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REAL ANALYTICITY AWAY FROM THE NUCLEUS OF PSEUDORELATIVISTIC HARTREE–FOCK ORBITALS

ANNA DALL'ACQUA, SØREN FOURNAIS,
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We prove that the Hartree–Fock orbitals of pseudorelativistic atoms, that is, atoms where the kinetic energy of the electrons is given by the pseudorelativistic operator $\sqrt{-\Delta + 1} - 1$, are real analytic away from the origin. As a consequence, the quantum mechanical ground state of such atoms is never a Hartree–Fock state.

Our proof is inspired by the classical proof of analyticity by nested balls of Morrey and Nirenberg. However, the technique has to be adapted to take care of the nonlocal pseudodifferential operator, the singularity of the potential at the origin, and the nonlinear terms in the equation.

1. Introduction and results

In [Dall'Acqua et al. 2008], three of the present authors studied the Hartree–Fock model for pseudorelativistic atoms, and proved the existence of Hartree–Fock minimizers. Furthermore, they proved that the corresponding Hartree–Fock orbitals (solutions to the associated Euler–Lagrange equation) are smooth away from the nucleus, and that they decay exponentially. In this paper we prove that all of these orbitals are, in fact, real analytic away from the origin. Apart from intrinsic mathematical interest, analyticity of solutions has important consequences. For example, in the nonrelativistic case, the analyticity of the orbitals was used in [Friesecke 2003; Lewin 2004a] to prove that the quantum mechanical ground state is never a Hartree–Fock state (or, more generally, is never a finite linear combination of Slater determinants). A direct consequence of our main regularity result is that this also holds in the pseudorelativistic case. Our proof also shows that any $H^{1/2}$-solution $\varphi : \mathbb{R}^3 \to \mathbb{C}$ to the nonlinear equation

$$(\sqrt{-\Delta + 1})\varphi - \frac{Z}{|\cdot|}\varphi \pm \big(|\varphi|^2 * |\cdot|^{-1}\big)\varphi = \lambda\varphi \tag{1}$$

which is smooth away from $x = 0$, is in fact real analytic there. As will be clear from the proof, our method yields the same result for solutions to equations of the form

$$(-\Delta + m)^s \varphi + V\varphi + |\varphi|^k \varphi = \lambda\varphi, \tag{2}$$

where V has a finite number of point singularities (but is analytic elsewhere), under certain conditions on m, s, V, and k (see Remark 1.2 below). We believe this result is of independent interest, but stick concretely to the case of pseudorelativistic Hartree–Fock orbitals, since this was the original motivation for the present work.

We consider a model for an atom with N electrons and nuclear charge Z (fixed at the origin), where the kinetic energy of the electrons is described by the expression $\sqrt{(|\boldsymbol{p}|c)^2 + (mc^2)^2} - mc^2$. This model takes into account some (kinematic) relativistic effects; in units where $\hbar = e = m = 1$, the Hamiltonian becomes

$$H = \sum_{j=1}^{N} \alpha^{-1}\{T(-\mathrm{i}\nabla_j) - V(\boldsymbol{x}_j)\} + \sum_{1 \le i < j \le N} \frac{1}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}, \tag{3}$$

with $T(\boldsymbol{p}) = E(\boldsymbol{p}) - \alpha^{-1} = \sqrt{|\boldsymbol{p}|^2 + \alpha^{-2}} - \alpha^{-1}$ and $V(\boldsymbol{x}) = Z\alpha/|\boldsymbol{x}|$. Here, α is Sommerfeld's fine structure constant; physically, $\alpha \simeq 1/137$.

The operator H acts on a dense subspace of the N-particle Hilbert space $\mathscr{H}_F = \wedge_{i=1}^{N} L^2(\mathbb{R}^3)$ of antisymmetric functions. (We will not consider spin since it is irrelevant for our discussion.) It is bounded from below on this subspace if and only if $Z\alpha \le 2/\pi$ (see [Lieb and Yau 1988]; for a number of other works on this operator, see [Carmona et al. 1990; Daubechies and Lieb 1983; Fefferman and de la Llave 1986; Herbst 1977; Lewis et al. 1997; Nardini 1986; Weder 1975; Zhislin and Vugalter 2002]).

The (*quantum*) *ground state energy* is the infimum of the quadratic form q defined by H, over the subset of elements of norm 1 of the corresponding form domain. Hence, it coincides with the infimum of the spectrum of H considered as an operator acting in $\mathscr{H}_F$. A corresponding minimizer is called a (*quantum*) *ground state* of H.

In the Hartree–Fock approximation, instead of minimizing the quadratic form q in the entire N-particle space $\mathscr{H}_F$, one restricts to wavefunctions Ψ which are pure wedge products, also called Slater determinants:

$$\Psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) = \frac{1}{\sqrt{N!}} \det(u_i(\boldsymbol{x}_j))_{i,j=1}^{N}, \tag{4}$$

with $\{u_i\}_{i=1}^{N}$ orthonormal in $L^2(\mathbb{R}^3)$ (called *orbitals*). Notice that this way, $\Psi \in \mathscr{H}_F$ and $\|\Psi\|_{L^2(\mathbb{R}^{3N})} = 1$.

The *Hartree–Fock ground state energy* is the infimum of the quadratic form q defined by H over such Slater determinants:

$$E^{\mathrm{HF}}(N, Z, \alpha) := \inf\{\, \mathsf{q}(\Psi, \Psi) \mid \Psi \text{ Slater determinant}\,\}. \tag{5}$$

Inserting Ψ of the form in (4) into q formally yields

$$\mathscr{E}^{\mathrm{HF}}(u_1, \ldots, u_N) := \mathsf{q}(\Psi, \Psi)$$

$$= \alpha^{-1} \sum_{j=1}^{N} \int_{\mathbb{R}^3} \left\{ \overline{u_j(\boldsymbol{x})}\, [T(-\mathrm{i}\nabla)u_j](\boldsymbol{x}) - V(\boldsymbol{x})|u_j(\boldsymbol{x})|^2 \right\} d\boldsymbol{x}$$

$$+ \frac{1}{2} \sum_{1 \le i,j \le N} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|u_i(\boldsymbol{x})|^2 |u_j(\boldsymbol{y})|^2}{|\boldsymbol{x} - \boldsymbol{y}|}\, d\boldsymbol{x}\, d\boldsymbol{y} - \frac{1}{2} \sum_{1 \le i,j \le N} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\overline{u_j(\boldsymbol{x})}u_i(\boldsymbol{x})\overline{u_i(\boldsymbol{y})}u_j(\boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|}\, d\boldsymbol{x}\, d\boldsymbol{y}. \tag{6}$$

In fact, $u_i \in H^{1/2}(\mathbb{R}^3)$, $1 \le i \le N$, is needed for this to be well-defined (see Section 3 for a detailed discussion), and so (5)–(6) can be written

$$E^{\mathrm{HF}}(N, Z, \alpha) = \inf\{\mathscr{E}^{\mathrm{HF}}(u_1, \ldots, u_N) \mid (u_1, \ldots, u_N) \in \mathcal{M}_N\}, \tag{7}$$

$$\mathcal{M}_N = \left\{ (u_1, \ldots, u_N) \in [H^{1/2}(\mathbb{R}^3)]^N \mid (u_i, u_j) = \delta_{ij} \right\}. \tag{8}$$

Here $(\ ,\ )$ denotes the scalar product in $L^2(\mathbb{R}^3)$. The existence of minimizers for the problem (7)–(8) was proved in [Dall'Acqua et al. 2008] when $Z > N - 1$ and $Z\alpha < 2/\pi$. (Note that such minimizers are generally not unique since $\mathscr{E}^{\mathrm{HF}}$ is not convex; see [Fournais et al. 2009]). The existence of infinitely many distinct critical points of the functional $\mathscr{E}^{\mathrm{HF}}$ on $\mathcal{M}_N$ was proved recently (under the same conditions) in [Enstedt and Melgaard 2009].

The Euler–Lagrange equations of the problem (7)–(8) are the *Hartree–Fock equations*,

$$\big[(T(-i\nabla) - V)\varphi_i\big](\boldsymbol{x}) + \alpha\Big(\sum_{j=1}^N \int_{\mathbb{R}^3} \frac{|\varphi_j(\boldsymbol{y})|^2}{|\boldsymbol{x} - \boldsymbol{y}|}\, d\boldsymbol{y}\Big)\varphi_i(\boldsymbol{x})$$

$$- \alpha \sum_{j=1}^N \Big(\int_{\mathbb{R}^3} \frac{\overline{\varphi_j(\boldsymbol{y})}\varphi_i(\boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|}\, d\boldsymbol{y}\Big)\varphi_j(\boldsymbol{x}) = \varepsilon_i\varphi_i(\boldsymbol{x}), \quad 1 \le i \le N. \tag{9}$$

Here the ε_i are the Lagrange multipliers of the orthonormality constraints in (8). (The naive Euler–Lagrange equations are more complicated than (9), but can be transformed to (9); see [Fournais et al. 2009].) Note that (9) can be reformulated as

$$h_{\boldsymbol{\varphi}}\varphi_i = \varepsilon_i\varphi_i, \quad 1 \le i \le N, \tag{10}$$

with $h_{\boldsymbol{\varphi}}$ the *Hartree–Fock operator associated to* $\boldsymbol{\varphi} = \{\varphi_1, \ldots, \varphi_N\}$, formally given by

$$h_{\boldsymbol{\varphi}}u = [T(-i\nabla) - V]u + \alpha R_{\boldsymbol{\varphi}}u - \alpha K_{\boldsymbol{\varphi}}u, \tag{11}$$

where $R_{\boldsymbol{\varphi}}u$ is the *direct interaction*, given by the multiplication operator defined by

$$R_{\boldsymbol{\varphi}}(\boldsymbol{x}) := \sum_{j=1}^N \int_{\mathbb{R}^3} \frac{|\varphi_j(\boldsymbol{y})|^2}{|\boldsymbol{x} - \boldsymbol{y}|}\, d\boldsymbol{y} \tag{12}$$

and $K_{\boldsymbol{\varphi}}u$ is the *exchange term*, given by the integral operator

$$(K_{\boldsymbol{\varphi}}u)(\boldsymbol{x}) = \sum_{j=1}^N \Big(\int_{\mathbb{R}^3} \frac{\overline{\varphi_j(\boldsymbol{y})}u(\boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|}\, d\boldsymbol{y}\Big)\varphi_j(\boldsymbol{x}). \tag{13}$$

The equations (9) (or equivalently (10)) are called the *self-consistent Hartree–Fock equations*. One has that $\sigma_{\mathrm{ess}}(h_{\boldsymbol{\varphi}}) = [0, \infty)$ and that, when in addition $N < Z$, the operator $h_{\boldsymbol{\varphi}}$ has infinitely many eigenvalues in $[-\alpha^{-1}, 0)$ (see [Dall'Acqua et al. 2008, Lemma 2]; the argument given there holds for any $\boldsymbol{\varphi} = \{\varphi_1, \ldots, \varphi_N\}$, $\varphi_i \in H^{1/2}(\mathbb{R}^3)$, as long as $Z\alpha < 2/\pi$). If $(\varphi_1, \ldots, \varphi_N) \in \mathcal{M}_N$ is a minimizer for

the problem (7)–(8), then the φ_i solve (10) with $\varepsilon_1 \leq \varepsilon_2 \leq \cdots \leq \varepsilon_N < 0$ the N *lowest* eigenvalues of the operator $h_{\boldsymbol{\varphi}}$ [Dall'Acqua et al. 2008].

In [Dall'Acqua et al. 2008] it was proved that solutions $\{\varphi_1, \ldots, \varphi_N\}$ to (9) — and, more generally, all eigenfunctions of the corresponding Hartree–Fock operator $h_{\boldsymbol{\varphi}}$ — are smooth away from $\boldsymbol{x} = 0$ (the singularity of V), and that (for the φ_i for which $\varepsilon_i < 0$) they decay exponentially. (The solutions studied in [Dall'Acqua et al. 2008] came from a minimizer of $\mathscr{E}^{\text{HF}}$, but the proof trivially extends to the solutions $\{\boldsymbol{\varphi}_n\}_{n\in\mathbb{N}} = \{\{\varphi_1^n, \ldots, \varphi_N^n\}\}_{n\in\mathbb{N}}$ to (9) found in [Enstedt and Melgaard 2009], and to all the eigenfunctions of the corresponding Hartree–Fock operators mentioned above). The main theorem of this paper is the following, which completely settles the question of regularity away from the origin of solutions to the equations (9).

Theorem 1.1. *Let $Z\alpha < 2/\pi$, and let $N \geq 2$ be a positive integer such that $N < Z + 1$. Let $\boldsymbol{\varphi} = \{\varphi_1, \ldots, \varphi_N\}$, $\varphi_i \in H^{1/2}(\mathbb{R}^3)$, $i = 1, \ldots, N$, be solutions to the pseudorelativistic Hartree–Fock equations in* (9).

Then, for $i = 1, \ldots, N$,

$$\varphi_i \in C^{\omega}(\mathbb{R}^3 \setminus \{0\}), \tag{14}$$

that is, the Hartree–Fock orbitals are real analytic away from the origin in $\mathbb{R}^3$.

Remark 1.2. (i) The restrictions $Z\alpha < 2/\pi$, $N < Z + 1$, and $N \geq 2$ are only made to ensure *existence* of $H^{1/2}$-solutions to (9). In fact, our proof proves analyticity away from $\boldsymbol{x} = 0$ for $H^{1/2}$-solutions to (9) for *any* $Z\alpha$. For the case $N = 1$, (9) reduces to $(T - V)\varphi = \varepsilon\varphi$ and our result also holds for $H^{1/2}$-solutions to this equation (see also (iv) and (v) below about more general V for which the result also holds for the linear equation). More interestingly, the result also holds for $H^{1/2}$-solutions to (1) (which, strictly speaking, cannot be obtained from (9) by any choice of N).

