frac{x_1}{|x_1|} - \frac{x_2}{|x_2|}\right|^\alpha.$$

This finishes the proof of the lemma. □

The following obvious lemma is used repeatedly throughout the paper:

**Lemma 2.10.** *Assume* $f(r\omega) = r^2 G(\omega)$ *with* $G \in C^{1,1}(\mathbb{R}^n \setminus \{0\}) \cap L^\infty(\mathbb{R}^n)$. *Then* $f \in C^{1,1}(\mathbb{R}^n)$.

*Proof.* The first derivatives of $f$ trivially exist and are continuous. Therefore it suffices to show that all derivatives of $f$ of second order belong to $L^\infty_{\text{loc}}(\mathbb{R}^n)$; the result then follows from Remark 2.7 (iv),

$$\frac{\partial^2 f}{\partial x_j \partial x_k} = 2\delta_{j,k} G(\omega) + 2\Big(x_j \frac{\partial G}{\partial x_k} + x_k \frac{\partial G}{\partial x_j}\Big) + r^2 \frac{\partial^2 G}{\partial x_j \partial x_k} \in L^\infty_{\text{loc}}(\mathbb{R}^n),$$

since $G \in C^{1,1}(\mathbb{R}^n \setminus \{0\})$. This proves the lemma. □

Note that a better regularity cannot be expected without assuming continuity of $G$ at $x = 0$. On the other hand, if $G$ only depends on $\omega \in \mathbb{S}^{n-1}$, and $G$ is continuous at $x = 0$, then $G$ is a constant.

*2.3. Proof of Theorem 2.6.* We first investigate, for $x_0 \in B_n(z, R_1)$, the behaviour of the Newton potential $w$ as given in (2.2), namely

$$w(x_0) = \int_{B_n(z,R_1)} \Gamma(x_0 - y) g(y') f(y'')\, dy \tag{2.11}$$

with $y = (y', y'') \in \mathbb{R}^{k+d} = \mathbb{R}^n$.

Since $u$ and $w$ are $C^{1,\alpha}$ - solutions of (2.5) in $B_n(z, R_1)$ (see Proposition 2.2), $h = u - w$ is harmonic. Any harmonic function $h$ in a bounded domain $\Omega$ satisfies the following *a priori* estimate (see [7, Theorem 2.10]):

$$\sup_K |D_{ij} h| \leq \frac{C(n)}{\delta^2} \sup_\Omega |h| \quad , \quad i, j \in \{1, \ldots, n\}, \tag{2.12}$$

with $K$ compact, $K \subset \Omega \subset \mathbb{R}^n$, and $\delta = \mathrm{dist}(K, \partial\Omega)$. So, by (2.11) and (2.12), for $x_0 \in B_n(z, R)$ (recall that $h = u - w$)

$$|D_{ij}u(x_0)| \leq \frac{C(n)}{(R_1 - R)^2}\Big( \sup_{B_n(z,R_1)} |u| + C(n, R_1)\big(\sup_{\mathbb{S}^{k-1}} |g|\big)\big(\sup_{\pi_d B_n(z,R_1)} |f|\big)\Big) + |D_{ij}w(x_0)|. \tag{2.13}$$

Therefore to prove that $u \in W^{2,\infty}_{\mathrm{loc}}(\mathbb{R}^n)$ and that $u$ satisfies (2.6) it obviously remains to show that $w$ satisfies the *a priori* estimate (2.6). This will be done via Lemma 2.5 and will finish the proof of Theorem 2.6.

We proceed as follows: Define $N = \{(x', x'') \in \mathbb{R}^n \mid x' = 0\}$ and note that $|N| = 0$ ($|N|$ denotes $n$-dimensional Lebesgue measure of $N$) and that for every ball $B_n \subset \mathbb{R}^n$, $B_n \setminus N$ is still a domain. For this the assumption $k \geq 2$ is vital (see also Remark 2.7 (ii)). Note also that (still with $x_0 \in B_n(z, R_1)$) $w$ can be written as

$$w(x_0) = \int_{B_n(z,R_1)\setminus N} \Gamma(x_0 - y)g(y')f(y'')\,dy. \tag{2.14}$$

Taking into account the Hölder continuity assumptions on $g$ and $f$ it is easily seen that for every domain $\Omega \subset \mathbb{R}^n$, $gf \in C^\alpha(\Omega \setminus N)$. Hence (2.14) and Proposition 2.4 imply that $w \in C^{2,\alpha}\big(B_n(z, R_1) \setminus N\big)$.

Now we are ready to apply Lemma 2.5: Pick $\Omega = B_n(z, R_1)\setminus N$ and $\Omega_0 = B_n(z, R_2)$ with $R_1 < R_2$, then we obtain from (2.4), for $x_0 \in B_n(z, R_1) \setminus N$, that

$$\begin{aligned} D_{ij}w(x_0) &= \int_{B_n(z,R_2)} D_{ij}\Gamma(x_0 - y)\big((gf)(y) - (gf)(x_0)\big)\,dy \\ &\quad - (gf)(x_0)\int_{\partial B_n(z,R_2)} D_i\Gamma(x_0 - y)\nu_j(y)\,d\sigma(y) \\ &\equiv I(x_0) + J(x_0). \end{aligned} \tag{2.15}$$

Here as before $gf$ is extended by zero outside $B_n(z, R_1)\setminus N$. Noting again that $|N| = 0$, we can use this integral representation to derive the *a priori* estimates on $D_{ij}w$. We want to show that for $0 < R < R_1$,

$$\sup_{B_n(z,R)} |D_{ij}w| \leq C_2\Big[\big(\sup_{\mathbb{S}^{k-1}} |g|\big)\,\|f\|_{C^\alpha(\pi_d B_n(z,R_1))} + \big(\sup_{\pi_d B_n(z,R_1)} |f|\big)\,\|g\|_{C^\alpha(\mathbb{S}^{k-1})}\Big], \tag{2.16}$$

where $C_2 = C_2(n, \alpha, R_1 - R, R/R_1)$. Inequality (2.16) together with inequality (2.13) will yield the desired *a priori* estimate (2.6) and implies in particular that $u \in W^{2,\infty}_{\mathrm{loc}}(\mathbb{R}^{k+d})$. So to finish the proof of Theorem 2.6 it remains to prove inequality (2.16). For this we have to estimate the integrals $I(x_0)$ and $J(x_0)$ in (2.15). We state the estimates in the following lemma (Lemma 2.11), which we then apply to prove inequality (2.16). The proof of Lemma 2.11 is given afterwards. For convenience we shall henceforth use the following notation: $B = B_n(z, R)$, $B_j = B_n(z, R_j)$, $j = 1, 2$.

**Lemma 2.11.** *With* $I(x_0)$ *and* $J(x_0)$ *as in* (2.15) *we have the estimates*

$$|I(x_0)| \leq C(n) \Big(\frac{R_2}{R_1 - R}\Big)^n \big(\sup_{\mathbb{S}^{k-1}} |g|\big) \big(\sup_{\pi_d B_1} |f|\big) + C(n,\alpha)\,(R_1 - R)^\alpha \big(\sup_{\mathbb{S}^{k-1}} |g|\big) \big[f\big]_{\alpha,\pi_d B_1} + C(n,\alpha)\,\big(\sup_{\pi_d B_1} |f|\big)\,\|g\|_{C^\alpha(\mathbb{S}^{k-1})}, \tag{2.17}$$

$$|J(x_0)| \leq C(n) \sup_{B_n(z,R)} |gf| \Big(\frac{R_2}{R_2 - R}\Big)^{n-1} \tag{2.18}$$

*for* $x_0 \in B_n(z,R) \setminus N$.

Combining the inequalities (2.17) and (2.18) with (2.15) leads to the *a priori* estimate

$$\begin{aligned} &\sup_{x_0 \in B_n(z,R)} |D_{ij} w(x_0)| \\ &\leq C(n)\Big[\Big(\frac{R_2}{R_1 - R}\Big)^n + \Big(\frac{R_2}{R_2 - R}\Big)^{n-1}\Big]\big(\sup_{\mathbb{S}^{k-1}} |g|\big) \big(\sup_{\pi_d B_1} |f|\big) \\ &+ C(n,\alpha)\Big[(R_1 - R)^\alpha \big(\sup_{\mathbb{S}^{k-1}} |g|\big)\,\big[f\big]_{\alpha,\pi_d B_1} + \big(\sup_{\pi_d B_1} |f|\big)\,\|g\|_{C^\alpha(\mathbb{S}^{k-1})}\Big]. \end{aligned} \tag{2.19}$$

Finally we pick $R_2 = 2R_1$ and obtain, with $C = C(n, \alpha, R, R_1)$,

$$\sup_{B_n(z,R)} |D_{ij} w| \leq C\,\Big[\big(\sup_{\mathbb{S}^{k-1}} |g|\big)\,\|f\|_{C^\alpha(\pi_d B_1)} + \big(\sup_{\pi_d B_1} |f|\big)\,\|g\|_{C^\alpha(\mathbb{S}^{k-1})}\Big]. \tag{2.20}$$

This finishes the proof of (2.16) and according to our previous considerations the proof of Theorem 2.6. It remains to prove the estimates in Lemma 2.11.

*Proof of Lemma 2.11* . We start by proving the estimate (2.18) on $J(x_0)$. For $y \in \partial B_2$ and $x_0 \in B_n(z,R) \setminus N$ we have $|x_0 - y| \geq R_2 - R$. This, and

$$|D_i \Gamma(x_0 - y)| \leq \frac{C(n)}{|x_0 - y|^{n-1}},$$

yields

$$\begin{aligned} |J(x_0)| &\leq |(gf)(x_0)| \int_{\partial B_2} |D_i \Gamma(x_0 - y)\,\nu_j(y)| d\sigma(y) \\ &\leq C(n) \sup_{B_n(z,R)} |gf| \Big(\frac{R_2}{R_2 - R}\Big)^{n-1}, \end{aligned}$$

verifying (2.18).

It remains to prove the estimate (2.17) on $I(x_0)$. This is more involved. With $R' = R_1 - R$ and $\Omega = B_n(z, R_2) \setminus N$, write

$$I(x_0) = I_1(x_0, R') + I_2(x_0, R') \tag{2.21}$$

with

$$I_1(x_0, R') = \int_{\Omega\setminus B_n(x_0,R')} D_{ij}\Gamma(x_0 - y)\big((gf)(y) - (gf)(x_0)\big)\,dy,$$
$$I_2(x_0, R') = \int_{B_n(x_0,R')} D_{ij}\Gamma(x_0 - y)\big((gf)(y) - (gf)(x_0)\big)\,dy.$$

Clearly we have (since $gf \equiv 0$ on $B_2 \setminus B_1$ and $g$ is homogeneous)

$$|I_1(x_0, R')| \le 2\big(\sup_{B_1}|gf|\big)\int_{\Omega\setminus B_n(x_0,R')} |D_{ij}\Gamma(x_0 - y)|\,dy$$
$$\le C(n)\big(\sup_{\mathbb{S}^{k-1}}|g|\big)\,\big(\sup_{\pi_d B_1}|f|\big)\Big(\frac{R_2}{R'}\Big)^n. \tag{2.22}$$

The estimate for $I_2(x_0, R')$ will be more involved and we need several steps.

First notice that

$$(D_{ij}\Gamma)(x) = \frac{P_2(x)}{|x|^{n+2}}\,, \tag{2.23}$$

where $P_2$ is a homogeneous harmonic polynomial of degree 2 (which clearly depends on the indices $i, j$; we suppress these for simplicity). Use polar coordinates $x = r\omega$, $r = |x|$, $\omega = x/|x|$, and obtain (using $\int_{\mathbb{S}^{n-1}} P_2(\omega)\,d\omega = 0$, and (2.23)) that

$$I_2(x_0, R') = C(n)\int_0^{R'}\int_{\mathbb{S}^{n-1}} r^{-1}P_2(\omega)\big(gf\big)(x_0 + r\omega)\,d\omega\,dr. \tag{2.24}$$

Denote $x \in \mathbb{R}^n$ by $x = (x', x'') = r\omega = r(\omega', \omega'')$, where $\omega' \in \mathbb{R}^k$, $\omega'' \in \mathbb{R}^d$ (so that $|\omega'|^2 + |\omega''|^2 = 1$; when $d = 0$, $\omega'' \equiv 0$). With this, write

$$I_2(x_0, R') = C(n)\int_0^{R'} r^{-1}\big(I_2^{(1)}(x_0, r) + I_2^{(2)}(x_0, r)\big)\,dr \tag{2.25}$$

with ($I_2^{(1)} = 0$ when $d = 0$)

$$I_2^{(1)}(x_0, r) = \int_{\mathbb{S}^{n-1}} P_2(\omega)\,g(x_0' + r\omega')\big(f(x_0'' + r\omega'') - f(x_0'')\big)\,d\omega,$$
$$I_2^{(2)}(x_0, r) = f(x_0'')\int_{\mathbb{S}^{n-1}} P_2(\omega)\,g(x_0' + r\omega')\,d\omega.$$

We need to estimate $|I_2^{(1)}|$ and $|I_2^{(2)}|$ such that we gain a suitable $r$-behaviour for small, respectively, large $r$ which will enable us to estimate $|I_2(x_0, R')|$.

Firstly, due to Lemma 2.5, $(gf)(y)$ is defined to be zero for $y \in B_2 \setminus B_1$ in $I(x_0)$ and formula (2.15) holds for $x_0 \in B_1 \setminus N$. Using this formula just for $x_0 \in B_n(z, R) \setminus N$ we have $x_0 + r\omega \in \overline{B_1}$ for all $r$ with $0 \le r \le R' = R_1 - R$ and therefore (up to the zero set $N \cup \partial B_1$) we can make use of the Hölder continuity properties of $g$ and $f$ for the points $x_0$ and $x_0 + r\omega$ in the integrals above.

Using the Hölder continuity of $f$ and the homogeneity of $g$ we obtain

$$
\begin{aligned}
&|I_2^{(1)}(x_0, r)| \\
&\quad = r^\alpha \left| \int_{\mathbb{S}^{n-1}} |\omega''|^\alpha P_2(\omega)\, g(x_0' + r\omega')\, \frac{f(x_0'' + r\omega'') - f(x_0'')}{r^\alpha |\omega''|^\alpha}\, d\omega \right| \\
&\quad \leq C(n)\, r^\alpha \big( \sup_{\mathbb{S}^{k-1}} |g| \big)\, [f]_{\alpha,\, \pi_d B_1}
\end{aligned}
$$

(for $[f]_{\alpha,\, \pi_d B_1}$, see Definition 2.1). Hence

$$
\int_0^{R'} r^{-1} |I_2^{(1)}(x_0, r)|\, dr \leq \frac{C(n)}{\alpha}\, (R')^\alpha \big( \sup_{\mathbb{S}^{k-1}} |g| \big)\, [f]_{\alpha,\, \pi_d B_1}. \tag{2.26}
$$

To estimate the second term in (2.25), we write in the following $x_0' = |x_0'|\,\eta$ with $\eta \in \mathbb{S}^{k-1}$ and define $s$ by $r = |x_0'| s$. Then

$$
\begin{aligned}
&\Big| \int_0^{R'} r^{-1} I_2^{(2)}(x_0, r)\, dr \Big| \qquad\qquad (2.27) \\
&\qquad = \big| f(x_0'') \big| \, \Big| \int_0^{R'} r^{-1} \int_{\mathbb{S}^{n-1}} P_2(\omega)\, g(|x_0'|\eta + r\omega')\, d\omega\, dr \Big| \\
&\qquad = \big| f(x_0'') \big| \, \Big| \int_0^{\frac{R'}{|x_0'|}} s^{-1} \int_{\mathbb{S}^{n-1}} P_2(\omega)\, g(\eta + s\omega')\, d\omega\, ds \Big|,
\end{aligned}
$$

where we used that $g$ is homogeneous of degree zero and $|x_0'| \neq 0$. Because of the $s^{-1}$-term in the $s$-integral we have to control the $\omega$-integral for $s \to 0$ and for $|x_0'| \to 0$.