(ii) The statement also holds for any eigenfunction of the associated Hartree–Fock operator given by (11).

(iii) It is obvious from the proof that the theorem holds true if we include spin.

(iv) As will also be clear from the proof, the statement of Theorem 1.1 (appropriately modified) also holds for molecules. More explicitly, for a molecule with K nuclei of charges $Z_1, \ldots, Z_K$, fixed at $R_1, \ldots, R_K \in \mathbb{R}^3$, replace V in (9) by $\sum_{k=1}^{K} V_k$ with $V_k(\boldsymbol{x}) = Z_k\alpha/|\boldsymbol{x} - R_k|$, $Z_k\alpha < 2/\pi$. Then, for $N < 1 + \sum_{k=1}^{K} Z_k$, Hartree–Fock minimizers exist (see [Dall'Acqua et al. 2008, Remark 1(viii)]), and the corresponding Hartree–Fock orbitals are real analytic away from the positions of the nuclei, i.e., belong to $C^{\omega}(\mathbb{R}^3 \setminus \{R_1, \ldots, R_K\})$.

(v) Another approximation to the full quantum mechanical problem is the *multiconfiguration self-consistent field method* (MC-SCF). Here one minimizes the quadratic form $\mathfrak{q}$ defined by the operator H given in (3) (or, more generally, with V from (iv)) over the set of *finite* sums of Slater determinants instead of only on single Slater determinants as in Hartree–Fock theory. If minimizers exist they satisfy what is called the *multiconfiguration equations* (MC equations). For more details, see [Fournais et al. 2009; Friesecke 2003; Lewin 2004b]. As will be clear from the proof, the statement of Theorem 1.1 also holds for solutions to these equations.

(vi) In fact, for V we only need the analyticity of V away from finitely many points in $\mathbb{R}^3$, and certain integrability properties of $V\varphi_i$ in the vicinity of each of these points, and at infinity; for more details, see Remark 4.1.

(vii) As will be clear from the proof, the statement of Theorem 1.1 also holds for other nonlinearities than the Hartree–Fock term in (9), namely $|\varphi|^k\varphi$ as in (2) (for k even; for k odd, one needs to take φ^{k+1}). The L^p-space in which one needs to study the problem (see Proposition 2.1 and the description of the proof below for details) needs to be chosen depending on k in this case (the larger the k, the larger the p).

(viii) Also, as will be clear from the proof, the result holds if $T(-i\nabla) = |\nabla|$ (i.e., $T(\boldsymbol{p}) = |\boldsymbol{p}|$) in (9). In (35) below, $E(\boldsymbol{p})^{-1}$ should then be replaced by $(|\boldsymbol{p}| + 1)^{-1}$ (and 1 added to $\alpha^{-1} + \varepsilon_i$). The only properties of $E(\boldsymbol{p})^{-1}$ used are in Lemmas C.1 and C.2, which follow also for $(|\boldsymbol{p}| + 1)^{-1}$ from the same methods with minor modifications. Similarly, one can replace $T(\boldsymbol{p})$ with $(-\Delta + \alpha^{-2})^s$, $s \in [1/2, 1]$.

(ix) The result of Theorem 1.1 in the nonrelativistic case ($T(-i\nabla)$ replaced by $-\alpha\Delta$ in (3)) was proved in [Friesecke 2003; Lewin 2004a]; see also the discussion below. In this case, it is furthermore known [Fournais et al. 2009] that, for $\boldsymbol{x} \in B_r(0)$ for some $r > 0$, $\varphi_i(\boldsymbol{x}) = \varphi_i^{(1)}(\boldsymbol{x}) + |\boldsymbol{x}|\varphi_i^{(2)}(\boldsymbol{x})$ with $\varphi_i^{(1)}, \varphi_i^{(2)} \in C^\omega(B_r(0))$.

Combining the argument in [Friesecke 2003; Lewin 2004a] with the analyticity away from the position of the nucleus of solutions to the MC equations (see Remark 1.2(v)) we readily obtain the following result.

Theorem 1.3. *Let* Ψ *be a* (*quantum*) *ground state of the operator* H *given in* (3). *Then* Ψ *is not a* finite *linear combination of Slater determinants.*

Remark 1.4. The same holds with V as in Remark 1.2(iv).

Description of the proof of Theorem 1.1. The proof of Theorem 1.1 is inspired by the standard Morrey–Nirenberg proof of analyticity of solutions to general (linear) elliptic partial differential equations with real analytic coefficients by "nested balls" [Morrey and Nirenberg 1957]. A good presentation of this technique can be found in [Hörmander 1969]. (Other proofs using a complexification of the coordinates also exist and have been applied to both linear and nonlinear equations; see [Morrey 2008] and references therein.)

In [Hörmander 1969] one proves L^2-bounds on derivatives of order k of the solution in a ball B_r (of some radius r) around a given point. These bounds should behave suitably in k in order to make the Taylor series of the solution converge locally, thereby proving analyticity.

The proof of these bounds is inductive. In fact, for some ball B_R with $R > r$, one proves the bounds on all balls B_ρ with $r \le \rho \le R$, with the appropriate (with respect to k) behavior in $R - \rho$. The base of induction is provided by standard elliptic estimates. In the induction step, one has to bound $k + 1$ derivatives of the solution in the ball B_ρ. To do so, one divides the difference $B_R \setminus B_\rho$ into $k+1$ nested balls using $k + 1$ localization functions with successively larger supports. Commuting m of the k derivatives (in the case of an operator of order m) with these localization functions produces (local) differential operators of order $m - 1$, with support in a larger ball. These local commutator terms are controlled by

the induction hypothesis, since they contain one derivative less. For the last term — the term where no commutators occur — one then uses the equation.

This approach poses new technical difficulties in our case, due to the nonlocality of the kinetic energy $T(\boldsymbol{p}) = \sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1}$ and the nonlinearity of the terms $R_{\boldsymbol{\varphi}}\varphi_i$ and $K_{\boldsymbol{\varphi}}\varphi_i$.

The nonlocality of the operator $\sqrt{-\Delta + \alpha^{-2}}$ implies that, as opposed to the case of a differential operator, the commutator of the kinetic energy with a localization function is not localized in the support of the localization function. That is, when resorting to proving analyticity by differentiating the equation, the localization argument described above introduces commutators which are (nonlocal) pseudodifferential operators. Now the induction hypothesis does not provide control of these terms. Furthermore, it is far from obvious that the singularity of the potential V outside B_R does not influence the regularity in B_R of the solution through these operators (or rather, through the nonlocality of $\sqrt{-\Delta + \alpha^{-2}}$). Loosely speaking, the singularity of the nuclear potential can be felt everywhere. (Note that if we would not have a (singular) potential V one could proceed as in [Frank and Lenzmann 2010] and prove global analyticity by showing exponential decay of the solutions in Fourier space.)

We overcome this problem by a new localization argument which enable us to capture in more detail the action of high order derivatives on nested balls (manifested in Lemma B.1 in the appendix). This, together with very explicit bounds on the (smoothing) operators $\phi E(\boldsymbol{p})^{-1} D^{\beta} \chi$ for χ and ϕ with disjoint supports (see Lemma C.2), are the main ingredients in solving the problem of nonlocality. The estimates are on $\phi E(\boldsymbol{p})^{-1} D^{\beta} \chi$ (not $\phi E(\boldsymbol{p}) D^{\beta} \chi$), since we invert $E(\boldsymbol{p})$ (turning the equation into an integral operator equation, see (35)). Our method of proof would also work in the nonrelativistic case, since the integral operators $(-\Delta + 1)^{-1}$ and $E(\boldsymbol{p})^{-1}$ enjoy similar properties.

The second major obstacle is the (morally cubic) nonlinearity of the terms $R_{\boldsymbol{\varphi}}\varphi_i$ and $K_{\boldsymbol{\varphi}}\varphi_i$.

To illustrate the problem, we discuss proving analyticity by the above method (local L^2-estimates) for solutions u to the equation $\Delta u = u^3$. When differentiating this equation (and therefore u^3), the application of Leibniz's rule introduces a sum of terms. After using Hölder's inequality on each term (the product of three factors, each a number of derivatives on u), one needs to use a Sobolev inequality to "get back down to L^2" in order to use the induction hypothesis. Summing the many terms, the needed estimate does not come out (in fact, some Gevrey-regularity would follow, but not analyticity).

In the quadratic case this can be done (that is, for the equation $\Delta u = u^2$ this problem does *not* occur), but in the cubic case, one looses too many derivatives.

The second insight of our proof is that this problem of loss of derivatives may be overcome by characterizing analyticity by growth of derivatives in some L^p with $p > 2$. When working in L^p for $p > 2$, the loss of derivatives in the Sobolev inequality mentioned above is less (as seen in Theorem D.1). Choosing p sufficiently large allows us to prove the needed estimate. The operator estimates on $\phi E(\boldsymbol{p})^{-1} D^{\beta} \chi$ mentioned above therefore have to be L^p-estimates. In fact, using $L^p - L^q$ estimates, one can also deal with the problem that the singularity of the nuclear potential V can be felt everywhere.

Note that taking $p = \infty$ would avoid using a Sobolev inequality altogether (L^∞ being an algebra), but the needed estimates on $\phi E(\boldsymbol{p})^{-1} D^{\beta} \chi$ cannot hold in this case. For local equations an approach to handle the loss of derivatives (due to Sobolev inequalities) exists. This was carried out in [Friedman 1958],

where analyticity of solutions to elliptic partial differential equations with general analytic nonlinearities was proved. Friedman works in spaces of continuous functions. In this approach, one needs to have a sufficiently high degree of regularity of the solution beforehand (it is not proved along the way). Also, since the elliptic regularity in spaces of continuous functions have an inherent loss of derivative, one needs to work on a sufficiently small domain in order for the method to work. We prefer to work in Sobolev spaces since this is the natural setting for our equation and since the needed estimates on the resolvent are readily obtained in these spaces.

For an alternative method of proof (one *fixed* localization function, to the power k, and estimating in a higher order Sobolev space (instead of in L^2) which is also an algebra), see [Kato 1996] (for the equation $\Delta u = u^2$) and [Hashimoto 2006] (for general second order nonlinear analytic PDEs).

Additional technical difficulties occur due to the fact that the cubic terms, $R_\varphi \varphi_i$ and $K_\varphi \varphi_i$, are actually nonlocal.

Note that in the proof that *nonrelativistic* Hartree–Fock orbitals are analytic away from the positions of the nuclei (see [Friesecke 2003; Lewin 2004b]), the nonlinearities are dealt with by cleverly rewriting the Hartree–Fock equations as a system. One introduces new functions $\phi_{i,j} = [\varphi_i \overline{\varphi_j}] * | \cdot |^{-1}$, which satisfy $-\Delta \phi_{i,j} = 4\pi \varphi_i \overline{\varphi_j}$. This eliminates the terms $R_\varphi \varphi_i$, $K_\varphi \varphi_i$, turning these into quadratic products in the functions φ_i, $\phi_{i,j}$, hence one obtains a (quadratic and local) nonlinear system of elliptic second order equations with coefficients analytic away from the positions of the nuclei. The result now follows from the results cited above [Kato 1996; Morrey 2008]. (In fact, this argument extends to solutions of the more general multiconfiguration self-consistent field equations, see [Friesecke 2003; Lewin 2004b].)

This idea cannot readily be extended to our case. The operator $E(\boldsymbol{p})$ is a pseudodifferential operator of first order, so when rewriting the Hartree–Fock equations as described above, one obtains a system of pseudodifferential equations. This system is, as before, of second (differential) order in the auxiliary functions $\phi_{i,j}$, but only of first (pseudodifferential) order in the original functions φ_i. Hence, the leading (second) order matrix is singular elliptic. Hence (even if we ignore the fact that the square root is nonlocal) the above argument does not apply.

To summarize, our approach is as follows. We invert the kinetic energy in the equation for the orbitals thereby obtaining an integral equation to which we apply successive differentiations. The localization argument of Lemma B.1 together with the smoothing estimates on $\phi E(\boldsymbol{p})^{-1} D^\beta \chi$ handle the nonlocality of this equation. By working in L^p for suitably large p one can afford the necessary loss of derivatives from using Sobolev inequalities when treating the nonlinear terms.