Define, for $0 \leq s_1 < s_2 \leq \infty$,

$$
K(s_1, s_2) = \int_{s_1}^{s_2} s^{-1} \int_{\mathbb{S}^{n-1}} P_2(\omega) g(\eta + s\omega')\, d\omega\, ds. \tag{2.28}
$$

The behaviour of $K$ for different regimes of $s_1$ and $s_2$ is expressed in Lemma 2.12 below. Applying it, we get that (for all $|x_0'| \in (0, \infty)$) $\big| K\big(0, R'/|x_0'|\big) \big| \leq C(n, \alpha)\, \|g\|_{C^\alpha(\mathbb{S}^{k-1})}$ (for $\|g\|_{C^\alpha(\mathbb{S}^{k-1})}$, see Definition 2.1).

Since due to (2.27)

$$
\Big| \int_0^{R'} r^{-1} I_2^{(2)}(x_0, r)\, dr \Big| = |f(x_0'')|\, \big| K\big(0, R'/|x_0'|\big) \big|
$$

we obtain

$$
\Big| \int_0^{R'} r^{-1} I_2^{(2)}(x_0, r)\, dr \Big| \leq C(n, \alpha)\, \big( \sup_{\pi_d B_1} |f| \big)\, \|g\|_{C^\alpha(\mathbb{S}^{k-1})}. \tag{2.29}
$$

Further via (2.25), (2.26) and (2.29) lead to

$$
\begin{aligned}
|I_2(x_0, R')| \leq{}& C(n, \alpha)\, (R')^\alpha\, \big( \sup_{\mathbb{S}^{k-1}} |g| \big)\, \big[ f \big]_{\alpha,\, \pi_d B_1} \\
&+ C(n, \alpha)\, \big( \sup_{\pi_d B_1} |f| \big)\, \|g\|_{C^\alpha(\mathbb{S}^{k-1})}.
\end{aligned} \tag{2.30}
$$

The estimate (2.17) now follows from (2.21), (2.22), and (2.30).

Proving Lemma 2.12 below will finish the proof of Lemma 2.11. □

**Lemma 2.12.** *With $K$ as in* (2.28) *we have:*

(i) $s_1 = 0, s_2 \leq 1/2$:

$$\big|K(0, s_2)\big| \leq C(n,\alpha)[g]_{\alpha,\mathbb{S}^{k-1}}. \tag{2.31}$$

(ii) $1/2 \leq s_1 < s_2 \leq 4$:

$$\big|K(s_1, s_2)\big| \leq C(n) \sup_{\mathbb{S}^{k-1}} |g|. \tag{2.32}$$

(iii) $4 \leq s_1 < s_2$:

$$\big|K(s_1, s_2)\big| \leq C(n,\alpha)\big[g\big]_{\alpha,\mathbb{S}^{k-1}} + C(n) \sup_{\mathbb{S}^{k-1}} |g|. \tag{2.33}$$

*Proof of Lemma 2.12 .*
(i) Since $\int_{\mathbb{S}^{n-1}} P_2(\omega)\, d\omega = 0$ and $g$ is homogeneous of degree 0 we have

$$K(0, s_2) = \int_0^{s_2} s^{-1} \int_{\mathbb{S}^{n-1}} P_2(\omega)\Big(g\Big(\frac{\eta + s\omega'}{|\eta + s\omega'|}\Big) - g(\eta)\Big)\, d\omega\, ds.$$

Note that $|\eta + s\omega'| \geq 1 - s \geq 1/2$. Since $g \in C^\alpha(\mathbb{S}^{k-1})$ we obtain

$$\big|K(0, s_2)\big| \leq C(n) \,\big[g\big]_{\alpha,\mathbb{S}^{k-1}} \int_0^{s_2} s^{-1} \Big|\frac{\eta + s\omega'}{|\eta + s\omega'|} - \eta\Big|^\alpha ds.$$

This, and

$$\Big|\frac{\eta + s\omega'}{|\eta + s\omega'|} - \eta\Big| \leq \frac{s + \big|1 - |\eta + s\omega'|\,\big|}{|\eta + s\omega'|} \leq \frac{2s}{|\eta + s\omega'|} \leq \frac{2s}{1-s} \leq 4s$$

imply (2.31).
(ii) This follows directly from the definition of $K$ (see (2.28)).
(iii) This is the most involved case. We write the unit sphere $\mathbb{S}^{n-1}$ as the union of

$$\Sigma(s) = \big\{\omega \in \mathbb{S}^{n-1} \;\big|\; s|\omega'| \leq \sqrt{s}\,\big\} = \big\{\omega \in \mathbb{S}^{n-1} \;\big|\; |\omega'| \leq \frac{1}{\sqrt{s}}\,\big\} \tag{2.34}$$

and its complement $\Sigma(s)^c$ (when $d = 0$, $\Sigma(s) = \emptyset$ for $s > 1$) and write $K(s_1, s_2) = A_1 + A_2 + A_3$ where (when $d = 0$, $A_2 = 0$ for $s_1 > 1$)

$$A_1 = \int_{s_1}^{s_2} s^{-1} \int_{\Sigma(s)^c} P_2(\omega)\; (g(\eta + s\omega') - g(s\omega'))\, d\omega\, ds,$$
$$A_2 = \int_{s_1}^{s_2} s^{-1} \int_{\Sigma(s)} P_2(\omega)\; (g(\eta + s\omega') - g(s\omega'))\, d\omega\, ds,$$
$$A_3 = \int_{s_1}^{s_2} s^{-1} \int_{\mathbb{S}^{n-1}} P_2(\omega)\; g(s\omega')\, d\omega\, ds.$$

The estimate (2.33) is a direct consequence of the following lemma. Proving it will finish the proof of Lemma 2.12. □

**Lemma 2.13.** *We have*

$$|A_1| \leq C(n,\alpha)\big[g\big]_{\alpha,\,\mathbb{S}^{k-1}}, \tag{2.35}$$

$$|A_2| \leq C(n) \sup_{\mathbb{S}^{k-1}} |g|, \tag{2.36}$$

$$A_3 = 0. \tag{2.37}$$

*Proof.* $\mathbf{A_1}$ : Note first that since $s|\omega'| \geq 2$ and $|\eta + s\omega'| \geq 1$ in $\Sigma(s)^c$ we obtain, using the homogeneity of degree zero of $g$ and the Hölder continuity of $g$ on $\mathbb{S}^{k-1}$, that

$$|A_1| \leq C(n)\big[g\big]_{\alpha,\mathbb{S}^{k-1}} \int_{s_1}^{s_2} s^{-1} \int_{\Sigma^c(s)} \Big|\frac{\eta + s\omega'}{|\eta + s\omega'|} - \frac{s\omega'}{|s\omega'|}\Big|^{\alpha}\, d\omega\, ds.$$

Then by using the triangle inequality and that $s|\omega'| \geq \sqrt{s} \geq 2$, we get

$$\begin{aligned}\Big|\frac{\eta + s\omega'}{|\eta + s\omega'|} - \frac{s\omega'}{|s\omega'|}\Big| &\leq \frac{1 + \big|\,|s\omega'| - |\eta + s\omega'|\,\big|}{|\eta + s\omega'|} \\ &\leq \frac{2}{|\eta + s\omega'|} \leq \frac{2}{\sqrt{s} - 1} \leq \frac{4}{\sqrt{s}}\end{aligned}$$

which leads to

$$|A_1| \leq C(n,\alpha)\big[g\big]_{\alpha,\,\mathbb{S}^{k-1}} s_1^{-\frac{\alpha}{2}} \leq C(n,\alpha)\big[g\big]_{\alpha,\,\mathbb{S}^{k-1}},$$

verifying (2.35).

$\mathbf{A_2}$ : For $d = 0$, $A_2 = 0$. For $d > 0$, the estimate (2.36) is a consequence of the following lemma, which is not hard to prove using polar coordinates in $\mathbb{R}^n$ (we omit the proof):

**Lemma 2.14.** *Let* $|\Sigma(s)|$ *denote the* $n-1$*-dimensional surface measure of* $\Sigma(s)$*. Then*

$$\big|\Sigma(s)\big| \leq C(n)s^{-1/2}. \tag{2.38}$$

From (2.38) we immediately get (2.36):

$$|A_2| \leq \Big(\int_4^{\infty} s^{-1}\big|\Sigma(s)\big|\, ds\Big)\, C(n) \sup_{\mathbb{S}^{k-1}} |g| \leq C(n) \sup_{\mathbb{S}^{k-1}} |g|.$$

$\mathbf{A_3}$ : We have

$$A_3 = 0 \tag{2.39}$$

as a consequence of the lemma below (when $d = 0$, (2.39) is trivially true, due to the assumptions on $g$), since, by assumption, $g|_{\mathbb{S}^{k-1}}$ is orthogonal to $\mathfrak{h}_2^{(k)}$ (the subspace of $L^2(\mathbb{S}^{k-1})$ spanned by the spherical harmonics of degree 2).

**Lemma 2.15.** *Let* $0 < k < n$ *and suppose* $\phi \in L^2(\mathbb{S}^{k-1})$ *is orthogonal to* $\mathfrak{h}_2^{(k)}$*. Let* $\tilde{\phi}$ *denote the following 'natural' extension of* $\phi$*:*

$$\tilde{\phi}\Big(\frac{(x,y)}{|(x,y)|}\Big) = \begin{cases}\phi\Big(\frac{x}{|x|}\Big) & \textit{for } |x| \neq 0, \\ 0 & \textit{for } |x| = 0.\end{cases}$$

*Then* $\tilde{\phi} \in L^2(\mathbb{S}^{n-1})$ *and* $\tilde{\phi}$ *is orthogonal to* $\mathfrak{h}_2^{(n)}$*.*

*Proof.* Since $\phi$ can be expanded in the natural basis of $L^2(\mathbb{S}^{k-1})$ it suffices to consider a $\phi$ which is the restriction to $\mathbb{S}^{k-1}$ of a harmonic, homogeneous polynomial $P_s$ of degree $s \neq 2$. Then $\tilde{P}_s(x,y) = P_s(x)$ for $(x,y) \in \mathbb{R}^n$ is a harmonic homogeneous polynomial in $\mathbb{R}^n$ of degree $s \neq 2$. Therefore $\tilde{\phi}$, being the restriction of $\tilde{P}_s$ to $\mathbb{S}^{n-1}$, is orthogonal in $L^2(\mathbb{S}^{n-1})$ to $\mathfrak{h}_2^{(n)}$. $\square$

This finishes the proof of Lemma 2.13, and therefore finally the proof of Theorem 2.6. $\square$

## 3. Proofs of Theorems 1.1 and 1.5

We recall that for notational simplicity we shall give the proofs of Theorems 1.1 and 1.5 only for the atomic case.

*3.1. Proof of Theorem 1.1.* Let $\psi$ satisfy $(H - V)\psi = 0$ in $\mathbb{R}^{3N}$, with $V$ as in (1.1), and let $F_2$ and $F_3$ be given as in (1.9) and (1.10). Define $\phi_3$ by the equation $\psi = e^{F_2+F_3}\phi_3$. Recall that $\Delta F_2 = V$. We now make use of Lemma 3.1 below which, together with Theorem 2.6, is the main ingredient in the proof of Theorem 1.1. Due to this lemma, there exists a function $K_3 : \mathbb{R}^{3N} \to \mathbb{R}$ such that $\Delta K_3 = -|\nabla F_2|^2$, and $G_3 \equiv K_3 - F_3 \in C^{1,1}(\mathbb{R}^{3N})$. Define $\zeta_3$ by

$$\psi = e^{F_2+K_3}\zeta_3 \tag{3.1}$$

that is, $\zeta_3 = e^{-G_3}\phi_3$. Since $G_3 \in C^{1,1}(\mathbb{R}^{3N})$, it remains to prove Lemma 3.1 below and that $\zeta_3 \in C^{1,1}(\mathbb{R}^{3N})$, then $\phi_3 \in C^{1,1}(\mathbb{R}^{3N})$ will follow.

**Lemma 3.1.** *There exists a function $G_3 : \mathbb{R}^{3N} \to \mathbb{R}$, $G_3 \in C^{1,1}(\mathbb{R}^{3N})$ such that the function*

$$\begin{aligned} K_3(\mathbf{x}) = K_3(x_1, \dots, x_N) = Z\frac{(2-\pi)}{12\pi} &\sum_{1\le j<k\le N} (x_j \cdot x_k)\ln(x_j^2 + x_k^2) \\ &+ G_3(\mathbf{x}) \end{aligned} \tag{3.2}$$

*solves the equation $\Delta K_3 = -|\nabla F_2|^2$, with $F_2$ as in* (1.9).

*Remark 3.2.* Note that the function $(x \cdot y)\ln(x^2 + y^2)$ belongs to $C^{1,\alpha}(\mathbb{R}^6)$ for all $\alpha \in (0, 1)$, but not to $C^{1,1}(\mathbb{R}^6)$.

*Proof.* Note that

$$\nabla F_2 = -\frac{Z}{2}\Big(\frac{x_1}{|x_1|}, \dots, \frac{x_N}{|x_N|}\Big) + \frac{1}{4}\Big(\sum_{j=2}^{N} \frac{x_1 - x_j}{|x_1 - x_j|}, \dots, \sum_{j=1}^{N-1} \frac{x_N - x_j}{|x_N - x_j|}\Big), \tag{3.3}$$

so that

$$\begin{aligned} |\nabla F_2|^2 = \Big(\frac{NZ^2}{4} + \frac{N(N-1)}{16}\Big) - \frac{Z}{4} &\sum_{1\le j<k\le N} \gamma_2(x_j, x_k) \\ + \frac{1}{8} &\sum_{1\le j<k<l\le N} \gamma_3(x_j, x_k, x_l) \\ \equiv \Gamma_1 + \Gamma_2(\mathbf{x}) + \Gamma_3(\mathbf{x}), \end{aligned} \tag{3.4}$$

with $(x, y, z \in \mathbb{R}^3)$

$$\gamma_2(x, y) = \Big(\frac{x}{|x|} - \frac{y}{|y|}\Big) \cdot \frac{x-y}{|x-y|}, \tag{3.5}$$
$$\gamma_3(x, y, z) = \frac{x-y}{|x-y|} \cdot \frac{x-z}{|x-z|} + \frac{y-x}{|y-x|} \cdot \frac{y-z}{|y-z|} + \frac{z-x}{|z-x|} \cdot \frac{z-y}{|z-y|}.$$

Therefore it is natural to make the 'Ansatz'

$$K_3 = \hat{\mu} + \hat{\kappa} + \hat{\nu},$$

and look for $\hat{\mu}, \hat{\kappa}, \hat{\nu}$ solving

$$\Delta\hat{\mu} = -\Gamma_1 \quad , \quad \Delta\hat{\kappa} = -\Gamma_2 \quad , \quad \Delta\hat{\nu} = -\Gamma_3.$$

First, it is easily seen that with $\mu(x) = |x|^2$, $x \in \mathbb{R}^3$, the function

$$\hat{\mu}(\mathbf{x}) = -\frac{1}{6}\Big(\sum_{j=1}^{N} \frac{Z^2}{4}\mu(x_j) + \sum_{1\le j<k\le N} \frac{1}{16}\mu(x_j - x_k)\Big),$$

satisfies $\Delta\hat{\mu} = -\Gamma_1$, $\hat{\mu} \in C^\infty(\mathbb{R}^{3N})$.