2. Proof of analyticity

In order to prove that the φ_i are real analytic in $\mathbb{R}^3 \setminus \{0\}$ it is sufficient, by [Krantz and Parks 2002, Proposition 2.2.10], to prove that for every $\boldsymbol{x}_0 \in \mathbb{R}^3 \setminus \{0\}$ there exists an open set $U \subseteq \mathbb{R}^3 \setminus \{0\}$ containing $\boldsymbol{x}_0$, and constants $\mathscr{C}, \mathscr{R} > 0$, such that (with $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$)

$$|\partial^\beta \varphi_i(\boldsymbol{x})| \le \mathscr{C} \frac{\beta!}{\mathscr{R}^{|\beta|}} \quad \text{for all } \boldsymbol{x} \in U \text{ and all } \beta \in \mathbb{N}_0^3. \tag{15}$$

Let $\boldsymbol{x}_0 \in \mathbb{R}^3 \setminus \{0\}$, and let ω be the ball $B_R(\boldsymbol{x}_0)$ with center $\boldsymbol{x}_0$ and radius $R := \min\{1, |\boldsymbol{x}_0|/4\}$. For $\delta > 0$ we denote by ω_δ the set of points in ω at distance larger than δ from $\partial\omega$, i.e.,

$$\omega_\delta := \{\boldsymbol{x} \in \omega \mid d(\boldsymbol{x}, \partial\omega) > \delta\}. \tag{16}$$

By our choice of ω we have $\omega_\delta = B_{R-\delta}(\boldsymbol{x}_0)$. Therefore $\omega_\delta = \varnothing$ for $\delta \geq R$. In particular, by our choice of R,

$$\omega_\delta = \varnothing \quad \text{for } \delta \geq 1. \tag{17}$$

For $\Omega \subseteq \mathbb{R}^n$ and $p \geq 1$ we let $L^p(\Omega)$ denote the usual L^p-space with norm $\|f\|_{L^p(\Omega)} = \left(\int_\Omega |f(\boldsymbol{x})|^p \, d\boldsymbol{x} \right)^{1/p}$. We write $\|f\|_p \equiv \|f\|_{L^p(\mathbb{R}^3)}$. In the following we equip the Sobolev space $W^{m,p}(\Omega)$, $\Omega \subseteq \mathbb{R}^n$, $m \in \mathbb{N}$ and $p \in [1, \infty)$, with the norm

$$\|u\|_{W^{m,p}(\Omega)} := \sum_{|\sigma| \leq m} \|D^\sigma u\|_{L^p(\Omega)}. \tag{18}$$

Theorem 1.1 follows from the following proposition.

Proposition 2.1. *Let $Z\alpha < 2/\pi$, and let $N \geq 2$ be a positive integer such that $N < Z + 1$. Let $\boldsymbol{\varphi} = \{\varphi_1, \ldots, \varphi_N\}$, $\varphi_i \in H^{1/2}(\mathbb{R}^3)$, $i = 1, \ldots, N$, be solutions to the pseudorelativistic Hartree–Fock equations in (9). Let $\boldsymbol{x}_0 \in \mathbb{R}^3 \setminus \{0\}$, $R = \min\{1, |\boldsymbol{x}_0|/4\}$, and $\omega = B_R(\boldsymbol{x}_0)$. Define $\omega_\delta = B_{R-\delta}(\boldsymbol{x}_0)$ for $\delta > 0$.*

Then for all $p \geq 5$ there exist constants $C, B > 1$ such that for all $j \in \mathbb{N}$, for all $\epsilon > 0$ such that $\epsilon j \leq R/2$, and for all $i \in \{1, \ldots, N\}$ we have

$$\epsilon^{|\beta|} \|D^\beta \varphi_i\|_{L^p(\omega_{\epsilon j})} \leq C B^{|\beta|} \quad \text{for all } \beta \in \mathbb{N}_0^3 \text{ with } |\beta| \leq j. \tag{19}$$

Given Proposition 2.1, the proof that the φ_i are real analytic is standard, using Sobolev embedding. We give the argument here for completeness. We then give the proof of Proposition 2.1 in the next section.

Let $U = B_{R/2}(\boldsymbol{x}_0) = \omega_{R/2} \subseteq \omega$. Using Theorem D.5 and (19) we have $\varphi_i \in C(\overline{U})$. Therefore it suffices to prove (15) for $|\beta| \geq 1$. Fix $i \in \{1, \ldots, N\}$ and consider $\beta \in \mathbb{N}_0^3 \setminus \{0\}$ an arbitrary multiindex. Setting $j = |\beta|$ and $\epsilon = (R/2)/j$ it follows from Proposition 2.1 (since $\epsilon j = R/2$) that there exist constants $C, B > 1$ such that

$$\|D^\beta \varphi_i\|_{L^p(\omega_{R/2})} \leq C \left(\frac{B}{\epsilon} \right)^{|\beta|} = C \left(\frac{2B}{R} \right)^{|\beta|} |\beta|^{|\beta|}, \tag{20}$$

with C, B independent of the choice of β. By Theorem D.5 (see also Remark D.6) there exists a constant $K_4 = K_4(p, \boldsymbol{x}_0)$ such that, for all $\beta' \in \mathbb{N}_0^3 \setminus \{0\}$,

$$\sup_{\boldsymbol{x} \in U} |D^{\beta'} \varphi_i(\boldsymbol{x})| \leq K_4 \sum_{|\sigma| \leq 1} \|D^{\beta'+\sigma} \varphi_i\|_{L^p(\omega_{R/2})} \leq K_4 \sum_{|\sigma| \leq 1} C \left(\frac{2B}{R} \right)^{|\sigma|+|\beta'|} \left(|\sigma| + |\beta'| \right)^{|\sigma|+|\beta'|},$$

using (20). Using that $R \leq 1 \leq B$, that $\#\{\sigma \in \mathbb{N}_0^3 \mid |\sigma| = 1\} = 3$, and that, from (A.7),

$$\left(1 + |\beta'| \right)^{1+|\beta'|} \leq \frac{\mathrm{e}}{\sqrt{2\pi}} \, \mathrm{e}^{2|\beta'|} \, |\beta'|!,$$

this implies that for all $\beta' \in \mathbb{N}_0^3 \setminus \{0\}$,

$$\sup_{\boldsymbol{x} \in U} |D^{\beta'} \varphi_i(\boldsymbol{x})| \leq \Big(\frac{8\mathrm{e}K_4 CB}{\sqrt{2\pi}R}\Big)\Big(\frac{2\mathrm{e}^2 B}{R}\Big)^{|\beta'|} |\beta'|!. \tag{21}$$

Since $|\sigma|! \leq 3^{|\sigma|}\sigma!$ for all $\sigma \in \mathbb{N}_0^3$ (see (A.4) in the appendix), this implies that

$$\sup_{\boldsymbol{x} \in U} |D^{\beta'} \varphi_i(\boldsymbol{x})| \leq \mathscr{C} \frac{\beta'!}{\mathscr{R}^{|\beta'|}}, \tag{22}$$

for some $\mathscr{C}, \mathscr{R} > 0$. This proves (15). Hence φ_i is real analytic in $\mathbb{R}^3 \setminus \{0\}$. This finishes the proof of Theorem 1.1.

It therefore remains to prove Proposition 2.1.

Remark 2.2. We here give explicit choices for the constants C and B in Proposition 2.1.

Let

$$C_1 := \max_{1 \leq a,b \leq N} \Big\| \int_{\mathbb{R}^3} \frac{|\varphi_a(\boldsymbol{y})\varphi_b(\boldsymbol{y})|}{|\cdot - \boldsymbol{y}|} \, d\boldsymbol{y} \Big\|_\infty. \tag{23}$$

Note that by (29) below, this is finite since $\varphi_i \in H^{1/2}(\mathbb{R}^3)$, $i = 1, \dots, N$.

Furthermore, let $A = A(\boldsymbol{x}_0) \geq 1$ be such that, for all $\sigma \in \mathbb{N}_0^3$,

$$\sup_{\boldsymbol{x} \in \omega} |D^\sigma V(\boldsymbol{x})| \leq A^{|\sigma|+1}|\sigma|!. \tag{24}$$

The existence of A follows from the real analyticity in $\omega = B_R(\boldsymbol{x}_0)$ (recall that $R = \min\{1, |\boldsymbol{x}_0|/4\}$) of $V = Z\alpha|\cdot|^{-1}$ (see e.g. [Krantz and Parks 2002, Proposition 2.2.10]). Assume without restriction that $A \geq \alpha^{-1} + \max_{1 \leq i \leq N} |\varepsilon_i|$.

Let $K_1 = K_1(p)$, $K_2 = K_2(p)$, and $K_3 = K_3(p)$ be the constants in Lemma C.1, Corollary D.2, and Corollary D.4, respectively (see Appendices C and D below). Then let

$$C_2 = \max\big\{K_1, 256\sqrt{2}/\pi\big\}, \tag{25}$$

$$C_3 = \max\big\{4\pi(1 + 2C_1/R^2)K_3, 160\pi K_2^2 K_3\big\}. \tag{26}$$

Choose

$$C > \max_{i \in \{1,\dots,N\}} \Big\{1, \|\varphi_i\|_{W^{1,p}(\omega)}, \|\varphi_i\|_{L^{3p}(B_{2R}(\boldsymbol{x}_0))}, \frac{768}{\pi}|\boldsymbol{x}_0|^{3(2-p)/(2p)}\|\varphi_i\|_2,$$
$$\Big[\frac{48\sqrt{2}}{\pi}A + 48\sqrt{2}C_1\frac{N}{Z\pi} + \frac{1536\sqrt{2}}{\pi^2|\boldsymbol{x}_0|}\Big]\|\varphi_i\|_3\Big\}. \tag{27}$$

That $C < \infty$ follows from the smoothness away from $\boldsymbol{x} = 0$ of the φ_i [Dall'Acqua et al. 2008, Theorem 1(ii)] and the fact that, since $\varphi_i \in H^{1/2}(\mathbb{R}^3)$, $1 \leq i \leq N$, we have $\varphi_i \in L^3(\mathbb{R}^3)$, $1 \leq i \leq N$, by Sobolev's inequality. Then choose

$$B > \max\big\{48AC_2, C_*, \frac{16}{|\boldsymbol{x}_0|}, 4C_1^2, (160C^2 K_2 C_3)^2, (24NC_2/Z)^2, 16K_3\big\}, \tag{28}$$

where C_* is the constant (related to a smooth partition of unity) introduced in (B.3). In particular, $B > 48$. We will prove Proposition 2.1 with these choices of C and B.

3. Proof of the main estimate

We first make (6) more precise, thereby also explaining the choice of $\mathcal{M}_N$ in (8). By Kato's inequality [Kato 1995, (5.33) p. 307],

$$\int_{\mathbb{R}^3} \frac{|f(\boldsymbol{x})|^2}{|\boldsymbol{x}|} \, d\boldsymbol{x} \le \frac{\pi}{2} \int_{\mathbb{R}^3} |\boldsymbol{p}| |\hat{f}(\boldsymbol{p})|^2 \, d\boldsymbol{p} \quad \text{for } f \in H^{1/2}(\mathbb{R}^3) \tag{29}$$

(where $\hat{f}(\boldsymbol{p}) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{-i\boldsymbol{x}\cdot\boldsymbol{p}} f(\boldsymbol{x}) \, d\boldsymbol{x}$ denotes the Fourier transform of f), and the KLMN theorem [Reed and Simon 1975, Theorem X.17] the operator h_0 given as

$$h_0 = T(-i\nabla) - V \tag{30}$$

is well-defined on $H^{1/2}(\mathbb{R}^3)$ (and bounded below by $-\alpha^{-1}$) as a form sum when $Z\alpha < 2/\pi$, that is,

$$(u, h_0 v) = (E(\boldsymbol{p})^{1/2} u, E(\boldsymbol{p})^{1/2} v) - \alpha^{-1}(u, v) - (V^{1/2} u, V^{1/2} v) \quad \text{for } u, v \in H^{1/2}(\mathbb{R}^3). \tag{31}$$

By abuse of notation, we write $E(\boldsymbol{p})$ for the (strictly positive) operator $E(-i\nabla) = \sqrt{-\Delta + \alpha^{-2}}$. For $(\varphi_1, \ldots, \varphi_N) \in \mathcal{M}_N$, the function $R_{\boldsymbol{\varphi}}$ given in (12) belongs to $L^\infty(\mathbb{R}^3)$ (using Kato's inequality above), and the operator $K_{\boldsymbol{\varphi}}$ given in (13) is Hilbert–Schmidt (see [Dall'Acqua et al. 2008, Lemma 2]). As a consequence, when $Z\alpha < 2/\pi$, the operator $h_{\boldsymbol{\varphi}}$ in (11) is a well-defined self-adjoint operator with quadratic form domain $H^{1/2}(\mathbb{R}^3)$ such that

$$(u, h_{\boldsymbol{\varphi}} v) = (u, h_0 v) + \alpha(u, R_{\boldsymbol{\varphi}} v) - \alpha(u, K_{\boldsymbol{\varphi}} v) \quad \text{for } u, v \in H^{1/2}(\mathbb{R}^3). \tag{32}$$

Since $(u, R_{\boldsymbol{\varphi}} u) - (u, K_{\boldsymbol{\varphi}} u) \ge 0$ for any $u \in L^2(\mathbb{R}^3)$, also $h_{\boldsymbol{\varphi}}$ is bounded from below by $-\alpha^{-1}$.

Then, for $(u_1, \ldots, u_N) \in \mathcal{M}_N$, the precise version of (6) becomes

$$\mathcal{E}^{\mathrm{HF}}(u_1, \ldots, u_N) = \sum_{j=1}^{N} \alpha^{-1}(u_j, h_0 u_j)$$

$$+ \frac{1}{2} \sum_{1 \le i, j \le N} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u_i(\boldsymbol{x})|^2 |u_j(\boldsymbol{y})|^2}{|\boldsymbol{x} - \boldsymbol{y}|} \, d\boldsymbol{x} \, d\boldsymbol{y} - \frac{1}{2} \sum_{1 \le i, j \le N} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\overline{u_j(\boldsymbol{x})} u_i(\boldsymbol{x}) \overline{u_i(\boldsymbol{y})} u_j(\boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|} \, d\boldsymbol{x} \, d\boldsymbol{y}. \tag{33}$$

The considerations on $R_{\boldsymbol{\varphi}}$ and $K_{\boldsymbol{\varphi}}$ above imply that also the nonlinear terms in (33) are finite for $u_i \in H^{1/2}(\mathbb{R}^3)$, $1 \le i \le N$.

If $(\varphi_1, \ldots, \varphi_N) \in \mathcal{M}_N$ is a critical point of $\mathcal{E}^{\mathrm{HF}}$ in (33), then $\boldsymbol{\varphi} = \{\varphi_1, \ldots, \varphi_N\}$ satisfies the self-consistent HF-equations (10) with the operator $h_{\boldsymbol{\varphi}}$ defined above.

Note that $E(\boldsymbol{p})$ is a bounded operator from $H^{1/2}(\mathbb{R}^3)$ to $H^{-1/2}(\mathbb{R}^3)$, and recall that (29) shows that V also defines a bounded operator from $H^{1/2}(\mathbb{R}^3)$ to $H^{-1/2}(\mathbb{R}^3)$ (for any $Z\alpha$). As noted above, both $R_{\boldsymbol{\varphi}}$ and $K_{\boldsymbol{\varphi}}$ are bounded operators on $L^2(\mathbb{R}^3)$ when $(\varphi_1, \ldots, \varphi_N) \in \mathcal{M}_N$. In particular, this shows that if $(\varphi_1, \ldots, \varphi_N) \in \mathcal{M}_N$ solves (10), then

$$E(\boldsymbol{p})\varphi_i - \alpha^{-1}\varphi_i - V\varphi_i + \alpha R_{\boldsymbol{\varphi}}\varphi_i - \alpha K_{\boldsymbol{\varphi}}\varphi_i = \varepsilon_i \varphi_i, \quad 1 \le i \le N, \tag{34}$$

hold as equations in $H^{-1/2}(\mathbb{R}^3)$. Using that $E(\boldsymbol{p})^{-1}$ is a bounded operator from $H^{-1/2}(\mathbb{R}^3)$ to $H^{1/2}(\mathbb{R}^3)$, this implies that, as equalities in $H^{1/2}(\mathbb{R}^3)$ (and therefore, in particular, in $L^2(\mathbb{R}^3)$),

$$\varphi_i = E(\boldsymbol{p})^{-1} V \varphi_i - \alpha E(\boldsymbol{p})^{-1} R_{\boldsymbol{\varphi}} \varphi_i + \alpha E(\boldsymbol{p})^{-1} K_{\boldsymbol{\varphi}} \varphi_i + (\alpha^{-1} + \varepsilon_i) E(\boldsymbol{p})^{-1} \varphi_i, \quad 1 \le i \le N. \quad (35)$$

Proof of Proposition 2.1. The proof is by induction on $j \in \mathbb{N}_0$. More precisely:

Definition 3.1. For $p \ge 1$ and $j \in \mathbb{N}_0$, let $\mathcal{P}(p, j)$ be the statement:
  For all $\epsilon > 0$ with $\epsilon j \le R/2$, and all $i \in \{1, \dots, N\}$ we have

$$\epsilon^{|\beta|} \| D^\beta \varphi_i \|_{L^p(\omega_{\epsilon j})} \le C \, B^{|\beta|} \quad \text{for all } \beta \in \mathbb{N}_0^3 \text{ with } |\beta| \le j, \quad (36)$$

where $C, B > 1$ are the constants in Remark 2.2.

  Then Proposition 2.1 is equivalent to the statement: For all $p \ge 5$, $\mathcal{P}(p, j)$ holds for all $j \in \mathbb{N}_0$. This is the statement we will prove by induction on $j \in \mathbb{N}_0$.

Base of induction. For convenience, we prove $\mathcal{P}(p, j)$ for both $j = 0$ and $j = 1$. Note that $\mathcal{P}(p, 0)$ trivially holds since (see Remark 2.2)

$$C = C(p) > \max_{1 \le i \le N} \| \varphi_i \|_{L^p(\omega)}. \quad (37)$$

Also $\mathcal{P}(p, 1)$ holds by the choice of C, since

$$C = C(p) > \max_{\substack{1 \le i \le N, \\ \nu \in \{1,2,3\}}} \| D_\nu \varphi_i \|_{L^p(\omega)}. \quad (38)$$

Namely, since $\omega_\epsilon \subseteq \omega$, (36) holds for $|\beta| = 0$ (and *all* $\epsilon > 0$) using (37). For $\beta \in \mathbb{N}_0$ with $|\beta| = 1 = j$ (i.e., $\beta = e_\nu$ for some $\nu \in \{1, 2, 3\}$), and all $\epsilon > 0$ with $\epsilon = \epsilon j \le R/2 < 1$,

$$\epsilon^{|\beta|} \| D^\beta \varphi_i \|_{L^p(\omega_{\epsilon j})} = \epsilon \| D_\nu \varphi_i \|_{L^p(\omega_\epsilon)} \le \| D_\nu \varphi_i \|_{L^p(\omega)} \le C \le C B = C B^{|\beta|}. \quad (39)$$

Here we again used that $\omega_\epsilon \subseteq \omega$, (38), and that $B > 1$ (see Remark 2.2).

Induction hypothesis:

$$\text{Let } p \ge 5 \text{ and } j \in \mathbb{N}_0, \, j \ge 1. \text{ Then } \mathcal{P}(p, \tilde{j}) \text{ holds for all } \tilde{j} \le j. \quad (40)$$

  We now prove that $\mathcal{P}(p, j+1)$ holds. Note that to prove this, it suffices to study $\beta \in \mathbb{N}_0^3$ with $|\beta| = j+1$. Namely, assume $\epsilon > 0$ is such that $\epsilon(j+1) \le R/2$ and let $\beta \in \mathbb{N}_0^3$ with $|\beta| < j+1$. Then $|\beta| \le j$ and $\epsilon j \le R/2$ so, by the definition of ω_δ and the induction hypothesis,

$$\epsilon^{|\beta|} \| D^\beta \varphi_i \|_{L^p(\omega_{\epsilon(j+1)})} \le \epsilon^{|\beta|} \| D^\beta \varphi_i \|_{L^p(\omega_{\epsilon j})} \le C B^{|\beta|}. \quad (41)$$

It therefore remains to prove that

$$\epsilon^{|\beta|} \| D^\beta \varphi_i \|_{L^p(\omega_{\epsilon(j+1)})} \le C \, B^{|\beta|} \quad \text{for all } \epsilon > 0 \text{ with } \epsilon(j+1) \le R/2 \text{ and all } \beta \in \mathbb{N}_0^3 \text{ with } |\beta| = j+1. \quad (42)$$

Remark 3.2. To use the induction hypothesis in its full strength, it is convenient to write, for $\ell > 0$, $\epsilon > 0$ such that $\epsilon \ell \le R/2$, and $\sigma \in \mathbb{N}_0^3$ with $0 < |\sigma| \le j$,

$$\|D^\sigma \varphi_i\|_{L^p(\omega_{\epsilon\ell})} = \|D^\sigma \varphi_i\|_{L^p(\omega_{\tilde{\epsilon}\tilde{j}})} \quad \text{with } \tilde{\epsilon} = \frac{\epsilon\ell}{|\sigma|}, \ \tilde{j} = |\sigma|,$$

so that, by the induction hypothesis (applied on the term with $\tilde{\epsilon}$ and $\tilde{j}$) we get that

$$\|D^\sigma \varphi_i\|_{L^p(\omega_{\epsilon\ell})} \le C\left(\frac{B}{\tilde{\epsilon}}\right)^{|\sigma|} = C\left(\frac{|\sigma|}{\ell}\right)^{|\sigma|}\left(\frac{B}{\epsilon}\right)^{|\sigma|}. \tag{43}$$

Compare this with (36). With the convention that $0^0 = 1$, (43) also holds for $|\sigma| = 0$.

We choose a function Φ (depending on j) satisfying

$$\Phi \in C_0^\infty(\omega_{\epsilon(j+3/4)}), \quad 0 \le \Phi \le 1, \quad \text{with } \Phi \equiv 1 \text{ on } \omega_{\epsilon(j+1)}. \tag{44}$$

Then

$$\|D^\beta \varphi_i\|_{L^p(\omega_{\epsilon(j+1)})} \le \|\Phi D^\beta \varphi_i\|_p. \tag{45}$$

The estimate (42) — and hence, by induction, the proof of Proposition 2.1 — now follows from the equations (35) for the φ_i, (45) and the following two lemmas.

Lemma 3.3. *Assume the induction hypothesis* (40) *holds. Let Φ be as in* (44). *Then for all $i \in \{1, \ldots, N\}$, all $\epsilon > 0$ with $\epsilon(j+1) \le R/2$, and all $\beta \in \mathbb{N}_0^3$ with $|\beta| = j+1$, both $\Phi D^\beta E(\boldsymbol{p})^{-1} V \varphi_i$ and $\Phi D^\beta E(\boldsymbol{p})^{-1} \varphi_i$ belong to $L^p(\mathbb{R}^3)$, and*

$$\|\Phi D^\beta E(\boldsymbol{p})^{-1} V \varphi_i\|_p \le \frac{C}{4}\left(\frac{B}{\epsilon}\right)^{|\beta|}, \tag{46}$$

$$\|(\alpha^{-1} + \varepsilon_i)\Phi D^\beta E(\boldsymbol{p})^{-1} \varphi_i\|_p \le \frac{C}{4}\left(\frac{B}{\epsilon}\right)^{|\beta|}, \tag{47}$$

where $C, B > 1$ are the constants in (36) *(see also Remark 2.2).*

Lemma 3.4. *Assume the induction hypothesis* (40) *holds. Let Φ be as in* (44). *Then for all $i \in \{1, \ldots, N\}$, all $\epsilon > 0$ with $\epsilon(j+1) \le R/2$, and all $\beta \in \mathbb{N}_0^3$ with $|\beta| = j+1$, both $\Phi D^\beta E(\boldsymbol{p})^{-1} R_{\boldsymbol{\varphi}} \varphi_i$ and $\Phi D^\beta E(\boldsymbol{p})^{-1} K_{\boldsymbol{\varphi}} \varphi_i$ belong to $L^p(\mathbb{R}^3)$, and*

$$\|\alpha \, \Phi D^\beta E(\boldsymbol{p})^{-1} R_{\boldsymbol{\varphi}} \varphi_i\|_p \le \frac{C}{4}\left(\frac{B}{\epsilon}\right)^{|\beta|},$$

$$\|\alpha \, \Phi D^\beta E(\boldsymbol{p})^{-1} K_{\boldsymbol{\varphi}} \varphi_i\|_p \le \frac{C}{4}\left(\frac{B}{\epsilon}\right)^{|\beta|},$$

where $C, B > 1$ are the constants in (36) *(see also Remark 2.2).*

Remark 3.5. For $a, b \in \{1, \ldots, N\}$, let $U_{a,b}$ denote the function

$$U_{a,b}(\boldsymbol{x}) = \int_{\mathbb{R}^3} \frac{\varphi_a(\boldsymbol{y})\overline{\varphi_b(\boldsymbol{y})}}{|\boldsymbol{x} - \boldsymbol{y}|} \, d\boldsymbol{y}, \quad \boldsymbol{x} \in \mathbb{R}^3. \tag{48}$$

In particular, $\|U_{a,b}\|_\infty \leq C_1$ for all $a, b \in \{1, \ldots, N\}$ (see (23)). Using (12) and (13), we can write

$$R_{\boldsymbol{\varphi}}\varphi_i = \sum_{\ell=1}^{N} U_{\ell,\ell}\varphi_i, \quad K_{\boldsymbol{\varphi}}\varphi_i = \sum_{\ell=1}^{N} U_{i,\ell}\varphi_\ell. \tag{49}$$

Hence Lemma 3.4 follows from the following lemma and the fact that $Z\alpha < 2/\pi < 1$.

Lemma 3.6. *Assume the induction hypothesis* (40) *holds. Let* Φ *be as in* (44). *For* $a, b \in \{1, \ldots, N\}$, *let* $U_{a,b}$ *be given by* (48). *Then for all* $a, b, i \in \{1, \ldots, N\}$, *all* $\epsilon > 0$ *with* $\epsilon(j+1) \leq R/2$, *and all* $\beta \in \mathbb{N}_0^3$ *with* $|\beta| = j+1$, $\Phi D^\beta E(\boldsymbol{p})^{-1} U_{a,b}\varphi_i$ *belong to* $L^p(\mathbb{R}^3)$, *and*

$$\|\Phi D^\beta E(\boldsymbol{p})^{-1}U_{a,b}\varphi_i\|_p \leq \frac{CZ}{4N}\left(\frac{B}{\epsilon}\right)^{|\beta|}, \tag{50}$$

where $C, B > 1$ *are the constants in* (36) *(see also Remark 2.2).*

It therefore remains to prove Lemmas 3.3 and 3.6. This will be done in the two following sections. $\square$

4. Proof of Lemma 3.3

We prove Lemma 3.3 by proving (46) and (47) separately.

Proof of (46). Let $\sigma \in \mathbb{N}_0^3$ and $\nu \in \{1, 2, 3\}$ be such that $\beta = \sigma + e_\nu$, so that $D^\beta = D_\nu D^\sigma$. Notice that $|\sigma| = j$. Choose localization functions $\{\chi_k\}_{k=0}^{j}$ and $\{\eta_k\}_{k=0}^{j}$ as in Appendix B. Since $V\varphi_i \in H^{-1/2}(\mathbb{R}^3)$, and $E(\boldsymbol{p})^{-1}$ maps $H^s(\mathbb{R}^3)$ to $H^{s+1}(\mathbb{R}^3)$ for all $s \in \mathbb{R}$, Lemma B.1 (with $\ell = j$) implies that

$$\Phi D^\beta E(\boldsymbol{p})^{-1}[V\varphi_i] = \sum_{k=0}^{j} \Phi D_\nu E(\boldsymbol{p})^{-1}D^{\beta_k}\chi_k D^{\sigma-\beta_k}[V\varphi_i] + \sum_{k=0}^{j-1}\Phi D_\nu E(\boldsymbol{p})^{-1}D^{\beta_k}[\eta_k, D^{\mu_k}]D^{\sigma-\beta_{k+1}}[V\varphi_i]$$
$$+ \Phi D_\nu E(\boldsymbol{p})^{-1}D^\sigma[\eta_j V\varphi_i], \quad (51)$$

as an identity in $H^{-|\beta|+1/2}(\mathbb{R}^3)$ (we have also used that $E(\boldsymbol{p})^{-1}$ commutes with derivatives on any $H^s(\mathbb{R}^3)$). Here, $[\cdot, \cdot]$ denotes the commutator. Also, $|\beta_k| = k$, $|\mu_k| = 1$, and $0 \leq \eta_k, \chi_k \leq 1$. (For the support properties of η_k, χ_k, see Appendix B.) We will prove that each term on the right side of (51) belong to $L^p(\mathbb{R}^3)$, and bound their norms. The proof of (46) will follow by summing these bounds.