Further, it suffices to find functions $\kappa$ and $\nu$ such that

$$\kappa(x, y) = \frac{2-\pi}{3\pi}\,(x \cdot y)\log(x^2 + y^2) + \kappa_1(x, y)\ ,\ \ \kappa_1 \in C^{1,1}(\mathbb{R}^6),$$
$$\text{with} \qquad (\Delta_x + \Delta_y)\kappa(x, y) = \gamma_2(x, y), \tag{3.6}$$

and $\nu \in C^{1,1}(\mathbb{R}^9)$ with

$$(\Delta_x + \Delta_y + \Delta_z)\nu(x, y, z) = \gamma_3(x, y, z), \tag{3.7}$$

since letting

$$\hat{\kappa}(\mathbf{x}) = \frac{Z}{4}\sum_{1\le j<k\le N} \kappa(x_j, x_k) \quad , \quad \hat{\nu}(\mathbf{x}) = -\frac{1}{8}\sum_{1\le j<k<l\le N} \nu(x_j, x_k, x_l)$$

gives $(\Delta = \sum_{j=1}^{N} \Delta_j)$

$$\Delta\hat{\kappa}(\mathbf{x}) = \frac{Z}{4}\sum_{1\le j<k\le N} \big((\Delta_j + \Delta_k)\kappa\big)(x_j, x_k) = -\Gamma_2(\mathbf{x}),$$
$$\Delta\hat{\nu}(\mathbf{x}) = -\frac{1}{8}\sum_{1\le j<k<l\le N} \big((\Delta_j + \Delta_k + \Delta_l)\nu\big)(x_j, x_k, x_l) = -\Gamma_3(\mathbf{x}).$$

The functions $\kappa$ and $\nu$ are constructed in Appendices A and B. Lemma 3.1 then follows from Lemma A.1 and Lemma B.1. □

*Remark 3.3.* Summarizing, one can say that only those points where the coordinates of (at least) 2 electrons coincide with that of the nucleus ($x_i = x_j = 0$) give rise to the logarithmic terms in $K_3$. These terms stem from the function $\kappa$ and are due to the type of singularity of the $\gamma_2$-terms in $|\nabla F_2|^2$. There is no such contribution from the function $\nu$, i.e., from the $\gamma_3$-terms in $|\nabla F_2|^2$. This is due to the permutational symmetry of $\nu$ with respect to the electron coordinates as will be seen from the proof of Lemma B.1.

To finish the proof of Theorem 1.1 it remains to prove that $\zeta_3 \in C^{1,1}(\mathbb{R}^{3N})$.

Using $(H - E)\psi = 0$ and $H = -\Delta + V$, we get the following equation for $\zeta_3$ (see (1.5) and (3.1); set $F = F_2 + K_3$ and $\phi = \zeta_3$, and use that $\Delta F_2 = V$)

$$\Delta\zeta_3 + 2\nabla\big(F_2 + K_3\big)\cdot\nabla\zeta_3 + \Big(\Delta K_3 + |\nabla\big(F_2 + K_3\big)|^2 + E\Big)\zeta_3 = 0. \tag{3.8}$$

Note that, by Lemma 3.1 and (3.3), the coefficients in (3.8) are (locally) in $L^\infty$. Therefore, by Proposition 2.2, $\zeta_3 \in C^{1,\alpha}(\mathbb{R}^{3N})$ for all $\alpha \in (0, 1)$. We need to improve this to $C^{1,1}(\mathbb{R}^{3N})$.

Using $\Delta K_3 = -|\nabla F_2|^2$ reduces (3.8) to the equation

$$\Delta\zeta_3 + 2\nabla\big(F_2 + K_3\big)\cdot\nabla\zeta_3 + \big(|\nabla K_3|^2 + 2\nabla F_2\cdot\nabla K_3 + E\big)\zeta_3 = 0. \tag{3.9}$$

This eliminated one of the terms in Eq. (3.8) for $\zeta_3$ that was only in $L^\infty(\mathbb{R}^{3N})$, and not continuous, namely $|\nabla F_2|^2$.

To deal with the two remaining ones (containing $\nabla F_2$), re-arrange Eq. (3.9):

$$\Delta\zeta_3 + \nabla F_2\cdot\Big(2\nabla\zeta_3 + 2\zeta_3\nabla K_3\Big) + \Big(|\nabla K_3|^2 + E\Big)\zeta_3 + 2\nabla K_3\cdot\nabla\zeta_3 = 0. \tag{3.10}$$

Define $\Psi = (\Psi_1, \ldots, \Psi_N) : \mathbb{R}^{3N} \to \mathbb{R}^{3N}$ by

$$\Psi(x_1, \ldots, x_N) = 2\nabla\zeta_3 + 2\zeta_3\nabla K_3. \tag{3.11}$$

That is, $\Psi_j = (\Psi_{j,1}, \Psi_{j,2}, \Psi_{j,3}) : \mathbb{R}^{3N} \to \mathbb{R}^3$ with

$$\Psi_{j,i} = 2\frac{\partial\zeta_3}{\partial x_{j,i}} + 2\zeta_3\frac{\partial K_3}{\partial x_{j,i}}\,,\;\; j \in \{1, \ldots, N\}\,,\;\; i \in \{1, 2, 3\}. \tag{3.12}$$

Then

$$\nabla F_2\cdot\big(2\nabla\zeta_3 + 2\zeta_3\nabla K_3\big) = \nabla F_2\cdot\Psi. \tag{3.13}$$

Since $K_3, \zeta_3 \in C^{1,\alpha}(\mathbb{R}^{3N})$ for all $\alpha \in (0, 1)$, we have $\Psi_{j,i} \in C^\alpha(\mathbb{R}^{3N})$ for all $j \in \{1, \ldots, N\}$, $i \in \{1, 2, 3\}$ and $\alpha \in (0, 1)$.

Next, let $\hat{\Psi}_{j,i} : \mathbb{R}^{3(N-1)} \to \mathbb{R}$ be defined by

$$\hat{\Psi}_{j,i}(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_N) = \Psi_{j,i}(x_1, \ldots, x_{j-1}, 0, x_{j+1}, \ldots, x_N), \tag{3.14}$$

that is, by setting $x_j$ equal to zero in $\Psi_{j,i}$.

Furthermore, define, for $j < k$, $j, k \in \{1, \ldots, N\}$, the functions $\Phi_{(j,k)} : \mathbb{R}^{3N} \to \mathbb{R}^3$ by

$$\begin{aligned}\Phi_{(j,k)}(x_1, \ldots, x_N) = {}& \\ \Psi_j(x_1, \ldots, x_{j-1}, \tfrac{1}{2}(x_j + x_k), x_{j+1}, \ldots, x_{k-1}, \tfrac{1}{2}(x_j + x_k), x_{k+1}, \ldots, x_N)& \\ - & \\ \Psi_k(x_1, \ldots, x_{j-1}, \tfrac{1}{2}(x_j + x_k), x_{j+1}, \ldots, x_{k-1}, \tfrac{1}{2}(x_j + x_k), x_{k+1}, \ldots, x_N).&\end{aligned} \tag{3.15}$$

The proof of Theorem 1.1 will follow from the following two lemmas:

**Lemma 3.4.** *Let $\hat{\Psi}_{j,i}$, $\Phi_{(j,k),i}$ be defined according to* (3.12), (3.14) *and* (3.15). *Assume the functions $u_{j,i}$, $v_{(j,k),i}$ solve the equations*

$$\Delta u_{j,i} = \frac{Z}{2}\frac{x_{j,i}}{|x_j|}\,\hat{\Psi}_{j,i}, \tag{3.16}$$

$$\Delta v_{(j,k),i} = -\frac{1}{4}\frac{x_{j,i}-x_{k,i}}{|x_j-x_k|}\,\Phi_{(j,k),i}. \tag{3.17}$$

*Then $u_{j,i}, v_{(j,k),i} \in C^{1,1}(\mathbb{R}^{3N})$.*

**Lemma 3.5.** *Let $\hat{\Psi}_j$, $\Phi_{(j,k)}$ be defined according to* (3.12), (3.14) *and* (3.15). *Then the functions*

$$\frac{1}{4}\frac{x_j-x_k}{|x_j-x_k|}\cdot\Big\{\big(\Psi_j-\Psi_k\big)-\Phi_{(j,k)}\Big\}, \tag{3.18}$$

$$\frac{Z}{2}\frac{x_j}{|x_j|}\cdot\big(\Psi_j-\hat{\Psi}_j\big) \tag{3.19}$$

*all belong to $C^{\alpha}(\mathbb{R}^{3N})$ for all $\alpha \in (0,1)$.*

Let us first finish the proof of Theorem 1.1, using the two lemmas.

Let the function $U : \mathbb{R}^{3N} \to \mathbb{R}$ be defined by

$$U = \sum_{i=1}^{3}\sum_{j=1}^{N} u_{j,i} + \sum_{i=1}^{3}\sum_{1\le j<k\le N} v_{(j,k),i} \tag{3.20}$$

with the functions $u_{j,i}$, $v_{(j,k),i}$ solving Eqs. (3.16) and (3.17). Then

$$\Delta U = \sum_{j=1}^{N}\frac{Z}{2}\frac{x_j}{|x_j|}\cdot\hat{\Psi}_j - \sum_{1\le j<k\le N}\frac{1}{4}\frac{x_j-x_k}{|x_j-x_k|}\cdot\Phi_{(j,k)}, \tag{3.21}$$

and, due to Lemma 3.4, $U \in C^{1,1}(\mathbb{R}^{3N})$.

Let $W = \zeta_3 - U$, then due to (3.10), (3.21), and the form of $\nabla F_2$ (see (3.3))

$$\begin{aligned}\Delta W = \sum_{j=1}^{N} -\frac{Z}{2}\frac{x_j}{|x_j|}\cdot\big(\Psi_j-\hat{\Psi}_j\big) - \Big(|\nabla K_3|^2+E\Big)\zeta_3 - 2\nabla K_3\cdot\nabla\zeta_3 \\ - \sum_{1\le j<k\le N}\frac{1}{4}\frac{x_j-x_k}{|x_j-x_k|}\cdot\Big\{\big(\Psi_j-\Psi_k\big)-\Phi_{(j,k)}\Big\}.\end{aligned} \tag{3.22}$$

Using the fact that $K_3, \zeta_3 \in C^{1,\alpha}(\mathbb{R}^{3N})$, and Lemma 3.5, we conclude that the RHS in (3.22) belongs to $C^{\alpha}(\mathbb{R}^{3N})$ for all $\alpha \in (0,1)$ . Due to Proposition 2.4, $W \in C^{2,\alpha}(\mathbb{R}^{3N})$ for all $\alpha \in (0,1)$, and so $\zeta_3 = W + U \in C^{1,1}(\mathbb{R}^{3N})$ (since $U \in C^{1,1}(\mathbb{R}^{3N})$ as mentioned above).

This finishes the proof that $\zeta_3 \in C^{1,1}(\mathbb{R}^{3N})$, and therefore $\phi_3 = e^{G_3}\zeta_3 \in C^{1,1}(\mathbb{R}^{3N})$, since $G_3 \in C^{1,1}(\mathbb{R}^{3N})$.

To finish the proof of Theorem 1.1, it therefore remains to prove Lemma 3.4 and Lemma 3.5.

*Proof of Lemma 3.4* . Firstly, for $u_{j,i}$, this is a straightforward application of Theorem 2.6, with $k = 3,\ d = 3(N-1)$ and

$$g \equiv \frac{x_{j,i}}{|x_j|} \quad , \quad x' \equiv x_j \in \mathbb{R}^3,$$
$$f \equiv \frac{Z}{2}\,\hat{\Psi}_{j,i} \quad , \quad x'' \equiv (x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_N) \in \mathbb{R}^{3(N-1)}.$$

It has already been noted that $\Psi_{j,i} \in C^\alpha(\mathbb{R}^{3N})$ for all $\alpha \in (0,1)$ and therefore (see (3.14)) also $\hat{\Psi}_{j,i} \in C^\alpha(\mathbb{R}^{3(N-1)})$ for all $\alpha \in (0,1)$. Clearly, $\frac{x_{j,i}}{|x_j|} \in C^\infty(\mathbb{R}^3\backslash\{0\}) \subset C^\alpha(\mathbb{R}^3\backslash\{0\})$, and $\mathcal{P}_2^{(3)}\big(\frac{x_{j,i}}{|x_j|}\big) = 0$, due to the anti-symmetry of the function $\frac{x_{j,i}}{|x_j|}$. Therefore, all assumptions of Theorem 2.6 are fullfilled and it follows that $u_{j,i} \in C^{1,1}(\mathbb{R}^{3N})$.

Secondly, for $v_{(j,k),i}$, we make an orthogonal change of coordinates: $a = \frac{1}{\sqrt{2}}(x_j - x_k),\ b = \frac{1}{\sqrt{2}}(x_j + x_k)$, the other coordinates remaining unchanged. Due to the specific definition of $\Phi_{(j,k),i}$, this brings us to a setup exactly as the one above for $u_{j,i}$. Since the orthogonal change of coordinates does not change the regularity, the conclusion follows as before.

This finishes the proof of Lemma 3.4. □

*Proof of Lemma 3.5* . First, note that the function $G_j = \Psi_j - \hat{\Psi}_j$ satisfies $G_j \in C^\alpha(\mathbb{R}^{3N})$ for all $\alpha \in (0,1)$, and

$$G_j(x_1, \ldots, x_{j-1}, 0, x_{j+1}, \ldots, x_N) = 0 \quad \text{for all } (x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_N) \in \mathbb{R}^{3(N-1)}.$$

Therefore, due to Lemma 2.9,

$$\frac{Z}{2}\frac{x_j}{|x_j|} \cdot \big(\Psi_j - \hat{\Psi}_j\big) \in C^\alpha(\mathbb{R}^{3N}) \quad \text{for all} \quad \alpha \in (0,1).$$

Secondly, for the function

$$\frac{1}{4}\frac{x_j - x_k}{|x_j - x_k|} \cdot \Big\{\big(\Psi_j - \Psi_k\big) - \Phi_{(j,k)}\Big\},$$

the same orthogonal change of coordinates as in the proof of Lemma 3.4 brings us in the same situation as the above, again due to the specific definition of $\Phi_{(j,k)}$. The conclusion follows as above.

This finishes the proof of Lemma 3.5. □

This finishes the proof of Theorem 1.1. □

*3.2. Proof of Theorem 1.5.* By Remark 1.6 it suffices to prove that (1.24) holds. We proceed similarly to the proof of Theorem 1.1, but here we need to estimate carefully all the involved quantities uniformly (i.e., independently of $\mathbf{x}_0 \in \mathbb{R}^{3N}$). For notational simplicity, we will prove (1.24) only in the case $R' = 2R$.

For the proof we need the following regularised version of Lemma 3.1.

**Lemma 3.1'.** *There exists a function* $G_{3,\mathrm{cut}} : \mathbb{R}^{3N} \to \mathbb{R}$*,* $G_{3,\mathrm{cut}} \in C^{1,1}(\mathbb{R}^{3N})$*, such that the function*

$$K_{3,\mathrm{cut}}(\mathbf{x}) = Z\,\frac{2-\pi}{12\pi} \sum_{1 \le j<k \le N} (x_j \cdot x_k)\chi(|x_j|)\chi(|x_k|)\ln(x_j^2 + x_k^2) + G_{3,\mathrm{cut}}(\mathbf{x}) = F_{3,\mathrm{cut}}(\mathbf{x}) + G_{3,\mathrm{cut}}(\mathbf{x}) \tag{3.23}$$

*(for* $F_{3,\mathrm{cut}}$*, see* (1.21)*) solves the equation*

$$\Delta K_{3,\mathrm{cut}} = -|\nabla F_{2,\mathrm{cut}}|^2 + r_{\mathrm{cut}},$$

*with* $F_{2,\mathrm{cut}}$ *as defined in* (1.20) *and* $r_{\mathrm{cut}} \in C^{\alpha}(\mathbb{R}^{3N})$ *for all* $\alpha \in (0,1)$*. Furthermore,* $G_{3,\mathrm{cut}}$ *can be chosen such that for all* $\rho > 0$ *the following estimate holds:*

$$\|G_{3,\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,\rho))} + \|r_{\mathrm{cut}}\|_{C^{\alpha}(B_{3N}(\mathbf{x}_0,\rho))} \le C, \tag{3.24}$$

*for some constant* $C = C(\rho) > 0$ *independent of* $\mathbf{x}_0 \in \mathbb{R}^{3N}$*.*

*Proof.* The proof of Lemma 3.1' is analogous to that of Lemma 3.1. Instead of $\mu, \kappa, \nu$ we will use functions $\mu_{\mathrm{cut}}, \kappa_{\mathrm{cut}}$ and $\nu_{\mathrm{cut}}$ to be defined presently. With $\chi$ being the function defined in (1.18) we define

$$\mu_{\mathrm{cut}}(x) = \chi(|x|)\mu(x) = \chi(|x|)|x|^2, \tag{3.25}$$

$$\begin{aligned} \kappa_{\mathrm{cut}}(x,y) &= \chi(|x|)\chi(|y|)\kappa(x,y) \qquad (3.26)\\ &\quad - \frac{1}{4}\chi(3|y|)\big(1-\chi(|x|)\big)\Big(|y|^2\frac{x\cdot y}{|x||y|}\Big)\\ &\quad - \frac{1}{4}\chi(3|x|)\big(1-\chi(|y|)\big)\Big(|x|^2\frac{x\cdot y}{|x||y|}\Big)\\ &\equiv \chi(|x|)\chi(|y|)\frac{2-\pi}{3\pi}(x\cdot y)\ln(x^2+y^2) + \kappa_{1,\mathrm{cut}}(x,y). \end{aligned}$$

(Note that $\kappa_{1,\mathrm{cut}}(x,y) \neq \chi(|x|)\chi(|y|)\kappa_1(x,y)$). Let $\nu_{\mathrm{cut}}$ be as in Lemma B.2, we then have

$$\begin{aligned} &\Delta\nu_{\mathrm{cut}} = \gamma_3 + h_\nu, \qquad (3.27)\\ &\|\nu_{\mathrm{cut}}\|_{C^{1,1}(B_9((x_0,y_0,z_0),\rho))} + \|h_\nu\|_{C^{\alpha}(B_9((x_0,y_0,z_0),\rho))} \le C, \end{aligned}$$

with $\gamma_3$ as in (3.5) and with $C$ independent of $(x_0, y_0, z_0) \in \mathbb{R}^9$ and $\rho > 0$.

For $\mu_{\mathrm{cut}}$, note that

$$\begin{aligned} \Delta\mu_{\mathrm{cut}} &= \Delta|x|^2 + \Delta(\mu_{\mathrm{cut}} - |x|^2) \qquad (3.28)\\ &= 6 - \Delta\big((1-\chi(|x|))|x|^2\big) \equiv 6 - h_\mu, \end{aligned}$$

where obviously,

$$\|\mu_{\mathrm{cut}}\|_{C^{1,1}(B_3(x_0,\rho))} + \big\|h_\mu\big\|_{C^{\alpha}(B_3(x_0,\rho))} \le C, \tag{3.29}$$

with $C$ independent of $x_0 \in \mathbb{R}^3$ and $\rho > 0$.

For $\kappa_{\text{cut}}$, using $\Delta\kappa = \gamma_2$ (see (3.5) and (3.6)), that $\Delta_y(|y|^2 \frac{x\cdot y}{|x||y|}) = 4\frac{x\cdot y}{|x||y|}$, and the support properties of $\chi$, we have that

$$\begin{aligned}
\Delta\kappa_{\text{cut}} &= \gamma_2 - \{1 - \chi(|x|)\chi(|y|)\}\big(1 - \chi(3|x|) - \chi(3|y|)\big)\gamma_2 \\
&\quad - \Big\{\chi(3|y|)\big(1 - \chi(|x|)\big) + \chi(3|x|)\big(1 - \chi(|y|)\big)\Big\}\big(\gamma_2 + \frac{x\cdot y}{|x||y|}\big) \\
&\quad + R_1 + R_2 + R_3, \\
&\equiv \gamma_2 - \mathcal{H}\gamma_2 - \mathcal{G}\big(\gamma_2 + \frac{x\cdot y}{|x||y|}\big) + R_1 + R_2 + R_3,
\end{aligned} \tag{3.30}$$

where

$$\begin{aligned}
R_1 &= \chi(|y|)\kappa\Delta_x\chi(|x|) + \chi(|y|)2\nabla_x\chi(|x|)\cdot\nabla_x\kappa \\
&\quad + \chi(|x|)\kappa\Delta_y\chi(|y|) + \chi(|x|)2\nabla_y\chi(|y|)\cdot\nabla_y\kappa, \\
R_2 &= -\frac{1}{4}\chi(3|y|)|y|^2\frac{y}{|y|}\cdot\Delta_x\big((1 - \chi(|x|))\frac{x}{|x|}\big) \\
&\quad - \frac{1}{4}\big(\Delta_y\chi(3|y|)\big)|y|^2\frac{y}{|y|}\cdot\big((1 - \chi(|x|)\frac{x}{|x|}\big) \\
&\quad - \frac{1}{2}\big(\nabla_y\chi(3|y|)\big)\cdot\nabla_y\Big(\frac{x\cdot y}{|x||y|}|y|^2\big(1 - \chi(|x|)\big)\Big),
\end{aligned}$$

and where $R_3$ is $R_2$ with $x$ and $y$ interchanged.

Using that $\kappa \in C^{1,\alpha}(\mathbb{R}^6)$ for all $\alpha \in (0, 1)$, and the support properties of $\chi$, it is easily seen that

$$\|R_j\|_{C^\alpha(B_6((x_0,y_0),\rho))} \le C, \tag{3.31}$$

with a constant $C$ independent of $(x_0, y_0)) \in \mathbb{R}^6$ and $\rho > 0$.

Since for all $(x, y) \in \mathbb{R}^6$,

$$\big|\nabla\gamma_2\big| \le 6\sqrt{2}\Big(\frac{1}{|x|} + \frac{1}{|y|}\Big), \quad \Big|\nabla\big(\gamma_2 + \frac{x\cdot y}{|x||y|}\big)\Big| \le \frac{8\sqrt{2}}{|x-y|}$$

we get, using the support properties of $\mathcal{H}$ and $\mathcal{G}$, that

$$\|\mathcal{H}\nabla\gamma_2\|_{L^\infty(\mathbb{R}^6)} \le C \quad , \quad \big\|\mathcal{G}\nabla\big(\gamma_2 + \tfrac{x\cdot y}{|x||y|}\big)\big\|_{L^\infty(\mathbb{R}^6)} \le C.$$

Again using the support properties of $\mathcal{H}$ and $\mathcal{G}$, this implies that

$$\begin{aligned}
&\|\mathcal{H}\gamma_2\|_{C^{0,1}(B_6((x_0,y_0),\rho))} \le C, \\
&\big\|\mathcal{G}\big(\gamma_2 + \tfrac{x\cdot y}{|x||y|}\big)\big\|_{C^{0,1}(B_6((x_0,y_0),\rho))} \le C,
\end{aligned} \tag{3.32}$$

with a constant $C$ independent of $(x_0, y_0) \in \mathbb{R}^6$ and $\rho > 0$.

From (3.30), (3.31), and (3.32) we get

$$\Delta\kappa_{\text{cut}} = \gamma_2 + h_\kappa \quad , \quad \|h_\kappa\|_{C^\alpha(B_6((x_0,y_0),\rho))} \le C, \tag{3.33}$$

with a constant $C$ independent of $(x_0, y_0) \in \mathbb{R}^6$ and $\rho > 0$. Note that (see (3.26) and (A.2))

$$\kappa_{1,\mathrm{cut}}(x, y) = \chi(|x|)\chi(|y|)\Big((x^2 + y^2)G_{\kappa_1}\big(\frac{(x, y)}{|(x, y)|}\big)\Big)\,,\ G_{\kappa_1} \in C^{1,1}(\mathbb{S}^5).$$

Therefore, due to the compact support of $\chi$,

$$\|\kappa_{1,\mathrm{cut}}\|_{C^{1,1}(B_6((x_0,y_0),\rho))} \leq C \tag{3.34}$$

with $C$ independent of $(x_0, y_0) \in \mathbb{R}^6$ and $\rho > 0$.

Observe that

$$|\nabla F_2|^2 = |\nabla F_{2,\mathrm{cut}}|^2 + \nabla(F_2 - F_{2,\mathrm{cut}}) \cdot \nabla(F_2 + F_{2,\mathrm{cut}}) \tag{3.35}$$

and that

$$\begin{aligned}
&\nabla(F_2 - F_{2,\mathrm{cut}}) \cdot \nabla(F_2 + F_{2,\mathrm{cut}}) \\
&\qquad = \sum_{j=1}^{N} \nabla_j(F_2 - F_{2,\mathrm{cut}}) \cdot \nabla_j(F_2 + F_{2,\mathrm{cut}}) \\
&\qquad = \sum_{j=1}^{N} \vec{b}_j \cdot \frac{x_j}{|x_j|} + \sum_{1\leq j<k\leq N} \vec{b}_{(j,k)} \cdot \frac{x_j - x_k}{|x_j - x_k|},
\end{aligned}$$

where

$$\begin{aligned}
\vec{b}_j &= -\frac{Z}{2}\Big\{1 + \chi(|x_j|) + \chi'(|x_j|)|x_j|\Big\}\Big(\vec{a}_j + \sum_{l=1,l\neq j}^{N} \vec{a}_{(j,l)}\Big),\\
\vec{b}_{(j,k)} &= \frac{1}{4}\Big\{1 + \chi(|x_j - x_k|) + \chi'(|x_j - x_k|)|x_j - x_k|\Big\} \times\\
&\qquad \times \Big(\vec{a}_j - \vec{a}_k + \sum_{l=1,l\neq j}^{N} \vec{a}_{(j,l)} - \sum_{l=1,l\neq k}^{N} \vec{a}_{(k,l)}\Big),\\
\vec{a}_j &= -\frac{Z}{2}\Big\{\Big(1 - \chi(|x_j|)\Big) - \chi'(|x_j|)|x_j|\Big\}\frac{x_j}{|x_j|},\\
\vec{a}_{(j,k)} &= \frac{1}{4}\Big\{\Big(1 - \chi(|x_j - x_k|)\Big) - \chi'(|x_j - x_k|)|x_j - x_k|\Big\}\frac{x_j - x_k}{|x_j - x_k|}.
\end{aligned}$$

Clearly (using the support properties of $\chi$), for all $\beta \in \mathbb{N}^{3N}$,

$$\|\partial^\beta \vec{b}_j\|_{L^\infty(\mathbb{R}^{3N})} + \|\partial^\beta \vec{b}_{(j,k)}\|_{L^\infty(\mathbb{R}^{3N})} \leq C(\beta). \tag{3.36}$$

Define

$$\begin{aligned}
G_{1,\mathrm{cut}} &= \frac{1}{4}\sum_{j=1}^{N} \vec{b}_j \cdot \Big(|x_j|^2 \frac{x_j}{|x_j|}\Big)\chi(|x_j|)\\
&\qquad + \frac{1}{4}\sum_{1\leq j<k\leq N} \vec{b}_{(j,k)} \cdot \Big(\Big|\frac{x_j - x_k}{\sqrt{2}}\Big|^2 \frac{x_j - x_k}{|x_j - x_k|}\Big)\chi(|x_j - x_k|).
\end{aligned}$$

Then, due to (3.36) and the support properties of $\chi$,

$$\|G_{1,\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,\rho))} \le C, \tag{3.37}$$

for some constant $C = C(\rho) > 0$ independent of $\mathbf{x}_0 \in \mathbb{R}^{3N}$.

Using $\Delta(|x_j|^2 \frac{x_j}{|x_j|}) = 4\frac{x_j}{|x_j|}$ and $\Delta(|\frac{x_j - x_k}{\sqrt{2}}|^2 \frac{x_j - x_k}{|x_j - x_k|}) = 4\frac{x_j - x_k}{|x_j - x_k|}$, we see that

$$\Delta G_{1,\mathrm{cut}} = \nabla(F_2 - F_{2,\mathrm{cut}}) \cdot \nabla(F_2 + F_{2,\mathrm{cut}}) + R, \tag{3.38}$$

with

$$\begin{aligned}
R &= \frac{1}{4}\sum_{j=1}^{N} \Delta\big(\chi(|x_j|)\vec{b}_j\big) \cdot \Big(|x_j|^2 \frac{x_j}{|x_j|}\Big) \\
&\quad + \frac{1}{2}\sum_{j=1}^{N}\sum_{i=1}^{3} \nabla_j\big(\chi(|x_j|)\vec{b}_{j,i}\big) \cdot \nabla_j\Big(|x_j|^2 \frac{x_{j,i}}{|x_j|}\Big) \\
&\quad + \frac{1}{4}\sum_{1\le j<k\le N} \Delta\big(\chi(|x_j - x_k|)\vec{b}_{(j,k)}\big) \cdot \Big(\Big|\frac{x_j - x_k}{\sqrt{2}}\Big|^2 \frac{x_j - x_k}{|x_j - x_k|}\Big) \\
&\quad + \frac{1}{2}\sum_{j<k}\sum_{i=1}^{3} \nabla_j\big(\chi(|x_j - x_k|)\vec{b}_{(j,k),i}\big) \cdot \nabla_j\Big(\Big|\frac{x_j - x_k}{\sqrt{2}}\Big|^2 \frac{x_{j,i} - x_{k,i}}{|x_j - x_k|}\Big) \\
&\quad + \sum_{j=1}^{N} \vec{b}_j \cdot \frac{x_j}{|x_j|}\big(1 - \chi(|x_j|)\big) \\
&\quad + \sum_{1\le j<k\le N} \vec{b}_{(j,k)} \cdot \frac{x_j - x_k}{|x_j - x_k|}\big(1 - \chi(|x_j - x_k|)\big).
\end{aligned}$$

From (3.36) and the support properties of $\chi$, we see that

$$\|R\|_{C^{0,1}(B_{3N}(\mathbf{x}_0,\rho))} \le C, \tag{3.39}$$

for some constant $C$ independent of $\mathbf{x}_0 \in \mathbb{R}^{3N}$ and $\rho > 0$.

Define

$$G_{3,\mathrm{cut}} = G_{1,\mathrm{cut}} + G_{2,\mathrm{cut}} \tag{3.40}$$

with

$$\begin{aligned}
G_{2,\mathrm{cut}} &= \hat{\mu}_{\mathrm{cut}} + \hat{\kappa}_{1,\mathrm{cut}} + \hat{\nu}_{\mathrm{cut}}, \\
\hat{\mu}_{\mathrm{cut}}(\mathbf{x}) &= -\frac{1}{6}\Big(\sum_{j=1}^{N} \frac{Z^2}{4}\mu_{\mathrm{cut}}(x_j) + \sum_{1\le j<k\le N} \frac{1}{16}\mu_{\mathrm{cut}}(x_j - x_k)\Big), \\
\hat{\kappa}_{1,\mathrm{cut}}(\mathbf{x}) &= \frac{Z}{4}\sum_{1\le j<k\le N} \kappa_{1,\mathrm{cut}}(x_j, x_k), \\
\hat{\nu}_{\mathrm{cut}}(\mathbf{x}) &= -\frac{1}{8}\sum_{1\le j<k<l\le N} \nu_{\mathrm{cut}}(x_j, x_k, x_l).
\end{aligned}$$

Then, with $K_{3,\mathrm{cut}}$ defined as in (3.23), we have, using (3.38), (3.27), (3.33), (3.28), (3.35), (3.4),

$$\begin{aligned}\Delta K_{3,\mathrm{cut}} &= |\nabla F_2|^2 - |\nabla F_{2,\mathrm{cut}}|^2 - \Gamma_1 - \Gamma_2 - \Gamma_3 + r_{\mathrm{cut}} \\ &= -|\nabla F_{2,\mathrm{cut}}|^2 + r_{\mathrm{cut}},\end{aligned} \tag{3.41}$$

where, due to (3.27), (3.33), (3.39), (3.29),

$$\|r_{\mathrm{cut}}\|_{C^{\alpha}(B_{3N}(\mathbf{x}_0,\rho))} \leq C, \tag{3.42}$$

for some constant $C = C(\rho) > 0$ independent of $\mathbf{x}_0 \in \mathbb{R}^{3N}$.