The first sum in (51). Let θ_k be the characteristic function of the support of χ_k (which is contained in ω). Since V is smooth on the closure of ω it follows from the induction hypothesis that the $D^{\sigma-\beta_k}[V\varphi_i]$ belong to $L^p(\omega')$ for any $\omega' \Subset \omega$. Also, the operator $\Phi D_\nu E(\boldsymbol{p})^{-1}D^{\beta_k}\chi_k$ is bounded on $L^p(\mathbb{R}^3)$ (as we will observe below). Therefore we can estimate, for $k \in \{0, \ldots, j\}$,

$$\|\Phi D_\nu E(\boldsymbol{p})^{-1}D^{\beta_k}\chi_k D^{\sigma-\beta_k}[V\varphi_i]\|_p = \|(\Phi E(\boldsymbol{p})^{-1}D_\nu D^{\beta_k}\chi_k)\theta_k D^{\sigma-\beta_k}[V\varphi_i]\|_p$$
$$\leq \|\Phi E(\boldsymbol{p})^{-1}D_\nu D^{\beta_k}\chi_k\|_{\mathscr{B}_p} \|\theta_k D^{\sigma-\beta_k}[V\varphi_i]\|_p. \tag{52}$$

Here, $\|\cdot\|_{\mathscr{B}_p}$ is the operator norm on $\mathscr{B}_p := B(L^p(\mathbb{R}^3))$, the bounded operators on $L^p(\mathbb{R}^3)$.

For $k = 0$, the first factor on the right side of (52) can be estimated using Lemma C.1 (since $|\beta_0| = 0$). This way, since $\|\chi_0\|_\infty = \|\Phi\|_\infty = 1$,

$$\|\Phi E(\boldsymbol{p})^{-1}D_\nu\chi_0\|_{\mathscr{B}_p} \leq K_1, \tag{53}$$

with $K_1 = K_1(p)$ the constant in (C.1).

For $k > 0$, the first factor on the right side of (52) can be estimated using (C.4) in Lemma C.2 (with $\mathfrak{r} = 1$, $\mathfrak{q}^* = \mathfrak{p} = p$). Since

$$\text{dist}(\text{supp } \chi_k, \text{supp } \Phi) \geq \epsilon(k - 1 + 1/4)$$

and $\|\chi_k\|_\infty = \|\Phi\|_\infty = 1$, this gives (since $(\beta_k + e_\nu)! \leq (|\beta_k| + 1)! = (k + 1)!$) that

$$\|\Phi E(\boldsymbol{p})^{-1} D_\nu D^{\beta_k} \chi_k\|_{\mathscr{B}_p} \leq \frac{32\sqrt{2}}{\pi} \frac{(k+1)!}{k} \left(\frac{8}{\epsilon(k-1+1/4)}\right)^k \leq \frac{256\sqrt{2}}{\pi}\left(\frac{8}{\epsilon}\right)^k. \tag{54}$$

It follows from (53) and (54) that, for all $k \in \{0, \ldots, j\}$, $\nu \in \{1, 2, 3\}$,

$$\|\Phi E(\boldsymbol{p})^{-1} D_\nu D^{\beta_k} \chi_k\|_{\mathscr{B}_p} \leq C_2 \left(\frac{8}{\epsilon}\right)^k, \tag{55}$$

with C_2 as defined in (25).

It remains to estimate the second factor in (52). Recall the definition of the constant A in (24). It follows from (24) and (17) that, for all $\epsilon > 0$, $\ell \in \mathbb{N}_0$, and $\sigma \in \mathbb{N}_0^3$,

$$\epsilon^{|\sigma|} \sup_{\boldsymbol{x} \in \omega_{\epsilon\ell}} |D^\sigma V(\boldsymbol{x})| \leq A^{|\sigma|+1} |\sigma|! \, \ell^{-|\sigma|}, \tag{56}$$

with $\omega_{\epsilon\ell} \subseteq \omega$ as in defined in (16).

For $k = j$, since $\beta_j = \sigma$, we find, by (56) and the choice of C (see Remark 2.2), that

$$\|\theta_j V \varphi_i\|_p \leq \|V\|_{L^\infty(\omega)} \|\varphi_i\|_{L^p(\omega)} \leq CA. \tag{57}$$

The estimate for $k \in \{0, \ldots, j-1\}$ is a bit more involved. We get, by Leibniz's rule, that

$$\|\theta_k D^{\sigma - \beta_k}[V\varphi_i]\|_p \leq \sum_{\mu \leq \sigma - \beta_k} \binom{\sigma - \beta_k}{\mu} \|\theta_k D^\mu V\|_\infty \|\theta_k D^{\sigma - \beta_k - \mu} \varphi_i\|_p. \tag{58}$$

Now, $\text{supp } \theta_k = \text{supp } \chi_k \subseteq \omega_{\epsilon(j-k+1/4)}$, so by (56), for all $\mu \leq \sigma - \beta_k$,

$$\|\theta_k D^\mu V\|_\infty \leq \sup_{\boldsymbol{x} \in \omega_{\epsilon(j-k+1/4)}} |D^\mu V(\boldsymbol{x})| \leq \epsilon^{-|\mu|} A^{|\mu|+1} |\mu|! \, (j-k)^{-|\mu|}. \tag{59}$$

By the induction hypothesis (in the form discussed in Remark 3.2),

$$\|\theta_k D^{\sigma - \beta_k - \mu} \varphi_i\|_p \leq \|D^{\sigma - \beta_k - \mu} \varphi_i\|_{L^p(\omega_{\epsilon(j-k)})} \leq C \left(\frac{|\sigma - \beta_k - \mu|}{j-k}\right)^{|\sigma - \beta_k - \mu|} \left(\frac{B}{\epsilon}\right)^{|\sigma - \beta_k - \mu|}. \tag{60}$$

It follows from (58), (59), and (60) that (using that $|\sigma| = j$, $|\beta_k| = k$, and (A.6), summing over $m = |\mu|$)

$$\|\theta_k D^{\sigma - \beta_k}[V\varphi_i]\|_p \leq CA \left(\frac{B}{\epsilon}\right)^{j-k} \sum_{m=0}^{j-k} \binom{j-k}{m} \frac{m! \, (j-k-m)^{j-k-m}}{(j-k)^{j-k}} \left(\frac{A}{B}\right)^m. \tag{61}$$

Note that, by (A.7), for $0 < m < j - k$,

$$\binom{j-k}{m} \frac{m! \, (j-k-m)^{j-k-m}}{(j-k)^{j-k}} \leq \frac{e^{1/12} \sqrt{j-k}}{\sqrt{j-k-m} \, e^m} \leq 1. \tag{62}$$

To see the last inequality, look at the cases $0 < m \le (j-k)/2$ and $j - k > m \ge (j-k)/2$ separately.

Hence (since $B > 2A$, see Remark 2.2), for any $k \in \{0, \ldots, j-1\}$,

$$\|\theta_k D^{\sigma-\beta_k}[V\varphi_i]\|_p \le CA\Big(\frac{B}{\epsilon}\Big)^{j-k} \sum_{m=0}^{j-k} \Big(\frac{A}{B}\Big)^m \le 2CA\Big(\frac{B}{\epsilon}\Big)^{j-k}. \tag{63}$$

Note that, by (57), the same estimate holds true if $k = j$.

So, from (52), (55), (63), the fact that $\epsilon \le 1$ (since $\epsilon(j+1) \le R/2 \le 1/2$), and the choice of B (in particular, $B > 16$; see Remark 2.2), it follows that

$$\Big\|\sum_{k=0}^{j} \Phi D_\nu E(\boldsymbol{p})^{-1} D^{\beta_k} \chi_k D^{\sigma-\beta_k}[V\varphi_i]\Big\|_p \le 2CAC_2\Big(\frac{B}{\epsilon}\Big)^{j} \sum_{k=0}^{j} \Big(\frac{8}{B}\Big)^k$$

$$\le C(4AC_2)\Big(\frac{B}{\epsilon}\Big)^{j} \le \frac{C}{12}\Big(\frac{B}{\epsilon}\Big)^{j+1}. \tag{64}$$

The second sum in (51). Note first that $[\eta_k, D^{\mu_k}] = -(D^{\mu_k}\eta_k)$ (recall that $|\mu_k| = 1$; see Lemma B.1).

Comparing the second sum in (51) with the first sum in (51), one sees that the second sum is the first one with j replaced by $j-1$ and χ_k replaced by $-D^{\mu_k}\eta_k$. Having now a derivative on the localization functions we have one derivative less falling on the term $V\varphi_i$. More precisely, the operator $D^{\sigma-\beta_{k+1}}$ contains $|\sigma - \beta_{k+1}| = j - (k+1) = (j-1) - k$ derivatives instead of $|\sigma - \beta_k| = j - k$ in $D^{\sigma-\beta_k}$. Then, to control $D^{\sigma-\beta_{k+1}}[V\varphi_i]$ (with the same method used above for $D^{\sigma-\beta_k}[V\varphi_i]$) we need that supp $D^{\mu_k}\eta_k$ is contained in $\omega_{\epsilon((j-1)-k+1/4)}$. Indeed we have much more: as for χ_k we have supp $D^{\mu_k}\eta_k \subseteq \omega_{\epsilon(j-k+1/4)} \subseteq \omega_{\epsilon((j-1)-k+1/4)}$. Finally, $\|D^{\mu_k}\eta_k\|_\infty \le C_*/\epsilon$, with $C_* > 0$ the constant in (B.3) in the appendix.

It follows that the second sum in (51) can be estimated as the first one, up to *one* extra factor of C_*/ϵ *and* up to replacing j by $j-1$ in the estimate (64). Hence, using that $\epsilon \le 1$, and the choice of B (see Remark 2.2), we get that

$$\Big\|\sum_{k=0}^{j-1} \Phi D_\nu E(\boldsymbol{p})^{-1} D^{\beta_k}[\eta_k, D^{\mu_k}]D^{\sigma-\beta_{k+1}}[V\varphi_i]\Big\|_p \le \frac{C_*}{\epsilon} C(4AC_2)\Big(\frac{B}{\epsilon}\Big)^{j-1}$$

$$\le C(4AC_2)\Big(\frac{B}{\epsilon}\Big)^{j} \le \frac{C}{12}\Big(\frac{B}{\epsilon}\Big)^{j+1}. \tag{65}$$

The last term in (51). It remains to study

$$\Phi D^{\beta} E(\boldsymbol{p})^{-1}[\eta_j V\varphi_i]. \tag{66}$$

We split V in two parts, one supported around $\boldsymbol{x} = 0$, and one supported away from $\boldsymbol{x} = 0$, and study the two terms separately. We will prove below that this way, $\eta_j V\varphi_i$ is actually a function in $L^1(\mathbb{R}^3) + L^3(\mathbb{R}^3)$. Upon using suitable operator bounds on $\Phi D^\beta E(\boldsymbol{p})^{-1}\chi$ (for some suitable smooth χ's), combined with bounds on the norms of the two parts of $\eta_j V\varphi_i$, we will finish the proof.

Let $\rho = |\boldsymbol{x}_0|/4$, and let θ_ρ and $\theta_{\rho/2}$ be the characteristic functions of the balls $B_\rho(0)$ and $B_{\rho/2}(0)$, respectively. Choose $\widetilde{\chi}_\rho \in C_0^\infty(\mathbb{R}^3)$ with supp $\widetilde{\chi}_\rho \subseteq B_\rho(0)$, $0 \le \widetilde{\chi}_\rho \le 1$, and $\widetilde{\chi}_\rho = 1$ on $B_{\rho/2}(0)$. Note that

then

$$\text{dist}(\text{supp }\Phi, \text{supp }\widetilde{\chi}_\rho) \geq \frac{|\boldsymbol{x}_0|}{2} = 2\rho, \tag{67}$$

by the choice of $\omega = B_R(\boldsymbol{x}_0)$, $R = \min\{1, |\boldsymbol{x}_0|/4\}$, since supp $\Phi \subseteq \omega_{\epsilon(j+1)} \subseteq \omega$.