Also, using (3.40), (3.27), (3.29), (3.37) and (3.34),

$$\|G_{3,\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,\rho))} \leq C, \tag{3.43}$$

for some constant $C$ independent of $\mathbf{x}_0 \in \mathbb{R}^{3N}$ and $\rho > 0$. Now, (3.24) follows from (3.42) and (3.43). This finishes the proof of Lemma 3.1'. □

Let $K_{3,\mathrm{cut}}$ be the function constructed in Lemma 3.1' above. Define (see (3.23), (1.19), and (1.22))

$$\zeta_{3,\mathrm{cut}} = e^{-F_{2,\mathrm{cut}} - K_{3,\mathrm{cut}}}\psi = e^{-G_{3,\mathrm{cut}}}\phi_{3,\mathrm{cut}}. \tag{3.44}$$

Note that for all $\rho > 0$ (using Lemma 3.1'),

$$\|F_{3,\mathrm{cut}} - K_{3,\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,\rho))} = \|G_{3,\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,\rho))}$$

and this quantity is bounded independently of $\mathbf{x}_0$. Hence proving (1.24) is equivalent to showing that

$$\|\zeta_{3,\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,R))} \leq C(R)\|\zeta_{3,\mathrm{cut}}\|_{L^{\infty}(B_{3N}(\mathbf{x}_0,2R))}. \tag{3.45}$$

Using that $\zeta_{3,\mathrm{cut}} = e^{-G_{3,\mathrm{cut}}}\phi_{3,\mathrm{cut}}$, the estimate (3.24) (twice), and the bound (1.25), we get, for all $0 < \rho < \rho'$,

$$\|\zeta_{3,\mathrm{cut}}\|_{C^{1,\alpha}(B_{3N}(\mathbf{x}_0,\rho))} \leq C\|\zeta_{3,\mathrm{cut}}\|_{L^{\infty}(B_{3N}(\mathbf{x}_0,\rho'))}, \tag{3.46}$$

with $C = C(\rho, \rho')$. Proving (3.45) is improving (3.46) to $\alpha = 1$.

The function $\zeta_{3,\mathrm{cut}}$ satisfies the equation

$$\begin{aligned}&\Delta\zeta_{3,\mathrm{cut}} + 2\big(\nabla F_{2,\mathrm{cut}} + \nabla K_{3,\mathrm{cut}}\big)\cdot\nabla\zeta_{3,\mathrm{cut}} \\ &+ \big(\Delta F_{2,\mathrm{cut}} + \Delta K_{3,\mathrm{cut}} + |\nabla F_{2,\mathrm{cut}} + \nabla K_{3,\mathrm{cut}}|^2 + (E - V)\big)\zeta_{3,\mathrm{cut}} = 0.\end{aligned}$$

We can rewrite this as

$$\begin{aligned}\Delta\zeta_{3,\mathrm{cut}} + 2\nabla F_{2,\mathrm{cut}}\cdot\big(\nabla\zeta_{3,\mathrm{cut}} + \zeta_{3,\mathrm{cut}}\nabla K_{3,\mathrm{cut}}\big)& \\ + r_{1,\mathrm{cut}}\cdot\nabla\zeta_{3,\mathrm{cut}} + r_{2,\mathrm{cut}}\zeta_{3,\mathrm{cut}} &= 0,\end{aligned} \tag{3.47}$$

with (since $\Delta F_2 = V$ and $\Delta K_{3,\mathrm{cut}} = -|\nabla F_{2,\mathrm{cut}}|^2 + r_{\mathrm{cut}}$)

$$\begin{aligned}r_{1,\mathrm{cut}} &= 2\nabla K_{3,\mathrm{cut}}, \\ r_{2,\mathrm{cut}} &= \Delta F_{2,\mathrm{cut}} + r_{\mathrm{cut}} + |\nabla K_{3,\mathrm{cut}}|^2 + (E - V) \\ &= \Delta(F_{2,\mathrm{cut}} - F_2) + r_{\mathrm{cut}} + |\nabla K_{3,\mathrm{cut}}|^2 + E.\end{aligned}$$

By the construction of $F_2$ and $F_{2,\mathrm{cut}}$ (see (1.9), (1.18), and (1.20)) it is clear that for all $\rho > 0$,

$$\|\Delta(F_{2,\mathrm{cut}} - F_2)\|_{C^\alpha(B_{3N}(\mathbf{x}_0,\rho))} \leq C,$$

with $C = C(\rho)$ independent of $\mathbf{x}_0 \in \mathbb{R}^{3N}$. Due to Lemma 3.1' (see also (1.18)), $\nabla K_{3,\mathrm{cut}}$ is $C^\alpha$, and we have for all $\rho > 0$,

$$\|\nabla K_{3,\mathrm{cut}}\|_{C^\alpha(B_{3N}(\mathbf{x}_0,\rho))} \leq C, \tag{3.48}$$

with $C = C(\rho)$ independent of $\mathbf{x}_0 \in \mathbb{R}^{3N}$. This, together with (3.24), means that

$$\|r_{j,\mathrm{cut}}\|_{C^\alpha(B_{3N}(\mathbf{x}_0,\rho))} \leq C, \qquad j = 1, 2, \tag{3.49}$$

where $C = C(\rho)$ is independent of $\mathbf{x}_0 \in \mathbb{R}^{3N}$.

In order to finish the proof, we introduce a localisation. Let $f : \mathbb{R} \to \mathbb{R},\ 0 \leq f \leq 1$, be decreasing and such that $f(t) = 1$ for $t < 0$ and $f(t) = 0$ for $t > 1$, and define, for $\rho > 0, \lambda > 1$,

$$\theta(x) \equiv \theta_{\rho,\lambda}(x) = f\big(\tfrac{1}{\lambda-1}(\tfrac{|x-x_0|}{\rho} - 1)\big). \tag{3.50}$$

(So $\theta(x) = 1$ on $B_{3N}(x_0, \rho)$ and $\theta(x) = 0$ outside $B_{3N}(x_0, \lambda\rho)$).

Clearly the derivatives of $\theta$ are bounded independently of $\mathbf{x}_0$. Below, all constants $C = C(\rho)$ also depend on $\lambda > 1$; we omit this dependence in the notation. On the set $B_{3N}(\mathbf{x}_0, \rho))$, $\theta\zeta_{3,\mathrm{cut}}$ satisfies the following equation:

$$\begin{aligned}\Delta(\theta\zeta_{3,\mathrm{cut}}) + 2\nabla F_{2,\mathrm{cut}} \cdot \big(\nabla(\theta\zeta_{3,\mathrm{cut}}) + (\theta\zeta_{3,\mathrm{cut}})\nabla K_{3,\mathrm{cut}}\big)& \\ + r_{1,\mathrm{cut}} \cdot \nabla(\theta\zeta_{3,\mathrm{cut}}) + r_{2,\mathrm{cut}}(\theta\zeta_{3,\mathrm{cut}}) = 0.&\end{aligned} \tag{3.51}$$

Using (3.51) we will deduce that

$$\|\theta_{R,\sqrt{2}}\,\zeta_{3,\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,R))} \leq C(R)\|\zeta_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,2R))}, \tag{3.52}$$

from which (3.45) clearly follows (since $\theta \equiv 1$ on $B_{3N}(\mathbf{x}_0, R)$). To prove Theorem 1.5, it therefore remains to prove (3.52).

*Proof of* (3.52). Let $\Psi_{j,i,\mathrm{cut}}$ be defined as $\Psi_{j,i}$ was in (3.12) but with $\zeta_3$, $K_3$ replaced by $\theta\zeta_{3,\mathrm{cut}}$, $K_{3,\mathrm{cut}}$, that is ($j \in \{1, \ldots, N\}$, $i \in \{1, 2, 3\}$),

$$\Psi_{j,i,\mathrm{cut}} = 2\frac{\partial(\theta\zeta_{3,\mathrm{cut}})}{\partial x_{j,i}} + 2(\theta\zeta_{3,\mathrm{cut}})\frac{\partial K_{3,\mathrm{cut}}}{\partial x_{j,i}}. \tag{3.53}$$

(Here, $\theta \equiv \theta_{R,\sqrt{2}}$). We define $\hat{\Psi}_{j,i,\mathrm{cut}}$, $\Phi_{(j,k),i,\mathrm{cut}}$ analogously to $\hat{\Psi}_{j,i}$, $\Phi_{(j,k),i}$ defined in (3.14) and (3.15). Using (3.48) and (3.46) we get that for all $0 < \rho < \rho'$,

$$\begin{aligned}\big\|\Psi_{j,i,\mathrm{cut}}\big\|_{C^\alpha(B_{3N}(\mathbf{x}_0,\rho))} &\leq C(\rho)\|\theta\zeta_{3,\mathrm{cut}}\|_{C^{1,\alpha}(B_{3N}(\mathbf{x}_0,\rho))} \\ &\leq C(\rho, \rho', R)\|\zeta_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,\rho'))}.\end{aligned} \tag{3.54}$$

We then have the following result, similar to Lemma 3.4:

**Lemma 3.4'.** *Let* $u_{j,i,\mathrm{cut}}$, $v_{(j,k),i,\mathrm{cut}}$ *be the solutions to Eqs.* (3.16), (3.17) *(with* $\hat{\Psi}_{j,i}$, $\Phi_{(j,k),i}$ *replaced by* $\hat{\Psi}_{j,i,\mathrm{cut}}$, $\Phi_{(j,k),i,\mathrm{cut}}$*) given by the Newton potential on* $B_{3N}(\mathbf{x}_0, \sqrt{2}R)$*.*

*Then, for all* $\rho < \sqrt{2}R < \rho'$*, there exists a constant* $C = C(\rho, \rho', R)$ *(independent of* $\mathbf{x}_0 \in \mathbb{R}^{3N}$*) such that*

$$\|u_{j,i}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,\rho))} \leq C\|\zeta_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,\rho'))}, \tag{3.55}$$

$$\|v_{(j,k),i}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,\rho))} \leq C\|\zeta_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,\rho'))}. \tag{3.56}$$

*Proof.* Using Theorem 2.6 and Remark 2.7 (iv) and (v), we get the *a priori* estimate

$$\begin{aligned}\|u_{j,i,\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,\rho))} \leq C\Big( \sup\left|\frac{x_{j,i}}{|x_j|}\right| \, \|\hat{\Psi}_{j,i,\mathrm{cut}}\|_{C^\alpha(\pi_{3N-3}B_{3N}(\mathbf{x}_0,\sqrt{2}R))} \\ + \Big(\sup_{\pi_{3N-3}B_{3N}(\mathbf{x}_0,\sqrt{2}R))} |\hat{\Psi}_{j,i,\mathrm{cut}}|\Big)\left\|\frac{x_{j,i}}{|x_j|}\right\|_{C^\alpha(\mathbb{S}^2)}\Big).\end{aligned} \tag{3.57}$$

Using (3.53) and (3.48) we have

$$\begin{aligned}\|\hat{\Psi}_{j,i,\mathrm{cut}}\|_{C^\alpha(\pi_{3N-3}B_{3N}(\mathbf{x}_0,\sqrt{2}R))} &\leq \|\Psi_{j,i,\mathrm{cut}}\|_{C^\alpha((\pi_{3N-3}B_{3N}(\mathbf{x}_0,\sqrt{2}R))\times\mathbb{R}^3)} \\ &\leq C\|\theta\zeta_{3,\mathrm{cut}}\|_{C^{1,\alpha}((\pi_{3N-3}B_{3N}(\mathbf{x}_0,\sqrt{2}R))\times\mathbb{R}^3)}.\end{aligned}$$

This, the compact support of $\theta$, and (3.57) implies the estimate

$$\|u_{j,i,\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,\rho))} \leq C\,\|\zeta_{3,\mathrm{cut}}\|_{C^{1,\alpha}(B_{3N}(\mathbf{x}_0,\sqrt{2}R))}. \tag{3.58}$$

Combining (3.58) and (3.46), we arrive at (3.55). This finishes the proof of the estimate (3.55) for $u_{j,i,\mathrm{cut}}$.

The analogous estimate (3.56) for $v_{(j,k),i,\mathrm{cut}}$ is proved in the same manner using the same coordinate transformation as in the proof of Lemma 3.4 (see also the proof of Lemma 3.5' below). We omit the details. □

**Lemma 3.5'.** *Let* $\Psi_{j,i,\mathrm{cut}}$ *be defined by* (3.53) *and let* $\hat{\Psi}_{j,i,\mathrm{cut}}$ *and* $\Phi_{(j,k),i,\mathrm{cut}}$ *be defined by* (3.14) *and* (3.15) *(with* $\Psi_{j,i}$ *replaced by* $\Psi_{j,i,\mathrm{cut}}$*). Then the functions defined by* (3.18) *and* (3.19) *(again, with an extra index* 'cut'*) belong to* $C^\alpha(\mathbb{R}^{3N})$ *for all* $\alpha \in (0, 1)$*. Furthermore, for any* $\rho < \sqrt{2}R < \rho'$*, their* $C^\alpha$*-norms on the ball* $B_{3N}(\mathbf{x}_0, \rho)$ *are bounded by*

$$C\|\zeta_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,\rho'))} \tag{3.59}$$

*with* $C = C(\rho, \rho', R)$ *independent of* $\mathbf{x}_0 \in \mathbb{R}^{3N}$*.*

*Proof.* That the functions belong to $C^\alpha(\mathbb{R}^{3N})$ for all $\alpha \in (0, 1)$ follows like in the proof of Lemma 3.5.

To prove the bounds on the norms it suffices, by Lemma 2.9 and the triangle inequality, to prove them for

$$\left\|\Psi_{k,i,\mathrm{cut}}\right\|_{C^\alpha(B_{3N}(\mathbf{x}_0,\rho))} \quad \text{and} \quad \left\|\Phi_{(j,k),i,\mathrm{cut}})\right\|_{C^\alpha(B_{3N}(\mathbf{x}_0,\rho))}.$$

For $\Psi_{k,i,\mathrm{cut}}$, the estimate follows from (3.54).

To bound $\Phi_{(j,k),i,\mathrm{cut}}$, denote by $t_{j,k} : \mathbb{R}^{3N} \to \mathbb{R}^{3N}$ the linear transformation (see also (3.15)),

$$t_{j,k}(\mathbf{x}) = (x_1, \dots, x_{j-1}, \tfrac{1}{2}(x_j + x_k), x_{j+1}, \dots, x_{k-1}, \tfrac{1}{2}(x_j + x_k), x_{k+1}, \dots, x_N),$$

so that

$$\Phi_{(j,k),i,\mathrm{cut}}(\mathbf{x}) = \Psi_{j,i,\mathrm{cut}}(t_{j,k}(\mathbf{x})) - \Psi_{k,i,\mathrm{cut}}(t_{j,k}(\mathbf{x})).$$

Then, since $|t_{j,k}(\mathbf{z})| \leq |\mathbf{z}|$,

$$\frac{\big|\Phi_{(j,k),i,\mathrm{cut}}(\mathbf{x}) - \Phi_{(j,k),i,\mathrm{cut}}(\mathbf{y})\big|}{|\mathbf{x}-\mathbf{y}|^\alpha} \leq \frac{\big|\Psi_{j,i,\mathrm{cut}}(t_{j,k}(\mathbf{x})) - \Psi_{j,i,\mathrm{cut}}(t_{j,k}(\mathbf{y}))\big|}{|t_{j,k}(\mathbf{x}) - t_{j,k}(\mathbf{y})|^\alpha} + \frac{\big|\Psi_{k,i,\mathrm{cut}}(t_{j,k}(\mathbf{x})) - \Psi_{k,i,\mathrm{cut}}(t_{j,k}(\mathbf{y}))\big|}{|t_{j,k}(\mathbf{x}) - t_{j,k}(\mathbf{y})|^\alpha}. \tag{3.60}$$

Due to the localisation $\theta$ in the definition of $\Psi_{k,i,\mathrm{cut}}$ (see (3.53)), both of the terms on the RHS of (3.60) are bounded by

$$C(\rho)\|\zeta_{3,\mathrm{cut}}\|_{C^{1,\alpha}(B_{3N}(\mathbf{x}_0,\sqrt{2}R))}.$$

The bound (3.59) for $\Phi_{(j,k),i,\mathrm{cut}}$ now follows using (3.46). This finishes the proof of the bound (3.59) for the functions $(\Psi_{j,i,\mathrm{cut}} - \Psi_{k,i,\mathrm{cut}}) - \Phi_{(j,k),i,\mathrm{cut}}$.

The proof for the functions $\Psi_{j,i,\mathrm{cut}} - \hat{\Psi}_{j,i,\mathrm{cut}}$ is similar (see also the proof of Lemma 3.4' above), so we omit the details. □

To finish the proof of Theorem 1.5, define $U_{\mathrm{cut}}$ analogously to (3.20), using the functions $u_{j,i,\mathrm{cut}}$, $v_{(j,k),i,\mathrm{cut}}$ from Lemma 3.4'. Then, by Lemma 3.4', for any $\rho < \sqrt{2}R < \rho'$,

$$\Delta U_{\mathrm{cut}} = \sum_{j=1}^N \frac{Z}{2}\frac{x_j}{|x_j|} \cdot \hat{\Psi}_{j,\mathrm{cut}} - \sum_{1\leq j<k\leq N} \frac{1}{4}\frac{x_j - x_k}{|x_j - x_k|} \cdot \Phi_{(j,k),\mathrm{cut}}, \tag{3.61}$$

$$\|U_{\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,\rho))} \leq C\|\zeta_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,\rho'))}. \tag{3.62}$$

Define ($\theta \equiv \theta_{R,\sqrt{2}}$)

$$W_{\mathrm{cut}} = \theta\zeta_{3,\mathrm{cut}} - U_{\mathrm{cut}}, \tag{3.63}$$

then, using (3.51), (3.53), (3.61), and the form of $\nabla F_2$ (see (3.3)), we get the following equation for $W_{\mathrm{cut}}$:

$$\begin{aligned}\Delta W_{\mathrm{cut}} = &-\frac{Z}{2}\sum_{j=1}^N \frac{x_j}{|x_j|} \cdot \Big\{\Psi_{j,\mathrm{cut}} - \hat{\Psi}_{j,\mathrm{cut}}\Big\} \\ &- \frac{1}{4}\sum_{1\leq j<k\leq N} \frac{x_j - x_k}{|x_j - x_k|} \cdot \Big\{\big(\Psi_{j,\mathrm{cut}} - \Psi_{k,\mathrm{cut}}\big) - \Phi_{(j,k),\mathrm{cut}}\Big\} \\ &+ \sum_{j=1}^N \nabla_j\big(F_2 - F_{2,\mathrm{cut}}\big) \cdot \Psi_{j,\mathrm{cut}} \\ &- \Big\{r_{1,\mathrm{cut}} \cdot \nabla(\theta\zeta_{3,\mathrm{cut}}) + r_{2,\mathrm{cut}}(\theta\zeta_{3,\mathrm{cut}})\Big\} \equiv \Lambda.\end{aligned} \tag{3.64}$$

Here, $\Lambda$ belongs to $C^\alpha$ for all $\alpha \in (0,1)$, and, for all $\rho < \sqrt{2}R < \rho'$,

$$\|\Lambda\|_{C^\alpha(B_{3N}(\mathbf{x}_0,\rho))} \leq C\|\zeta_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,\rho'))} \tag{3.65}$$

with $C = C(\rho,\rho',R)$ independent of $\mathbf{x}_0 \in \mathbb{R}^{3N}$. For the first two terms in (3.64) this follows from Lemma 3.5'. For the third term, it follows using the form of $F_2 - F_{2,\mathrm{cut}}$ (see (1.9), (1.18), and (1.20)) and (3.54). For the last term we use (3.49) and (3.46).

By Proposition 2.4 this means that $W_{\mathrm{cut}}$ belongs to $C^{2,\alpha}$, and we have the estimate

$$\begin{aligned}\|W_{\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,R))} &\leq \|W_{\mathrm{cut}}\|_{C^{2,\alpha}(B_{3N}(\mathbf{x}_0,R))} \\ &\leq C(R)\big(\|W_{\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,\sqrt[3]{2}R))} + \|\Lambda\|_{C^\alpha(B_{3N}(\mathbf{x}_0,\sqrt[3]{2}R))}\big).\end{aligned} \tag{3.66}$$

Using (3.63), the triangle inequality, and then (3.62) (with $\rho = \sqrt[3]{2}R$ and $\rho' = 2R$), we have

$$\|W_{\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,\sqrt[3]{2}R))} \leq C(R)\|\zeta_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,2R))}.$$

This, (3.66), and (3.65) with $\rho = \sqrt[3]{2}R$ and $\rho' = 2R$, gives the estimate

$$\|W_{\mathrm{cut}}\|_{C^{1,1}(B_{3N}(\mathbf{x}_0,R))} \leq C(R)\|\zeta_{3,\mathrm{cut}}\|_{L^\infty(B_{3N}(\mathbf{x}_0,2R))}. \tag{3.67}$$

Using $\theta\zeta_{3,\mathrm{cut}} = W_{\mathrm{cut}} + U_{\mathrm{cut}}$, (3.62) (with $\rho = R$ and $\rho' = 2R$) and (3.67), the estimate (3.52) follows. □

This finishes the proof of Theorem 1.5. □

## A. Construction of the Function $\kappa$

In this appendix we construct the function $\kappa$ that gives rise to the terms of order $r^2\ln(r)$ in the function $K_3$ solving $\Delta K_3 = -|\nabla F_2|^2$ (see the previous section, Remark 3.3 in particular). Therefore, $\kappa$ is responsible for the $C^{1,\alpha}$-singularities in the wavefunction $\psi$.

More precisely, we prove the following:

**Lemma A.1.** *Let the function $\gamma_2 : \mathbb{R}^6 \to \mathbb{R}$ be given by*

$$\gamma_2(x,y) = \Big(\frac{x}{|x|} - \frac{y}{|y|}\Big)\cdot\frac{x-y}{|x-y|} \quad , \quad x,y \in \mathbb{R}^3. \tag{A.1}$$

*Then there exists a function $\kappa : \mathbb{R}^6 \to \mathbb{R}$ of the form*

$$\begin{aligned}\kappa(x,y) &= \frac{2-\pi}{3\pi}\,(x\cdot y)\ln(x^2+y^2) + (x^2+y^2)\,G_{\kappa_1}\Big(\frac{(x,y)}{|(x,y)|}\Big) \\ &\equiv k(x,y) + \kappa_1(x,y) \quad , \quad G_{\kappa_1} \in C^{1,1}(\mathbb{S}^5)\end{aligned} \tag{A.2}$$

*satisfying $\Delta\kappa = \gamma_2$.*

*Remark A.1.* Note that by Lemma 2.10, $\kappa_1 \in C^{1,1}(\mathbb{R}^6)$.

*Proof.* Recall that $\mathfrak{h}_2^{(6)} = \mathrm{Ran}(\mathcal{P}_2^{(6)})$ is given by the linear span of the harmonic, homogeneous polynomials of degree 2 in $\mathbb{R}^6$ restricted to $\mathbb{S}^5$.

By Lemma C.1 we have that

$$(\mathcal{P}_2^{(6)}\gamma_2)(r\omega) = c_1 \frac{x \cdot y}{x^2 + y^2} \quad , \quad c_1 = \frac{16(2-\pi)}{3\pi},$$

where $r^2 = x^2 + y^2$, $\omega = (x, y)/r \in \mathbb{S}^5$. Let $k(x, y) = \frac{c_1}{16}(x \cdot y)\ln(x^2 + y^2)$. Then

$$\big(\Delta_x + \Delta_y\big)k(x, y) = c_1 \frac{x \cdot y}{x^2 + y^2} = (\mathcal{P}_2^{(6)}\gamma_2)(r\omega).$$

Letting $\kappa_1 = \kappa - k$ this reduces the problem (of finding $\kappa$ such that $(\Delta_x + \Delta_y)\kappa = \gamma_2$) to finding $\kappa_1$ such that

$$(\Delta_x + \Delta_y)\kappa_1 = \hat{\gamma}_2 \tag{A.3}$$

with

$$\hat{\gamma}_2 = \gamma_2 - c_1 \frac{x \cdot y}{x^2 + y^2}. \tag{A.4}$$

Due to the above,

$$(\mathcal{P}_2^{(6)}\hat{\gamma}_2)(r\omega) = 0.$$

Therefore, by Proposition 2.8, there exists a solution $\kappa_1$ to (A.3) such that $\kappa_1(r\omega) = r^2 G_{\kappa_1}(\omega)$, with $G_{\kappa_1} \in C^{1,\alpha}(\mathbb{S}^5)$ for all $\alpha \in (0, 1)$.

To verify (A.2) we need to prove that in fact $G_{\kappa_1} \in C^{1,1}(\mathbb{S}^5)$. We will do this by proving that $\kappa_1 \in C^{1,1}(\mathbb{R}^6 \setminus \{0\})$, since then $G_{\kappa_1} = \kappa_1/r^2 \in C^{1,1}(\mathbb{S}^5)$.

To prove $\kappa_1 \in C^{1,1}(\mathbb{R}^6 \setminus \{0\})$, we analyze Eq. (A.3) for $\kappa_1$ in the vicinity of singular points of the function $\hat{\gamma}_2$ on the sphere $\mathbb{S}^5$. There are two types of singular points: (a) $(x_0, x_0) \in \mathbb{S}^5$, (b) $(0, y_0) \in \mathbb{S}^5$ (resp. $(x_0, 0) \in \mathbb{S}^5$). The function $\kappa_1$ is $C^\infty$ in a neighbourhood of all other points on $\mathbb{S}^5$ due to Proposition 2.4 (since, for $r > 0$, $\hat{\gamma}_2$ is $C^\infty$ away from points of type (a) and (b), see (A.1) and (A.4)).

(a) Let $U_a \subset \mathbb{R}^6$ be a neighbourhood of a point $(x_0, x_0) \in \mathbb{S}^5$ (i.e., $2|x_0|^2 = 1$) such that for some $c > 0$, $|x| \geq c$, $|y| \geq c$ for $(x, y) \in U_a$. Choose new coordinates: Let

$$(x_1, x_2) = t(x, y) = (x - y, x + y).$$

Then

$$\big(\gamma_2 \circ t^{-1}\big)(x_1, x_2) = \frac{x_1}{|x_1|} \cdot \left(\frac{x_1 - x_2}{|x_1 - x_2|} + \frac{x_1 + x_2}{|x_1 + x_2|}\right) \equiv \frac{x_1}{|x_1|} \cdot G_a(x_1, x_2)$$

with $G_a \in C^\infty\big(t(U_a)\big)$. Since $G_a(0, x_2) = 0$ for $x_2 \neq 0$ (that is, for $x = y \neq 0$ in the original coordinates), we have, by Lemma 2.9, that $\gamma_2 \circ t^{-1} \in C^{0,1}\big(t(U_a)\big)$, and therefore $\gamma_2 \in C^{0,1}(U_a) \subset C^\alpha(U_a)$ for all $\alpha \in (0, 1)$. Since $(x \cdot y)/(x^2 + y^2) \in C^\infty(U_a)$, we have (see (A.4)) $\hat{\gamma}_2 \in C^\alpha(U_a)$ for all $\alpha \in (0, 1)$. By Proposition 2.4 we get from (A.3) that $\kappa_1 \in C^{2,\alpha}(U_a)$.

(b) Let $U_b \subset \mathbb{R}^6$ be a neighbourhood of a point $(0, y_0) \in \mathbb{S}^5$ (i.e., $|y_0| = 1$) such that for some $c > 0$, $|y| \geq c$, $|x - y| \geq c$ for $(x, y) \in U_b$. Then

$$\begin{aligned}\gamma_2(x, y) &= \Big(\frac{x}{|x|} - \frac{y}{|y|}\Big) \cdot \frac{x-y}{|x-y|} \\ &= -\frac{x}{|x|} \cdot \frac{y}{|y|} + \frac{x}{|x|} \cdot \Big(\frac{y}{|y|} - \frac{y-x}{|y-x|}\Big) - \frac{y}{|y|} \cdot \frac{x-y}{|x-y|}.\end{aligned}$$

Note that

$$-\frac{y}{|y|} \cdot \frac{x-y}{|x-y|} \in C^\infty(U_b)$$

and that

$$\frac{x}{|x|} \cdot \Big(\frac{y}{|y|} - \frac{y-x}{|y-x|}\Big) \equiv \frac{x}{|x|} \cdot G_b(x, y),$$

with $G_b \in C^\infty(U_b)$, $G_b(0, y) = 0$ for $y \neq 0$. Therefore, by Lemma 2.9 and (A.4),

$$\hat{\gamma}_2(x, y) - \Big(-\frac{x}{|x|} \cdot \frac{y}{|y|}\Big) \in C^{0,1}(U_b) \subset C^\alpha(U_b) \text{ for all } \alpha \in (0, 1).$$

Let $\kappa_2$ be such that

$$\big(\Delta_x + \Delta_y\big)\kappa_2 = -\frac{x}{|x|} \cdot \frac{y}{|y|} \quad , \quad \kappa_2 \in C^{1,1}(U_b).$$

The existence of such a function is ensured by Theorem 2.6, since $y \neq 0$ for $(x, y) \in U_b$, and $\mathcal{P}_2^{(3)}\big(\frac{x}{|x|}\big) = 0$ due to the anti-symmetry of $\frac{x}{|x|}$.

Then (see (A.3)) $\kappa_3 = \kappa_1 - \kappa_2$ solves

$$\big(\Delta_x + \Delta_y\big)\kappa_3 = \hat{\gamma}_2(x, y) - \Big(-\frac{x}{|x|} \cdot \frac{y}{|y|}\Big) \in C^\alpha(U_b) \text{ for all } \alpha \in (0, 1),$$

so by elliptic regularity $\kappa_3 \in C^{2,\alpha}(U_b) \subset C^{1,1}(U_b)$. Since $\kappa_2 \in C^{1,1}(U_b)$, this proves $\kappa_1 = \kappa_2 + \kappa_3 \in C^{1,1}(U_b)$. Together with $\kappa_1 \in C^{2,\alpha}(U_a)$ from above, this implies $G_{\kappa_1} = \kappa_1/r^2 \in C^{1,1}(\mathbb{S}^5)$, and so $\kappa_1 = r^2 G_{\kappa_1} \in C^{1,1}(\mathbb{R}^6)$.

This finishes the proof of the existence of $\kappa$ solving (3.6), and having the form (A.2), with $G = G_{\kappa_1}$.

## B. Construction of the Function $\nu$

In this appendix we construct a function $\nu$ solving (3.7).