Now,

$$\Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V \varphi_i] = \Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V \widetilde{\chi}_\rho \varphi_i] + \Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V (1 - \widetilde{\chi}_\rho) \varphi_i]. \tag{68}$$

For the first term in (68), we use Lemma C.2, with $\mathfrak{p} = 1$, $\mathfrak{q} = p/(p-1)$, and $\mathfrak{r} = p$. Then $\mathfrak{p}, \mathfrak{r} \in [1, \infty)$ and $\mathfrak{q} > 1$, and $\mathfrak{q}^{-1} + p^{-1} = 1$. We get that (recall (67) and that $\widetilde{\chi}_\rho \theta_\rho = \widetilde{\chi}_\rho$),

$$\|\Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V \widetilde{\chi}_\rho \varphi_i]\|_p \leq \|\Phi D^\beta E(\boldsymbol{p})^{-1} \widetilde{\chi}_\rho\|_{\mathcal{B}_{1,p}} \|\eta_j V \theta_\rho \varphi_i\|_1$$

$$\leq \frac{4\sqrt{2}}{\pi} \beta! \left(\frac{8}{2\rho}\right)^{|\beta|} (2\rho)^{3/\mathfrak{r}-2} \big(\mathfrak{r}(|\beta|+2) - 3\big)^{-1/\mathfrak{r}} \|V\theta_\rho \varphi_i\|_1. \tag{69}$$

Here we used that $\|\Phi\|_\infty = \|\widetilde{\chi}_\rho\|_\infty = 1$ and that $\eta_j \equiv 1$ where $\theta_\rho \neq 0$. Note that $j + 1 \leq \epsilon^{-1}$ (since, by assumption, $\epsilon(j+1) \leq R/2 \leq 1/2$). Therefore,

$$\beta! \leq |\beta|! = (j+1)! \leq (j+1)^{j+1} \leq \epsilon^{-(j+1)} = \epsilon^{-|\beta|}. \tag{70}$$

Note furthermore that since $|\beta| = j + 1 \geq 2$ and $\mathfrak{r} \geq 1$,

$$\big(\mathfrak{r}(|\beta|+2) - 3\big)^{-1/\mathfrak{r}} \leq 1, \tag{71}$$

independently of β. It follows that

$$\|\Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V \widetilde{\chi}_\rho \varphi_i]\|_p \leq \frac{4\sqrt{2}}{\pi} \left(\frac{|\boldsymbol{x}_0|}{2}\right)^{(3-2p)/p} \|V\theta_\rho \varphi_i\|_1 \left(\frac{16/|\boldsymbol{x}_0|}{\epsilon}\right)^{|\beta|}. \tag{72}$$

Using Schwarz's inequality and that $Z\alpha < 2/\pi$,

$$\|V\theta_\rho \varphi_i\|_1 \leq \|V\theta_\rho\|_2 \|\varphi_i\|_2 = Z\alpha \sqrt{|\boldsymbol{x}_0|\pi} \|\varphi_i\|_2 \leq \frac{2}{\sqrt{\pi}} \sqrt{|\boldsymbol{x}_0|} \|\varphi_i\|_2. \tag{73}$$

(Note that $\|V\theta_\rho\|_t < \infty \Leftrightarrow t < 3$.) It follows from (72), (73), and the choice of B and C (see Remark 2.2) that

$$\big\|\Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V \widetilde{\chi}_\rho \varphi_i]\big\|_p \leq \frac{32}{\pi} |\boldsymbol{x}_0|^{3(2-p)/(2p)} \|\varphi_i\|_2 \left(\frac{16/|\boldsymbol{x}_0|}{\epsilon}\right)^{|\beta|} \leq \frac{C}{24} \left(\frac{B}{\epsilon}\right)^{j+1}. \tag{74}$$

We now consider the second term in (68). Recall that Φ is supported in $\omega_{\epsilon(j+1)}$ and

$$\text{dist}(\text{supp }\Phi, \text{supp }\eta_j) \geq \epsilon(j + 1/4). \tag{75}$$

Again, we use Lemma C.2, this time with $\mathfrak{p} = 3$, $\mathfrak{q} = p/(p-1)$, and $\mathfrak{r} = 3p/(2p+3)$. Then

$$\mathfrak{p}^{-1} + \mathfrak{q}^{-1} + \mathfrak{r}^{-1} = 2, \quad \mathfrak{p} \in [1, \infty), \quad \mathfrak{q} > 1, \quad \mathfrak{r} \in [1, 3/2)$$

(since $p > 3$), and $\mathfrak{q}^{-1} + p^{-1} = 1$. This gives

$$\left\| \Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V(1-\widetilde{\chi}_\rho)\varphi_i] \right\|_p$$

$$\leq \left\| \Phi D^\beta E(\boldsymbol{p})^{-1}\eta_j \right\|_{\mathscr{B}_{3,p}} \left\| V(1-\widetilde{\chi}_\rho)\varphi_i \right\|_3$$

$$\leq \frac{4\sqrt{2}}{\pi}\beta!\left(\frac{8}{\epsilon(j+1/4)}\right)^{|\beta|}\left(\epsilon(j+1/4)\right)^{3/\mathfrak{r}-2}\left(\mathfrak{r}(|\beta|+2)-3\right)^{-1/\mathfrak{r}}\|V(1-\widetilde{\chi}_\rho)\|_\infty\|\varphi_i\|_3.$$

As before, we used that $\|\Phi\|_\infty = \|\eta_j\|_\infty = 1$. Note that

$$\beta!\left(\frac{8}{j+1/4}\right)^{|\beta|} \leq 32^{|\beta|}\frac{|\beta|!}{(j+1)^{|\beta|}} = 32^{|\beta|}\frac{(j+1)!}{(j+1)^{j+1}} \leq 32^{|\beta|}. \tag{76}$$

Since $\epsilon(j+1) \leq R/2 < 1$ and $\mathfrak{r} < 3/2$ it follows that $(\epsilon(j+1/4))^{3/\mathfrak{r}-2} \leq 1$. Also, by the choice of ρ, the definition of V, and since $Z\alpha < 2/\pi$,

$$\left|((1-\theta_{\rho/2})V)(\boldsymbol{x})\right| \leq \frac{8Z\alpha}{|\boldsymbol{x}_0|} \leq \frac{16}{\pi|\boldsymbol{x}_0|}, \quad \boldsymbol{x} \in \mathbb{R}^3. \tag{77}$$

It follows from (77) (and that $0 \leq 1-\widetilde{\chi}_\rho \leq 1-\theta_{\rho/2}$), (71), (76), and the choice of C and B (see Remark 2.2), that for all $i = 1, \ldots, N$ (recall that $|\beta| = j+1$)

$$\left\| \Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V(1-\widetilde{\chi}_\rho)\varphi_i] \right\|_p \leq \frac{4\sqrt{2}}{\pi}\frac{16}{\pi|\boldsymbol{x}_0|}\|\varphi_i\|_3\left(\frac{32}{\epsilon}\right)^{|\beta|} \leq \frac{C}{24}\left(\frac{B}{\epsilon}\right)^{j+1}. \tag{78}$$

It follows from (68), (74), and (78) that

$$\left\| \Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V\varphi_i] \right\|_p \leq \frac{C}{12}\left(\frac{B}{\epsilon}\right)^{j+1}. \tag{79}$$

The estimate (46) now follows from (51) and the estimates (64), (65), and (79). $\qquad\square$

Proof of (47). The constant functions $W_i(\boldsymbol{x}) = \alpha^{-1} + \varepsilon_i$ trivially satisfy the conditions on $V (= Z\alpha|\cdot|^{-1})$ needed in the proof above. In fact, having assumed $A \geq \alpha^{-1} + \max_{1\leq i\leq N}|\varepsilon_i|$ (see Remark 2.2), (24) (and therefore (56)) trivially holds for W_i. Also, for the term $\Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j W_i\varphi_i]$ we proceed directly as for the term $\Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V(1-\widetilde{\chi}_\rho)\varphi_i]$ above (but without any splitting in $\widetilde{\chi}_\rho$ and $1-\widetilde{\chi}_\rho$), using that $|W_i(\boldsymbol{x})| \leq A$, $\boldsymbol{x} \in \mathbb{R}^3$. The proof of (47) therefore follows from the proof of (46) above, by the choice of C and B (see Remark 2.2).

This finishes the proof of Lemma 3.3. $\qquad\square$

Remark 4.1. In fact, with a simple modification the arguments above (the local L^p-bound on the two terms in (68)) can be made to work just assuming that, for all $s > 0$,

$$V\varphi_i \in L^1(B_s(0)), \quad V\varphi_i \in L^3(\mathbb{R}^3 \setminus B_s(0)). \tag{80}$$

5. Proof of Lemma 3.6

Proof of (50). Similarly to the case of the term with V in Lemma 3.3, we here use the localization functions introduced in Appendix B. With the notation as in the previous section (in particular, $\beta = \sigma + e_\nu$

with $|\sigma| = j$), Lemma B.1 (with $\ell = j$) implies that

$$
\Phi D^\beta E(\boldsymbol{p})^{-1}[U_{a,b}\varphi_i]
$$

$$
= \sum_{k=0}^{j} \Phi D_\nu E(\boldsymbol{p})^{-1} D^{\beta_k} \chi_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i] + \sum_{k=0}^{j-1} \Phi D_\nu E(\boldsymbol{p})^{-1} D^{\beta_k}[\eta_k, D^{\mu_k}] D^{\sigma-\beta_{k+1}}[U_{a,b}\varphi_i]
$$

$$
+ \Phi D_\nu E(\boldsymbol{p})^{-1} D^\sigma[\eta_j U_{a,b}\varphi_i], \quad (81)
$$

as an identity in $H^{-|\beta|}(\mathbb{R}^3)$. As in the proof of Lemma 3.3, $[\,\cdot\,,\,\cdot\,]$ denotes the commutator, $|\beta_k| = k$, $|\mu_k| = 1$, and $0 \leq \eta_k, \chi_k \leq 1$. (For the support properties of η_k, χ_k, see Appendix B.) As in the previous section, we will prove that each term on the right side of (81) belong to $L^p(\mathbb{R}^3)$, and bound their norms. The claim of the lemma will follow by summing these bounds.

The first sum in (81). We first proceed like for the similar sum in the proof of Lemma 3.3 (see (52), and after). Let θ_k be the characteristic function of the support of χ_k. It follows from the induction hypothesis, using that $-\Delta U_{a,b} = 4\pi \varphi_a \overline{\varphi_b}$, and Theorems D.5 and D.3, that the $D^{\sigma-\beta_k}[U_{a,b}\varphi_i]$ belong to $L^p(\omega')$ for any $\omega' \Subset \omega$. As before, the operator $\Phi D_\nu E(\boldsymbol{p})^{-1} D^{\beta_k} \chi_k$ is bounded on $L^p(\mathbb{R}^3)$. Then, for $k \in \{0, \dots, j\}$,

$$
\left\| \Phi D_\nu E(\boldsymbol{p})^{-1} D^{\beta_k} \chi_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i] \right\|_p = \left\| (\Phi E(\boldsymbol{p})^{-1} D_\nu D^{\beta_k} \chi_k) \theta_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i] \right\|_p
$$

$$
\leq \left\| \Phi E(\boldsymbol{p})^{-1} D_\nu D^{\beta_k} \chi_k \right\|_{\mathcal{B}_p} \left\| \theta_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i] \right\|_p. \quad (82)
$$

The first factor on the right side of (82) was estimated in the proof of Lemma 3.3 (see (55)): For all $k \in \{0, \dots, j\}$, $\nu \in \{1, 2, 3\}$,

$$
\left\| \Phi E(\boldsymbol{p})^{-1} D_\nu D^{\beta_k} \chi_k \right\|_{\mathcal{B}_p} \leq C_2 \left(\frac{8}{\epsilon} \right)^k, \quad (83)
$$

with C_2 the constant in (25).

It remains to estimate the second factor in (82). For $k = j$, since $\beta_j = \sigma$, we find that, by (23) and the choice of C and B (see Remark 2.2),

$$
\|\theta_j U_{a,b}\varphi_i\|_p \leq \|U_{a,b}\|_\infty \|\varphi_i\|_{L^p(\omega)} \leq C_1 C \leq C \left(\frac{B}{\epsilon} \right)^{1/2}. \quad (84)
$$

In the last inequality we also used that $\epsilon \leq 1$ (since $\epsilon(j+1) \leq R/2 < 1$).

The estimate for $k \in \{0, \dots, j-1\}$ is more involved. We get, by Leibniz's rule, that

$$
\|\theta_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\|_p \leq \sum_{\mu \leq \sigma-\beta_k} \binom{\sigma-\beta_k}{\mu} \left\| \theta_k (D^\mu U_{a,b})(D^{\sigma-\beta_k-\mu}\varphi_i) \right\|_p. \quad (85)
$$

We estimate separately each term on the right side of (85).

We separate into two cases.

If $\mu = 0$ then, using the induction hypothesis (i.e., $\mathcal{P}(p, j-k)$; recall that supp $\theta_k \subseteq \omega_{\epsilon(j-k)}$) and (23),

$$
\|\theta_k U_{a,b} D^{\sigma-\beta_k}\varphi_i\|_p \leq C_1 C \left(\frac{B}{\epsilon} \right)^{j-k} \leq \frac{C}{2} \left(\frac{B}{\epsilon} \right)^{j-k+1/2}. \quad (86)
$$

In the last inequality we used the choice of B (see Remark 2.2) and that $\epsilon \leq 1$.

If $0 < \mu \leq \sigma - \beta_k$, then (since supp $\chi_k \subseteq \omega_{\epsilon(j-k+1/4)}$) Hölder's inequality (with $1/p = 1/(3p) + 2/(3p)$) and Corollary D.2 give

$$\|\theta_k(D^\mu U_{a,b})(D^{\sigma-\beta_k-\mu}\varphi_i)\|_p$$
$$\leq \|\theta_k D^\mu U_{a,b}\|_{3p/2}\|\theta_k D^{\sigma-\beta_k-\mu}\varphi_i\|_{3p}$$
$$\leq K_2\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega_{\epsilon(j-k+1/4)})}\|D^{\sigma-\beta_k-\mu}\varphi_i\|^\theta_{W^{1,p}(\omega_{\epsilon(j-k+1/4)})}\|D^{\sigma-\beta_k-\mu}\varphi_i\|^{1-\theta}_{L^p(\omega_{\epsilon(j-k+1/4)})}. \quad (87)$$

Here, K_2 is the constant in Corollary D.2, and $\theta = 2/p < 1$. Note that $\omega_{\epsilon(j-k+1/4)} = B_r(\mathbf{x}_0)$ with $r \in [R/2, 1]$, since $\epsilon(j+1) \leq R/2$ and $R = \min\{1, |\mathbf{x}_0|/4\}$

We will use Lemma 5.3 below to bound the first factor in (87). The last two factors we now bound using the induction hypothesis.

If $\mu \in \mathbb{N}_0^3$ is such that $0 < \mu \leq \sigma - \beta_k$, then the induction hypothesis (in the form discussed in Remark 3.2) gives (recall here (18) and that $|\sigma| = j$, $|\beta_k| = k$) that for the last two factors in (87) we have

$$\|D^{\sigma-\beta_k-\mu}\varphi_i\|^{1-\theta}_{L^p(\omega_{\epsilon(j-k+1/4)})} \leq \left[C\left(\frac{j-k-|\mu|}{j-k+1/4}\right)^{j-k-|\mu|}\left(\frac{B}{\epsilon}\right)^{j-k-|\mu|}\right]^{1-\theta} \quad (88)$$

and (using that $B > 1$ (see Remark 2.2) and $\epsilon(j-k+1/4) \leq \epsilon(j+1) \leq R/2 < 1$)

$$\|D^{\sigma-\beta_k-\mu}\varphi_i\|^\theta_{W^{1,p}(\omega_{\epsilon(j-k+1/4)})}$$
$$\leq \left[C\left(\frac{j-k-|\mu|}{j-k+1/4}\right)^{j-k-|\mu|}\left(\frac{B}{\epsilon}\right)^{j-k-|\mu|} + 3C\left(\frac{j-k-|\mu|+1}{j-k+1/4}\right)^{j-k-|\mu|+1}\left(\frac{B}{\epsilon}\right)^{j-k-|\mu|+1}\right]^\theta$$
$$\leq \left[4C\left(\frac{j-k-|\mu|+1}{j-k+1/4}\right)^{j-k-|\mu|+1}\left(\frac{B}{\epsilon}\right)^{j-k-|\mu|+1}\right]^\theta. \quad (89)$$

It follows from (88) and (89) that for all $\mu \in \mathbb{N}_0^3$ with $0 < \mu \leq \sigma - \beta_k$,

$$\|D^{\sigma-\beta_k-\mu}\varphi_i\|^\theta_{W^{1,p}(\omega_{\epsilon(j-k+1/4)})}\|D^{\sigma-\beta_k-\mu}\varphi_i\|^{1-\theta}_{L^p(\omega_{\epsilon(j-k+1/4)})} \leq C4^\theta\left(\frac{B}{\epsilon}\right)^{j-k-|\mu|+\theta}\left(\frac{j-k-|\mu|+1}{j-k+1/4}\right)^{j-k-|\mu|+\theta}. \quad (90)$$

From (87), Lemma 5.3, and (90) (using (A.6) in the appendix, summing over $m = |\mu|$), it follows that

$$\sum_{0<\mu\leq\sigma-\beta_k}\binom{\sigma-\beta_k}{\mu}\left\|\theta_k(D^\mu U_{a,b})(D^{\sigma-\beta_k-\mu}\varphi_i)\right\|_p$$
$$\leq C^3 C_3 K_2\left(\frac{B}{\epsilon}\right)^{j-k+\theta}\sum_{m=1}^{j-k}4^\theta\binom{j-k}{m}\frac{(j-k-m+1)^{j-k-m+\theta}(m+1/4)^m}{(j-k+1/4)^{j-k+\theta}}$$
$$\times\left[\left(\frac{1}{\sqrt{B}}\right)^m + \sqrt{m}\left(\frac{B(m+1/4)}{\epsilon(j-k+1/4)}\right)^{2\theta-2}\right]. \quad (91)$$

Here, C_3 is the constant from (26). Recall also that $\theta = 2/p$.

We prove that for $m \in \{1, \ldots, j-k\}$,

$$4^\theta\binom{j-k}{m}\frac{(j-k-m+1)^{j-k-m+\theta}(m+1/4)^m}{(j-k+1/4)^{j-k+\theta}} \leq 10\epsilon^{-1/2+\theta}\frac{1}{\sqrt{m}}. \quad (92)$$

Note first that, since $\epsilon(j - k + 1/4) \leq \epsilon(j + 1) \leq 1$,

$$(j - k + 1/4)^{1/2-\theta} \leq \epsilon^{-1/2+\theta}. \tag{93}$$

This shows that the inequality in (92) is true for $m = j - k > 0$, since $\theta < 1$. For $m < j - k$, we use (A.8) in the appendix, and (93), to get that (since $(1 + 1/n)^n \leq e$)

$$\binom{j-k}{m} \frac{(j-k-m+1)^{j-k-m+\theta}(m+1/4)^m}{(j-k+1/4)^{j-k+\theta}} \leq \frac{e^{25/12}}{\sqrt{2\pi}} \frac{(j-k-m+1)^{\theta}}{(j-k-m)^{1/2}} \epsilon^{-1/2+\theta} \frac{1}{\sqrt{m}}. \tag{94}$$

Since $\theta < 1/2$ and $m \leq j - k - 1$, we have that

$$\frac{(j-k-m+1)^{\theta}}{(j-k-m)^{1/2}} \leq 2^{\theta} \leq \sqrt{2}. \tag{95}$$

The estimate (92) for $m \in \{1, \ldots, j - k - 1\}$ now follows from (94)–(95) (since $4^{\theta}e^{25/12}/\sqrt{\pi} \leq 10$).

Inserting (92) in (91) (and using again $\epsilon(j - k + 1/4) \leq 1$ and $2\theta - 2 < 0$) we find that

$$\sum_{0 < \mu \leq \sigma - \beta_k} \binom{\sigma - \beta_k}{\mu} \left\| \theta_k (D^{\mu} U_{a,b})(D^{\sigma-\beta_k-\mu}\varphi_i) \right\|_p$$

$$\leq 10 C^3 C_3 K_2 \left(\frac{B}{\epsilon}\right)^{j-k+\theta} \epsilon^{-1/2+\theta} \sum_{m=1}^{j-k} \left[\left(\frac{1}{\sqrt{B}}\right)^m + \frac{1}{B^{2-2\theta}} \frac{1}{m^{2-2\theta}} \right]$$

$$\leq 10 C^3 C_3 K_2 \left(\frac{B}{\epsilon}\right)^{j-k+1/2} \frac{1}{\sqrt{B}} (2 + 6), \tag{96}$$

where we used that $\theta \leq 2/5$, $B \geq 4$ (see Remark 2.2), and $\sum_{m=1}^{\infty} m^{-6/5} \leq 1 + \int_1^{\infty} x^{-6/5}\, dx = 6$ to estimate

$$\sum_{m=1}^{\infty} \left(\frac{1}{\sqrt{B}}\right)^m \leq \frac{2}{\sqrt{B}}, \quad \frac{1}{B^{2-2\theta}} \sum_{m=1}^{\infty} \frac{1}{m^{2-2\theta}} \leq \frac{6}{\sqrt{B}}. \tag{97}$$

This is the very essential reason for needing $p \geq 5$.

By the choice of B (see Remark 2.2) it follows that

$$\sum_{0 < \mu \leq \sigma - \beta_k} \binom{\sigma - \beta_k}{\mu} \left\| \theta_k (D^{\mu} U_{a,b})(D^{\sigma-\beta_k-\mu}\varphi_i) \right\|_p \leq \frac{C}{2} \left(\frac{B}{\epsilon}\right)^{j-k+1/2}. \tag{98}$$

From (85), (86), and (98) it follows that for all $k \in \{0, \ldots, j - 1\}$,

$$\left\| \theta_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i] \right\|_p \leq C \left(\frac{B}{\epsilon}\right)^{j-k+1/2}. \tag{99}$$

Using (82), (83), (84), and (99) it follows for the first sum in (81) that

$$\left\|\sum_{k=0}^{j} \Phi D_\nu E(\boldsymbol{p})^{-1} D^{\beta_k} \chi_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\right\|_p \leq C_2 \sum_{k=0}^{j} 8^k \epsilon^{-k} \|\theta_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\|_p$$

$$\leq C_2 C\left(\frac{B}{\epsilon}\right)^{j+1/2} \sum_{k=0}^{j} \left(\frac{8}{B}\right)^k. \tag{100}$$

Since $B > 16$ (see Remark 2.2) the last sum is less than 2 and so for the first term in (81) we finally get, by the choice of B (see Remark 2.2) that

$$\left\|\sum_{k=0}^{j} \Phi D_\nu E(\boldsymbol{p})^{-1} D^{\beta_k} \chi_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\right\|_p \leq 2C_2 C\left(\frac{B}{\epsilon}\right)^{j+1/2} \leq \frac{CZ}{12N}\left(\frac{B}{\epsilon}\right)^{j+1}. \tag{101}$$

The second sum in (81). By the same arguments as for the second sum in (51) (see after (64)), it follows that the second sum in (81) can be estimated as the first one, up to *one* extra factor of C_*/ϵ (with $C_* > 0$ the constant in (B.3) in the appendix) *and* up to replacing j by $j-1$ in the estimate (101). Hence, by the choice of B (see Remark 2.2)

$$\left\|\sum_{k=0}^{j-1} \Phi D_\nu E(\boldsymbol{p})^{-1} D^{\beta_k}[\eta_k, D^{\mu_k}] D^{\sigma-\beta_{k+1}}[U_{a,b}\varphi_i]\right\|_p \leq \frac{C_*}{\epsilon}\frac{CZ}{12N}\left(\frac{B}{\epsilon}\right)^{j} \leq \frac{CZ}{12N}\left(\frac{B}{\epsilon}\right)^{j+1}. \tag{102}$$

The last term in (81). Since $\sigma + e_\nu = \beta$, the last term in (81) equals

$$\Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j U_{a,b}\varphi_i].$$

We proceed exactly as for the term $\Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j V(1-\widetilde{\chi}_\rho)\varphi_i]$ in (68) (but without any splitting in $\widetilde{\chi}_\rho$ and $1-\widetilde{\chi}_\rho$), except that the estimate in (77) is replaced by $\|U_{a,b}\|_\infty \leq C_1$ (see (23)). It follows, from the choice of B and C (see Remark 2.2) that (recall that $|\beta| = j+1$)

$$\|\Phi D^\beta E(\boldsymbol{p})^{-1}[\eta_j U_{a,b}\varphi_i]\|_p \leq \|\Phi D^\beta E(\boldsymbol{p})^{-1}\eta_j\|_{\mathscr{B}_{3,p}} \|U_{a,b}\varphi_i\|_3$$

$$\leq \frac{4\sqrt{2}}{\pi} C_1 \|\varphi_i\|_3 \left(\frac{32}{\epsilon}\right)^{|\beta|} \leq \frac{CZ}{12N}\left(\frac{B}{\epsilon}\right)^{j+1}. \tag{103}$$

The estimate (50) now follows from (81) and the estimates (101), (102), and (103).

This finishes the proof of Lemma 3.6. $\qquad\square$

It remains to prove Lemma 5.3 below ($L^{3p/2}$-bound on derivatives of the Newton potential $U_{a,b}$ of products of orbitals, $\varphi_a\varphi_b$).

In the next lemma we first give an $L^{3p/2}$-estimate on the derivatives of the product of the orbitals φ_i, needed for the proof of the bound in Lemma 5.3 below.

Lemma 5.1. *Assume the induction hypothesis* (40) *holds. Then, for all $a, b \in \{1, \ldots, N\}$, all $\beta \in \mathbb{N}_0^3$ with $|\beta| \leq j-1$, and all $\epsilon > 0$ with $\epsilon(|\beta|+1) \leq R/2$,*

$$\|D^\beta(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\epsilon(|\beta|+1)})} \leq 10 K_2^2 C^2 (1+\sqrt{|\beta|})\left(\frac{B}{\epsilon}\right)^{|\beta|+2\theta}, \tag{104}$$

with K_2 from Corollary D.2, C from Remark 2.2, and $\theta = \theta(p) = 2/p$.