**Lemma B.1.** *There exists a solution* $\nu = \nu(x, y, z)$ *to Eq.* (3.7) *satisfying*

(i) $\nu$ *is invariant under cyclic permutation, i.e.,* $\nu(x, y, z) = (\nu \circ \sigma)(x, y, z)$ *for all* $x, y, z \in \mathbb{R}^3$, *where* $\sigma(x, y, z) = (z, x, y)$.
(ii) $\nu \in C^{1,1}(\mathbb{R}^9)$.

The idea is to change coordinates, to the centre-of-mass frame for $(x, y, z)$. In these new coordinates, the problem of solving (3.7) turns out to reduce to a problem in 6 variables only. By an extra symmetry of the function $\gamma_3$ (see (3.5)), namely permutation of the three electron-coordinates $x$, $y$, and $z$, the logarithmic term that occured in the function $\kappa$ (see (A.2)) does not occur here. This is because the projection on $\mathfrak{h}_2^{(6)}$ of $\tilde{\gamma}_3$ (the function that $\gamma_3$ transforms into in the new coordinates, see (B.2) below) vanishes, due to this extra symmetry.

*Proof.* Make the following change of coordinates (each entry below is a diagonal $3 \times 3$-matrix with the listed number in the diagonal; we will use this notation repeatedly; here, $x, y, z \in \mathbb{R}^3$)

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \mathcal{T}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \tag{B.1}$$

Then

$$\begin{aligned}&\big(\gamma_3 \circ \mathcal{T}\big)(x_1, x_2, x_3) = \\ &\frac{x_2}{|x_2|}\cdot\frac{x_2+\sqrt{3}x_3}{|x_2+\sqrt{3}x_3|} + \frac{x_2}{|x_2|}\cdot\frac{x_2-\sqrt{3}x_3}{|x_2-\sqrt{3}x_3|} - \frac{x_2+\sqrt{3}x_3}{|x_2+\sqrt{3}x_3|}\cdot\frac{x_2-\sqrt{3}x_3}{|x_2-\sqrt{3}x_3|} \\ &\equiv \tilde{\gamma}_3(x_1, x_2, x_3).\end{aligned} \tag{B.2}$$

That $\tilde{\gamma}_3$ is independent of $x_1$ is the fact that $\gamma_3$ only depends on the inter-electron coordinates ($x - y$, $y - z$, $z - x$ respectively), and not on the centre-of-mass coordinate ($x_{CM} = \frac{1}{\sqrt{3}}(x + y + z) = x_1$).

The function $\gamma_3$ is invariant under cyclic permutation of the electron-coordinates $x$, $y$ and $z$, that is, $\big(\gamma_3 \circ \sigma\big)(x, y, z) = \gamma_3(x, y, z)$ for all $x, y, z \in \mathbb{R}^3$ with $\sigma(x, y, z) = (z, x, y)$. This gives that

$$\big(\tilde{\gamma}_3 \circ \mathcal{R}\big)(x_1, x_2, x_3) = \tilde{\gamma}_3(x_1, x_2, x_3) \text{ for all } x_1, x_2, x_3 \in \mathbb{R}^3, \tag{B.3}$$

with $\mathcal{R}$ the orthogonal transformation given by $\mathcal{R} = \mathcal{T}^{-1} \circ \sigma \circ \mathcal{T}$, that is by the $9 \times 9$-matrix (again, each entry is a diagonal $3 \times 3$-matrix)

$$\mathcal{R} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\frac{2\pi}{3}) & \sin(\frac{2\pi}{3}) \\ 0 & -\sin(\frac{2\pi}{3}) & \cos(\frac{2\pi}{3}) \end{pmatrix}.$$

Note that $\mathcal{R}$ is a rotation of $(x_2, x_3)$ by $\frac{2\pi}{3}$ around $x_1$ (all in $\mathbb{R}^9$), that is, $\mathcal{R}^3 = I_9$, where $I_9$ is the identity on $\mathbb{R}^9$.

Define the function $\bar{\gamma}_3$ by

$$\bar{\gamma}_3(x_2, x_3) = \tilde{\gamma}_3(x_1, x_2, x_3) \quad , \quad (x_2, x_3) \in \mathbb{R}^6 \tag{B.4}$$

(since $\tilde{\gamma}_3$ is independent of $x_1$, this is well defined). Then, due to (B.3),

$$\big(\bar{\gamma}_3 \circ \bar{\mathcal{R}}\big)(x_2, x_3) = \bar{\gamma}_3(x_2, x_3) \text{ for all } x_2, x_3 \in \mathbb{R}^3, \tag{B.5}$$

with (each entry still being a diagonal $3 \times 3$-matrix)

$$\bar{\mathcal{R}} = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} = \begin{pmatrix} \cos(\frac{2\pi}{3}) & \sin(\frac{2\pi}{3}) \\ -\sin(\frac{2\pi}{3}) & \cos(\frac{2\pi}{3}) \end{pmatrix}. \tag{B.6}$$

Observe that if $\bar{\nu} = \bar{\nu}(x_2, x_3)$ solves (for $\bar{\gamma}_3$, see (B.2) and (B.4))

$$\big(\Delta_{x_2} + \Delta_{x_3}\big)\bar{\nu} = \bar{\gamma}_3, \tag{B.7}$$

then trivially the function $\tilde{\nu}$ defined by $\tilde{\nu}(x_1, x_2, x_3) = \bar{\nu}(x_2, x_3)$ solves

$$\big(\Delta_{x_1} + \Delta_{x_2} + \Delta_{x_3}\big)\tilde{\nu} = \tilde{\gamma}_3.$$

Since $\mathcal{T}$ is orthogonal, the function $\nu = \tilde{\nu} \circ \mathcal{T}^{-1}$ will then solve (recall that $\tilde{\gamma}_3 = \gamma_3 \circ \mathcal{T}$) $\big(\Delta_x + \Delta_y + \Delta_z\big)\nu = \gamma_3$, that is, (3.7). The problem of solving (3.7) therefore reduces to solving (B.7).

Observe next that (see (B.2) and (B.4))

$$\bar{\gamma}_3(\mathcal{O}x_2, \mathcal{O}x_3) = \bar{\gamma}_3(x_2, x_3) \text{ for all } \mathcal{O} \in SO(3),\, x_2, x_3 \in \mathbb{R}^3.$$

This and (B.5) gives, by (iii) of Lemma C.2, that $\mathcal{P}_2^{(6)}\bar{\gamma}_3 = 0$ . Therefore, by Proposition 2.8, there exists a solution $\bar{\nu}$ to (B.7) with

$$\bar{\nu}(x_2, x_3) = (x_2^2 + x_3^2)\, G_{\bar{\nu}}\left(\frac{(x_2, x_3)}{|(x_2, x_3)|}\right),$$
$$G_{\bar{\nu}} \in C^{1,\alpha}(\mathbb{S}^5) \text{ for all } \alpha \in (0, 1).$$

We proceed to prove that in fact $G_{\bar{\nu}} \in C^{2,\alpha}(\mathbb{S}^5)$ for all $\alpha \in (0, 1)$. We do this by showing that $\bar{\nu} \in C^{2,\alpha}(\mathbb{R}^6 \setminus \{0\})$, using (B.7) and elliptic regularity (Proposition 2.4).

Note that there are two kinds of singular points of $\bar{\gamma}_3$ on $\mathbb{S}^5$: (a) $x_2 = 0$ (and so $x_3 \neq 0$), (b) $x_2 = \sqrt{3}x_3$ (and so $x_2 \neq 0 \neq x_3$) (resp. $x_2 = -\sqrt{3}x_3$). The function $\bar{\nu}$ (and therefore, $G_{\bar{\nu}}$) is $C^\infty$ in a neighbourhood of all other points on $\mathbb{S}^5$ due to elliptic regularity (Proposition 2.4).

(a) Let $U_a \subset \mathbb{R}^6$ be a neighbourhood of a point $(0, x_3^0) \in \mathbb{S}^5$ (i.e., $x_3^0 \neq 0$), such that for some $c > 0$, $|x_2 + \sqrt{3}x_3| \geq c$, $|x_2 - \sqrt{3}x_3| \geq c$ for $(x_2, x_3) \in U_a$. Note that

$$\bar{\gamma}_3(x_2, x_3) = \frac{x_2}{|x_2|} \cdot \left(\frac{x_2 + \sqrt{3}x_3}{|x_2 + \sqrt{3}x_3|} + \frac{x_2 - \sqrt{3}x_3}{|x_2 - \sqrt{3}x_3|}\right) - \frac{x_2 + \sqrt{3}x_3}{|x_2 + \sqrt{3}x_3|} \cdot \frac{x_2 - \sqrt{3}x_3}{|x_2 - \sqrt{3}x_3|}. \tag{B.8}$$

Write

$$\frac{x_2}{|x_2|} \cdot \left(\frac{x_2 + \sqrt{3}x_3}{|x_2 + \sqrt{3}x_3|} + \frac{x_2 - \sqrt{3}x_3}{|x_2 - \sqrt{3}x_3|}\right) \equiv \frac{x_2}{|x_2|} \cdot G_a(x_2, x_3),$$

where $G_a \in C^\infty(U_a)$, $G_a(0, x_3) = 0$. Furthermore,

$$\frac{x_2 + \sqrt{3}x_3}{|x_2 + \sqrt{3}x_3|} \cdot \frac{x_2 - \sqrt{3}x_3}{|x_2 - \sqrt{3}x_3|} \in C^\infty(U_a).$$

Therefore, due to Lemma 2.9, $\bar{\gamma}_3 \in C^{0,1}(U_a) \subset C^\alpha(U_a)$ for all $\alpha \in (0, 1)$, and so, by (B.7) and elliptic regularity (Proposition 2.4), $\bar{\nu} \in C^{2,\alpha}(U_a)$.

(b) Let $U_b$ be a neighbourhood of a point $(x_2^0, x_3^0) \in \mathbb{S}^5$ with $x_2^0 = \sqrt{3}x_3^0$ (i.e., $x_2^0 \neq 0 \neq x_3^0$), such that for some $c > 0$, $|x_2| \geq c$, $|x_2 + \sqrt{3}x_3| \geq c$ for $(x_2, x_3) \in U_b$. Choose new coordinates: Let

$$(u, v) = \tau(x_2, x_3) = (x_2 - \sqrt{3}x_3, x_2 + \sqrt{3}x_3).$$

Then

$$\big(\bar{\gamma}_3 \circ \tau^{-1}\big)(u, v) = \frac{u}{|u|} \cdot \left(\frac{u+v}{|u+v|} - \frac{v}{|v|}\right) + \frac{u+v}{|u+v|} \cdot \frac{v}{|v|}.$$

We proceed as above. Write

$$\frac{u}{|u|} \cdot \left(\frac{u+v}{|u+v|} - \frac{v}{|v|}\right) \equiv \frac{u}{|u|} \cdot G_b(u, v),$$

where $G_b \in C^\infty\big(\tau(U_b)\big)$ (since $v \neq 0, u + v \neq 0$ in $\tau(U_b)$), $G_b(0, v) = 0$ for $v \neq 0$. Furthermore,

$$\frac{u+v}{|u+v|} \cdot \frac{v}{|v|} \in C^\infty(U_b).$$

Lemma 2.9 implies that $\bar{\gamma}_3 \circ \tau^{-1} \in C^{0,1}\big(\tau(U_b)\big)$, and so $\bar{\gamma}_3 \in C^{0,1}(U_b) \subset C^\alpha(U_b)$ for all $\alpha \in (0, 1)$. By (B.7) and elliptic regularity (Proposition 2.4) follows that $\bar{\nu} \in C^{2,\alpha}(U_b)$.

Singular points of the form $x_2^0 = -\sqrt{3}x_3^0$ are treated analogously.

From the above follows that $\bar{\nu} \in C^{2,\alpha}(\mathbb{R}^6 \setminus \{0\})$, and therefore $G_{\bar{\nu}} \in C^{2,\alpha}(\mathbb{S}^5)$, for all $\alpha \in (0, 1)$.

This finishes the construction of a function $\bar{\nu} \in C^{1,1}(\mathbb{R}^6)$ that solves (B.7), and has the form

$$\bar{\nu}(x_2, x_3) = (x_2^2 + x_3^2)\, G_{\bar{\nu}}\left(\frac{(x_2, x_3)}{|(x_2, x_3)|}\right), \qquad G_{\bar{\nu}} \in C^{2,\alpha}(\mathbb{S}^5) \text{ for all } \alpha \in (0, 1). \tag{B.9}$$

As discussed above $\overline{\nu}$ defines a function $\nu$ solving Eq. (3.7). Clearly, since $\overline{\nu} \in C^{1,1}(\mathbb{R}^6)$, we get $\nu \in C^{1,1}(\mathbb{R}^9)$. The solution $\nu$ constructed in this manner does not necessarily satisfy the invariance property (i). In order to force this invariance, we consider

$$\nu_{\text{sym}} = \frac{1}{3}\sum_{j=1}^{3}(\nu \circ \sigma^j)(x, y, z).$$

Since the Laplace operator commutes with $\sigma$, and $\gamma_3$ is invariant under $\sigma$, $\nu_{\text{sym}}$ satisfies the conclusion of Lemma B.1. □

With the notation from the proof of Lemma B.1, we define

$$\overline{\nu}_{\text{cut}}(x_2, x_3) = \chi(x_2^2 + x_3^2)\, \overline{\nu}(x_2, x_3),$$

with $\chi$ as in (1.18), and $\tilde{\nu}_{\text{cut}}(x_1, x_2, x_3) \equiv \overline{\nu}_{\text{cut}}(x_2, x_3)$ (as already defined). As discussed above (for $\nu$) the function $\tilde{\nu}_{\text{cut}}$ defines a function $\nu_{\text{cut}} = \tilde{\nu}_{\text{cut}} \circ \mathcal{T}^{-1} : \mathbb{R}^9 \to \mathbb{R}$ (by the linear transformation $\mathcal{T}$ in (B.1)). We then get:

**Lemma B.2.** *The function* $\nu_{\rm cut}$ *satisfies*

$$\Delta \nu_{\rm cut} = \gamma_3 + h,$$

*with* $\gamma_3$ *as in* (3.5) *and* $h \in C^{\alpha}(\mathbb{R}^9)$ *for all* $\alpha \in (0,1)$. *Furthermore, we have the estimate*

$$\|\nu_{\rm cut}\|_{C^{1,1}(B_9((x_0,y_0,z_0),R))} + \|h\|_{C^{\alpha}(B_9((x_0,y_0,z_0),R))} \leq C, \tag{B.10}$$

*with* $C$ *independent of* $(x_0, y_0, z_0) \in \mathbb{R}^9$ *and* $R > 0$.

*Proof.* We calculate, using (B.7),

$$\begin{aligned}\big(\Delta_{x_1} + \Delta_{x_2} + \Delta_{x_3}\big)\tilde{\nu}_{\rm cut} &= \big(\Delta_{x_2} + \Delta_{x_3}\big)\overline{\nu}_{\rm cut} \equiv \Delta\overline{\nu}_{\rm cut}\\ &= \overline{\gamma}_3 + \big\{(\Delta\chi)\overline{\nu} + 2\nabla\chi\cdot\nabla\overline{\nu}\big\} - (1-\chi)\overline{\gamma}_3\\ &\equiv \tilde{\gamma}_3 + \tilde{h}.\end{aligned}$$

Using (B.8) and (B.9) we see that the term in $\{\cdot\}$ is $C^{\alpha}$ and has compact support. The function $(1-\chi)\overline{\gamma}_3$ is $C^{\alpha}$ (this was proved in the proof of Lemma B.1) and homogeneous of degree zero outside $B_6(0,2)$. Therefore,

$$\|\tilde{h}\|_{C^{\alpha}(B_9((x_1^0,x_2^0,x_3^0),R))} \leq C,$$

with $C$ independent of $(x_1^0, x_2^0, x_3^0) \in \mathbb{R}^9$ and $R > 0$. Since $\chi$ has compact support, and $\overline{\nu} \in C^{1,1}(\mathbb{R}^6)$, we have

$$\|\tilde{\nu}_{\rm cut}\|_{C^{1,1}(B_9((x_1^0,x_2^0,x_3^0),R))} \leq C,$$

with $C$ independent of $(x_1^0, x_2^0, x_3^0) \in \mathbb{R}^9$ and $R > 0$.

Since $\mathcal{T}$ is an orthogonal transformation, (B.10) follows. This finishes the proof of the lemma. □

## C. Computation of $\mathcal{P}_2^{(6)}\gamma_2$

In this appendix we compute $\mathcal{P}_2^{(6)}\gamma_2$, the singular part of the two-particle terms in $|\nabla F_2|^2$, see (3.4) and (3.5). This is Lemma C.1 below. It follows from general results on $\mathcal{P}_2^{(6)}\eta$ when $\eta$ has certain symmetry-properties (Lemma C.2). The latter is also responsible for the non-occurrence of terms of order $r^2\ln(r)$ (of regularity $C^{1,\alpha}$ only) in the function $\nu$ constructed in the previous appendix; see Lemma B.1.

**Lemma C.1.** *Let*

$$\gamma_2(x,y) = \Big(\frac{x}{|x|} - \frac{y}{|y|}\Big)\cdot\frac{x-y}{|x-y|}, \quad (x,y)\in\mathbb{R}^3\times\mathbb{R}^3. \tag{C.1}$$

*Then*

$$\big(\mathcal{P}_2^{(6)}\gamma_2\big)(x,y) = \frac{16(2-\pi)}{3\pi}\,\frac{x\cdot y}{x^2+y^2}, \quad (x,y)\in\mathbb{R}^3\times\mathbb{R}^3.$$

*Proof.* This will follow from Lemma C.2 and Lemma C.3 below. Namely, by (i) and (ii) in Lemma C.2 we get that, due to symmetry,

$$\big(\mathcal{P}_2^{(6)}\gamma_2\big)(x,y) = c_1\,\frac{x\cdot y}{x^2+y^2} \;\text{ for some }\; c_1\in\mathbb{R},$$

that is, only the function $x\cdot y$ (restricted to $\mathbb{S}^5$) contributes to the projection onto $\mathfrak{h}_2^{(6)}$ of the function $\gamma_2$ in (C.1). That $c_1 = \frac{16(2-\pi)}{3\pi}$ is the result of Lemma C.3 (which is merely two computations). □

**Lemma C.2.** *Assume $\eta\in L^2(\mathbb{S}^5)$ satisfies*

$$\eta(\mathcal{O}x,\mathcal{O}y) = \eta(x,y) \tag{C.2}$$

*for all $\mathcal{O}\in SO(3)$ and almost all $(x,y)\in\mathbb{S}^5\subset\mathbb{R}^3\times\mathbb{R}^3$. Let $\mathcal{Q}_1$ be the orthogonal projection (in $L^2(\mathbb{S}^5)$) onto*

$$\operatorname{Span}\left\{P_1|_{\mathbb{S}^5}\,,\;P_2|_{\mathbb{S}^5}\right\},$$

*and $\mathcal{Q}_2$ the orthogonal projection onto*

$$\operatorname{Span}\left\{P_1|_{\mathbb{S}^5}\right\},$$

*where $P_1(x,y)=x\cdot y$, $P_2(x,y)=x^2-y^2$, $(x,y)\in\mathbb{R}^3\times\mathbb{R}^3$.*

*Then*

(i) $\mathcal{P}_2^{(6)}\eta = \mathcal{Q}_1\eta$.

(ii) *Let $\eta$ satisfy*

$$\eta(x,y)=\eta(y,x)\text{ for almost all }(x,y)\in\mathbb{S}^5\subset\mathbb{R}^3\times\mathbb{R}^3. \tag{C.3}$$

*Then $\mathcal{P}_2^{(6)}\eta=\mathcal{Q}_2\eta$.*

(iii) *Let $\bar{\mathcal{R}}$ be as in* (B.6). *Assume $\eta$ satisfies*

$$\eta(\bar{\mathcal{R}}(x,y))=\eta(x,y)\text{ for almost all }(x,y)\in\mathbb{S}^5\subset\mathbb{R}^3\times\mathbb{R}^3. \tag{C.4}$$

*Then $\mathcal{P}_2^{(6)}\eta=0$.*

*Proof of Lemma C.2* . Suppose (i) is proven then the proofs of (ii) and (iii) are simple:

*Proof of* (ii) . Due to (i) we only need to prove that

$$\int_{\mathbb{S}^5}\eta(x,y)(x^2-y^2)\,d\omega = 0.$$

This follows using the symmetry (C.3) of $\eta$ (which preserves the measure $d\omega$ of $\mathbb{S}^5$):

$$\int_{\mathbb{S}^5}\eta(x,y)P(x,y)\,d\omega = \frac{1}{2}\int_{\mathbb{S}^5}\eta(x,y)\big(P(y,x)+P(x,y)\big)\,d\omega,$$

and when $P(x,y)=P_2(x,y)=x^2-y^2$, then $P(y,x)+P(x,y)=0$. This proves (ii). □

*Proof of* (iii). Using (i) and (C.4) it is enough to show that

$$P(x,y) + P(\bar{\mathcal{R}}(x,y)) + P(\bar{\mathcal{R}}^2(x,y)) = 0,$$

when $P(x,y) = x \cdot y$ or $x^2 - y^2$ (since $\bar{\mathcal{R}}$ preserves the measure $d\omega$ of $\mathbb{S}^5$). This follows by direct calculation. □

It remains to prove (i):

*Proof of* (i). Recall that $\mathfrak{h}_2^{(6)} = \mathrm{Ran}(\mathcal{P}_2^{(6)})$. Define $\mathfrak{h}_{2,inv}$ by

$$\mathfrak{h}_{2,inv} = \mathrm{Span}\left\{ f \in \mathfrak{h}_2^{(6)} \,\middle|\, f(\mathcal{O}x, \mathcal{O}y) = f(x,y) \text{ for all } \mathcal{O} \in SO(3) \right\}.$$

Note that $\mathcal{P}_2^{(6)}\eta \in \mathfrak{h}_{2,inv}$ because of (C.2). We need to prove that

$$\mathfrak{h}_{2,inv} = \mathrm{Span}\left\{ P_1|_{\mathbb{S}^5},\ P_2|_{\mathbb{S}^5} \right\}.$$

Since every function in $\mathfrak{h}_{2,inv}$ can be written as a finite sum of spherical harmonics of degree 2 it suffices to consider a real, harmonic polynomial $P$ which is homogeneous of degree 2, and which is invariant under the action of $SO(3)$:

$$P(\mathcal{O}x, \mathcal{O}y) = P(x,y) \text{ for all } \mathcal{O} \in SO(3). \tag{C.5}$$

Identifying $P$ with a quadratic form on $\mathbb{R}^6$, there exist real symmetric matrices $A$, $B$, and $C$, such that

$$P(x,y) = x \cdot Ax + y \cdot By + x \cdot Cy. \tag{C.6}$$

The condition of harmonicity of $P$ becomes $\mathrm{Tr}[A+B] = 0$. We prove that $A$, $B$, and $C$ have to be multiples of the identity matrix $I_3$ on $\mathbb{R}^3$. To do so, let us first restrict to $x = 0$. Using (C.5) and (C.6) we get

$$y \cdot By = P(0,y) = P(\mathcal{O}0, \mathcal{O}y) = \mathcal{O}y \cdot B\mathcal{O}y,$$

for all $\mathcal{O} \in SO(3)$. Let $\lambda$ be a (real) eigenvalue of $B$, with corresponding eigenvector $v$: $Bv = \lambda v$. Let $y$ be any vector in $\mathbb{R}^3$. Then there exists an $\mathcal{O}_y \in SO(3)$ such that $\mathcal{O}_y y = \mu_y v$ for some $\mu_y \in \mathbb{R}$, and therefore $y \cdot By = \mathcal{O}_y y \cdot B\mathcal{O}_y y = \lambda \|y\|^2$. Since this is true for all $y \in \mathbb{R}^3$, we get $B = \lambda I_3$. A similar argument (with $y = 0$, and letting $x$ vary) shows that also $A$ is a multiple of the identity. Finally, the condition of harmonicity, $\mathrm{Tr}[A+B] = 0$, implies that $A = -B = -\lambda I_3$.

Finally the term $x \cdot Cy$. This will be treated similarly. Due to the above (see (C.6)), $x \cdot Cy = P(x,y) - \lambda(y^2 - x^2)$. Therefore, (C.5) implies

$$x \cdot Cy = \mathcal{O}x \cdot C\mathcal{O}y \quad \text{for all } \mathcal{O} \in SO(3).$$

By arguments similar to the above, we find that $C$ is also a multiple of the identity $I_3$. Since $P(x,y) = \lambda(x^2 - y^2) + x \cdot Cy$, this finishes the proof of (i). □

This finishes the proof of Lemma C.2. □

**Lemma C.3.** *Let $\mathcal{Q}_2$ be the orthogonal projection (in $L^2(\mathbb{S}^5)$) onto*

$$\mathrm{Span}\left\{ P_1|_{\mathbb{S}^5} \right\} \quad , \quad P_1(x,y) = x \cdot y \quad , \quad (x,y) \in \mathbb{R}^3 \times \mathbb{R}^3,$$

*and let*

$$\gamma_2(x,y) = \left( \frac{x}{|x|} - \frac{y}{|y|} \right) \cdot \frac{x-y}{|x-y|}, \quad (x,y) \in \mathbb{R}^3 \times \mathbb{R}^3.$$

*Then*

$$\mathcal{Q}_2\gamma_2 = c_1 \frac{x \cdot y}{x^2 + y^2}, \quad c_1 = \frac{16(2-\pi)}{3\pi}. \tag{C.7}$$

*Proof.* Note that, with

$$Y(\omega) = \frac{P_1|_{\mathbb{S}^5}(\omega)}{\| \, P_1|_{\mathbb{S}^5} \, \|_{L^2(\mathbb{S}^5)}}, \quad \omega = \frac{(x,y)}{\sqrt{x^2+y^2}},$$

we have $\|Y\|_{L^2(\mathbb{S}^5)} = 1$, and so

$$\begin{aligned} \mathcal{Q}_2\gamma_2(\omega) &= Y(\omega) \int_{\mathbb{S}^5} Y(\omega)\gamma_2(\omega)\, d\omega \\ &= \left\{ \frac{1}{\| \, P_1|_{\mathbb{S}^5} \, \|^2_{L^2(\mathbb{S}^5)}} \cdot \int_{\mathbb{S}^5} P_1|_{\mathbb{S}^5}(\omega)\, \gamma_2(\omega)\, d\omega \right\} \cdot \frac{x \cdot y}{x^2+y^2}. \end{aligned} \tag{C.8}$$

We need to compute the two integrals in the brackets.

Since $P_1$ is homogeneous of order 2 and $\gamma_2$ of order 0 (as functions on $\mathbb{R}^6$), we have

$$\int_{B_6(0,R)} P_1(x,y)\gamma_2(x,y)\, dx\, dy = \frac{R^8}{8} \int_{\mathbb{S}^5} P_1|_{\mathbb{S}^5}(\omega)\, \gamma_2(\omega)\, d\omega.$$

Therefore,

$$\int_{\mathbb{S}^5} P_1|_{\mathbb{S}^5}(\omega)\, \gamma_2(\omega)\, d\omega = 8 \int_{B_6(0,1)} P_1(x,y)\gamma_2(x,y)\, dx\, dy. \tag{C.9}$$

Choose coordinates $(|x|, |y|, |x-y|, \Omega)$ for $\mathbb{R}^6$ (with $\Omega$ three necessary angles). Note that

$$P_1(x,y) = x \cdot y = \frac{1}{2}\left(|x|^2 + |y|^2 - |x-y|^2\right) \quad , \quad (x,y) \in \mathbb{R}^3 \times \mathbb{R}^3,$$

and

$$\gamma_2(x,y) = \frac{|x|+|y|}{|x-y|}\left(1 - \frac{|x|^2 + |y|^2 - |x-y|^2}{2|x||y|}\right), \; (x,y) \in \mathbb{R}^3 \times \mathbb{R}^3.$$

Then (see Hylleraas [12, (45d)]; let $s = |x|, t = |y|, r = |x - y|$)

$$\int_{B_6(0,1)} P_1(x,y)\gamma_2(x,y)\,dx\,dy = \frac{1}{4}\Big(\int d\Omega\Big) \times$$
$$\times \int_0^1 \int_0^{\sqrt{1-s^2}} \int_{|s-t|}^{s+t} (s^2+t^2-r^2)(s+t)\big(2st - (s^2+t^2-r^2)\big)\,dr\,dt\,ds$$
$$= \frac{1}{4}\frac{(2-\pi)}{48}\int d\Omega. \tag{C.10}$$

Using (C.9) and (C.10) this means that

$$\int_{\mathbb{S}^5} P_1|_{\mathbb{S}^5}(\omega)\,\gamma_2(\omega)\,d\omega = \frac{2-\pi}{24}\int d\Omega. \tag{C.11}$$

Next, observe that, again due to homogeneity, we have

$$\int_{B_6(0,R)} (x\cdot y)^2\,dx\,dy = \frac{R^{10}}{10}\,\big\|P_1\big|_{\mathbb{S}^5}\big\|^2_{L^2(\mathbb{S}^5)}$$

and so

$$\big\|P_1\big|_{\mathbb{S}^5}\big\|^2_{L^2(\mathbb{S}^5)} = 10\int_{B_6(0,1)} (x\cdot y)^2\,dx\,dy. \tag{C.12}$$

Since $x\cdot y = \frac{1}{2}\big(|x|^2+|y|^2-|x-y|^2\big)$ we get (using coordinates as above)

$$\int_{B_6(0,1)} (x\cdot y)^2\,dx\,dy$$
$$= \frac{1}{4}\Big(\int d\Omega\Big)\int_0^1 \int_0^{\sqrt{1-s^2}} \int_{|s-t|}^{s+t} \big(s^2+t^2-r^2\big)^2 srt\,dr\,dt\,ds$$
$$= \frac{\pi}{1280}\int d\Omega.$$

This means (see (C.12)) that

$$\big\|P_1\big|_{\mathbb{S}^5}\big\|^2_{L^2(\mathbb{S}^5)} = \frac{\pi}{128}\int d\Omega. \tag{C.13}$$

Now (C.7) follows from (C.8), (C.11), and (C.13). This finishes the proof of Lemma C.3. □

*Acknowledgement.* All four authors thank the organizers of the program *Partial Differential Equations and Spectral Theory* for invitations to the Mittag-Leffler Institute in 2002 where part of the work was done. Furthermore, parts of this work have been carried out at various institutions, whose hospitality is gratefully acknowledged: Aalborg University (SF, MHO, THO), The Erwin Schrödinger Institute (TØS), Université Paris-Sud (TØS), and the IHÉS (TØS). Financial support from the Danish Natural Science Research Council, European Science Foundation Programme *Spectral Theory and Partial Differential Equations* (SPECT), and EU IHP network *Postdoctoral Training Program in Mathematical Analysis of Large Quantum Systems*, contract no. HPRN-CT-2002-00277 is gratefully acknowledged.

SF has been supported by a Marie Curie Fellowship of the European Community Programme 'Improving the Human Research Potential and the Socio-Economic Knowledge Base' under contract number HPMF-CT-2002-01822, and by a grant from the Carlsberg Foundation.

Finally, SF and TØS wish to thank I. Herbst for useful discussions at the Mittag-Leffler Institute.

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Communicated by B. Simon