Proof. By Leibniz's rule and Schwarz's inequality we get

$$\|D^\beta(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\epsilon(|\beta|+1)})} \le \sum_{\mu\le\beta}\binom{\beta}{\mu}\|D^\mu\varphi_a\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})}\|D^{\beta-\mu}\varphi_b\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})}.$$

We use Corollary D.2 (with $\omega_{\epsilon(|\beta|+1)} = B_r(x_0)$, $r = R - \epsilon(|\beta| + 1)$; note that $r \in [R/2, 1]$, since $\epsilon(|\beta| + 1) \le R/2$ and $R = \min\{1, |x_0|/4\}$). This gives, with K_2 from Corollary D.2 and $\theta = 2/p$,

$$\|D^\beta(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\epsilon(|\beta|+1)})} \le K_2^2 \sum_{\mu\le\beta}\binom{\beta}{\mu}\|D^\mu\varphi_a\|_{W^{1,p}(\omega_{\epsilon(|\beta|+1)})}^\theta \|D^\mu\varphi_a\|_{L^p(\omega_{\epsilon(|\beta|+1)})}^{1-\theta}$$
$$\times \|D^{\beta-\mu}\varphi_b\|_{W^{1,p}(\omega_{\epsilon(|\beta|+1)})}^\theta \|D^{\beta-\mu}\varphi_b\|_{L^p(\omega_{\epsilon(|\beta|+1)})}^{1-\theta}. \quad (105)$$

We now use the induction hypothesis (in the form discussed in Remark 3.2) on each of the four factors in the sum on the right side of (105). Note that, by assumption, $\epsilon(|\beta| + 1) \le \epsilon j \le R/2$ and $|\mu| < |\mu| + 1 \le |\beta| + 1 \le j$ (similarly, $|\beta - \mu| < |\beta - \mu| + 1 \le j$). Recalling (18), we therefore get, for all $\mu \in \mathbb{N}_0^3$ such that $\mu \le \beta$,

$$\|D^\mu\varphi_a\|_{W^{1,p}(\omega_{\epsilon(|\beta|+1)})}^\theta\|D^\mu\varphi_a\|_{L^p(\omega_{\epsilon(|\beta|+1)})}^{1-\theta}$$

$$\le \left[C\left(\frac{|\mu|}{|\beta|+1}\right)^{|\mu|}\left(\frac{B}{\epsilon}\right)^{|\mu|}\right]^{1-\theta}\left[C\left(\frac{|\mu|}{|\beta|+1}\right)^{|\mu|}\left(\frac{B}{\epsilon}\right)^{|\mu|} + 3C\left(\frac{|\mu|+1}{|\beta|+1}\right)^{|\mu|+1}\left(\frac{B}{\epsilon}\right)^{|\mu|+1}\right]^\theta$$

$$\le 4^\theta C\left(\frac{B}{\epsilon}\right)^{|\mu|+\theta}\frac{(|\mu|+1)^{\theta(|\mu|+1)}|\mu|^{|\mu|(1-\theta)}}{(|\beta|+1)^{|\mu|+\theta}},$$

since (recall that $\epsilon(|\beta| + 1) \le R/2 < 1$ and $B > 1$)

$$\frac{|\mu|^{|\mu|}}{(|\mu|+1)^{|\mu|+1}}\,\epsilon(|\beta|+1)B^{-1} \le 1.$$

Proceeding similarly for the other two factors in (105), we get (using (A.6) in the appendix and summing over $m = |\mu|$) that

$$\sum_{\mu\le\beta}\binom{\beta}{\mu}\|D^\mu\varphi_a\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})}\|D^{\beta-\mu}\varphi_b\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})}$$
$$\le 16^\theta(CK_2)^2\left(\frac{B}{\epsilon}\right)^{|\beta|+2\theta}\sum_{m=0}^{|\beta|}\binom{|\beta|}{m}\frac{[(m+1)^{m+1}(|\beta|-m+1)^{|\beta|-m+1}]^\theta[m^m(|\beta|-m)^{|\beta|-m}]^{1-\theta}}{(|\beta|+1)^{|\beta|+2\theta}}. \quad (106)$$

We simplify the sum in m. Note that for $m = 0$ and $m = |\beta|$, the summand is bounded by 1. Therefore, for $|\beta| \le 1$ the estimate (104) follows from (106), since $2 \cdot 16^\theta \le 7$. It remains to consider $|\beta| \ge 2$. For $m \ge 1$, $m < |\beta|$, we can use (A.8) in the appendix to get (since $(1 + 1/n)^n \le e$) that

$$\sum_{0<\mu<\beta}\binom{\beta}{\mu}\|D^\mu\varphi_a\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})}\|D^{\beta-\mu}\varphi_b\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})}$$
$$\le \frac{e^{1/12}}{\sqrt{2\pi}}(CK_2)^2(16e^2)^\theta\left(\frac{B}{\epsilon}\right)^{|\beta|+2\theta}\frac{|\beta|^{|\beta|+1/2}}{(|\beta|+1)^{|\beta|+2\theta}}\sum_{m=1}^{|\beta|-1}\frac{[(m+1)(|\beta|-m+1)]^\theta}{\sqrt{m}\sqrt{|\beta|-m}}.$$

Since the function

$$f(x) = (x+1)(|\beta| - x + 1), \quad x \in [1, |\beta| - 1],$$

has its maximum (which is $(|\beta|/2 + 1)^2$) at $x = |\beta|/2$, and since

$$\sum_{m=1}^{|\beta|-1} \frac{1}{\sqrt{m}\sqrt{|\beta|-m}} \le \int_0^{|\beta|} \frac{1}{\sqrt{x}\sqrt{|\beta|-x}} \, dx = \pi,$$

we get

$$\sum_{0 < \mu < \beta} \binom{\beta}{\mu} \|D^\mu \varphi_a\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})} \|D^{\beta-\mu}\varphi_b\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})} \le \mathrm{e}^{1/12}(16\mathrm{e}^2)^\theta \sqrt{\frac{\pi}{2}} (CK_2)^2 \sqrt{|\beta|} \left(\frac{B}{\epsilon}\right)^{|\beta|+2\theta}. \quad (107)$$

The estimate (104) now follows from (105), (106), and (107), since $\mathrm{e}^{1/12}(16\mathrm{e}^2)^\theta \sqrt{\pi/2} \le 10$ and $2 \cdot 16^\theta \le 7$ (recall that $p \ge 5$). This finishes the proof of Lemma 5.1. $\qquad\square$

The next two lemmas, used in the proof above of Lemma 3.6, control the $L^{3p/2}$-norm of derivatives of $U_{a,b}$.

Lemma 5.2. *Define $U_{a,b}$ by (48). Then for all $a, b \in \{1, \ldots, N\}$, and all $\mu \in \mathbb{N}_0^3$ with $|\mu| \le 2$,*

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega)} \le 4\pi K_3 (C^2 + 2C_1/R^2), \quad (108)$$

with K_3 from Corollary D.4, C from Remark 2.2, C_1 from (23), and $R = \min\{1, |x_0|/4\}$.

Proof. Recall that $\omega = B_R(x_0)$, $R = \min\{1, |x_0|/4\}$. Using (18), and Corollary D.4, we get, for all $\mu \in \mathbb{N}_0^3$ with $|\mu| \le 2$,

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega)} \le \|U_{a,b}\|_{W^{2,3p/2}(B_R(x_0))} \le K_3 \left\{ \|\Delta U_{a,b}\|_{L^{3p/2}(B_{2R}(x_0))} + \frac{1}{R^2} \|U_{a,b}\|_{L^{3p/2}(B_{2R}(x_0))} \right\}. \quad (109)$$

By the definition of $U_{a,b}$ (see (48)) we have

$$-\Delta U_{a,b}(x) = 4\pi \, \varphi_a(x)\overline{\varphi_b}(x) \quad \text{for } x \in \mathbb{R}^3, \quad (110)$$

and $\|U_{a,b}\|_\infty \le C_1$ (see (23)). Hence, from (109), Hölder's inequality, and the choice of C (see Remark 2.2; recall also that $p \ge 5$)

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega)} \le 4\pi K_3 \left\{ \|\varphi_a\|_{L^{3p}(B_{2R}(x_0))} \|\varphi_b\|_{L^{3p}(B_{2R}(x_0))} + \frac{1}{R^2} \|U_{a,b}\|_\infty |B_{2R}(x_0)|^{2/3p} \right\}$$

$$\le 4\pi K_3 (C^2 + 2C_1/R^2). \qquad\square$$

Lemma 5.3. *Assume the induction hypothesis (40) holds, and define $U_{a,b}$ by (48). Then for all $a, b \in \{1, \ldots, N\}$, all $k \in \{0, \ldots, j-1\}$, all $\mu \in \mathbb{N}_0^3$ with $|\mu| \le j - k$, and all $\epsilon > 0$ with $\epsilon(j+1) \le R/2$,*

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega_{\epsilon(j-k+1/4)})}$$

$$\le C_3 C^2 \left(\frac{\sqrt{B}}{\epsilon}\right)^{|\mu|} \left(\frac{|\mu|+1/4}{j-k+1/4}\right)^{|\mu|} + C_3 C^2 \sqrt{|\mu|} \left(\frac{B}{\epsilon}\right)^{|\mu|+2\theta-2} \left(\frac{|\mu|+1/4}{j-k+1/4}\right)^{|\mu|+2\theta-2}, \quad (111)$$

with $\theta = \theta(p) = 2/p$, C and B from Remark 2.2, and C_3 the constant in (26).

Proof. If $m := |\mu| \leq 2$, (111) follows from Lemma 5.2 and the definition of C_3 in (26), since $\epsilon(j-k+1/4) \leq \epsilon(j+1) \leq R/2 < 1$, and $C, B > 1$ (see Remark 2.2).

If $m := |\mu| \geq 3$ then we write $\mu = \mu_{m-2} + e_{\nu_1} + e_{\nu_2}$ with $\nu_i \in \{1, 2, 3\}$, $i = 1, 2$, $|\mu_{m-2}| = m - 2$. Then by the definition of the $W^{2,3p/2}$-norm (recall (18)) we find that

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega_{\epsilon(j-k+1/4)})} \leq \|D^{\mu_{m-2}} U_{a,b}\|_{W^{2,3p/2}(\omega_{\epsilon(j-k+1/4)})}$$
$$= \|D^{\mu_{m-2}} U_{a,b}\|_{W^{2,3p/2}(\omega_{\tilde\epsilon_1(m-1+1/4)})}, \tag{112}$$

with $\tilde\epsilon_1$ such that

$$\tilde\epsilon_1(m - 1 + 1/4) = \epsilon(j - k + 1/4). \tag{113}$$

To estimate the norm in (112) we will again use that $U_{a,b}$ satisfies (110). Applying $D^{\mu_{m-2}}$ to (110) and using the elliptic *a priori* estimate in Corollary D.4 (with $r = r_1 = R - \tilde\epsilon_1(m-1+1/4)$ and $\delta = \delta_1 = \tilde\epsilon_1/4$; recall that $\omega_\rho = B_{R-\rho}(x_0)$) we get

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega_{\epsilon(j-k+1/4)})} \leq 4\pi K_3 \|D^{\mu_{m-2}}(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\tilde\epsilon_1(m-1)})} + \frac{16 K_3}{\tilde\epsilon_1^2} \|D^{\mu_{m-2}} U_{a,b}\|_{L^{3p/2}(\omega_{\tilde\epsilon_1(m-1)})}, \tag{114}$$

with $K_3 = K_3(p)$ the constant in (D.9). Notice that for this estimate we needed to enlarge the domain, taking the ball with a radius $\tilde\epsilon_1/4$ larger.

We now iterate the procedure (on the second term on the right side of (114)), with $\tilde\epsilon_i$ ($i = 2, \ldots, \lfloor\frac{m}{2}\rfloor$) such that

$$\tilde\epsilon_i(m - 2i + 1 + 1/4) = \tilde\epsilon_{i-1}(m - 2(i-1) + 1), \tag{115}$$

and with $r = r_i = R - \tilde\epsilon_i(m - 2i + 1 + 1/4)$ and $\delta = \delta_i = \tilde\epsilon_i/4$. Note that (113) and (115) imply that

$$\tilde\epsilon_i \geq \tilde\epsilon_{i-1} \geq \cdots \geq \tilde\epsilon_1 = \epsilon \frac{j - k + 1/4}{m - 1 + 1/4} \quad \text{for } i = 2, \ldots, \left\lfloor\frac{m}{2}\right\rfloor \tag{116}$$

and

$$\tilde\epsilon_i(m - 2i + 1) \leq \tilde\epsilon_{i-1}(m - 2(i-1) + 1) \leq \ldots \leq \tilde\epsilon_1(m-1) \leq \epsilon(j - k + 1/4). \tag{117}$$

We get (with $\prod_{\ell=1}^0 \equiv 1$ and $|\mu_{m-2i}| = m - 2i$),

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega_{\epsilon(j-k+1/4)})} \leq 4\pi K_3 \sum_{i=1}^{\lfloor\frac{m}{2}\rfloor} \left(\|D^{\mu_{m-2i}}(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\tilde\epsilon_i(m-2i+1)})} \prod_{\ell=1}^{i-1} \frac{16 K_3}{\tilde\epsilon_\ell^2} \right)$$
$$+ \left(\prod_{\ell=1}^{\lfloor\frac{m}{2}\rfloor} \frac{16 K_3}{\tilde\epsilon_\ell^2} \right) \|D^{\mu_{m-2\lfloor\frac{m}{2}\rfloor}} U_{a,b}\|_{L^{3p/2}(\omega_{\tilde\epsilon_{\lfloor\frac{m}{2}\rfloor}(m-2\lfloor\frac{m}{2}\rfloor+1)})}. \tag{118}$$

Using (116), and Lemma 5.1 for each $i = 1, \ldots, \lfloor\frac{m}{2}\rfloor$ fixed (note that $\tilde\epsilon_i(m - 2i + 1) \leq R/2$ by (117) since $\epsilon(j + 1) \leq R/2$) we get that

$$\|D^{\mu_{m-2i}}(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\tilde\epsilon_i(m-2i+1)})} \prod_{\ell=1}^{i-1} \frac{16 K_3}{\tilde\epsilon_\ell^2} \leq 20 K_2^2 C^2 \sqrt{m} \left(\frac{B}{\epsilon}\right)^{m+2\theta-2} \left(\frac{m-1+1/4}{j-k+1/4}\right)^{m+2\theta-2} \left(\frac{16 K_3}{B^2}\right)^{i-1},$$
$$\tag{119}$$

with K_2 from Corollary D.2, and $\theta = \theta(p) = 2/p$. Here we also used that $1 + \sqrt{m-2i} \le 2\sqrt{m}$. Note that $\sum_{i=1}^{\lfloor \frac{m}{2} \rfloor} (16K_3/B^2)^{i-1} < 2$ since $B^2 > 32K_3$ (see Remark 2.2). It follows that

$$4\pi K_3 \sum_{i=1}^{\lfloor \frac{m}{2} \rfloor} \left(\| D^{\mu_{m-2i}} (\varphi_a \overline{\varphi_b}) \|_{L^{3p/2}(\omega_{\tilde{\epsilon}_i(m-2i+1)})} \prod_{\ell=1}^{i-1} \frac{16K_3}{\tilde{\epsilon}_\ell^2} \right)$$
$$\le 160\pi K_2^2 K_3 C^2 \sqrt{m} \left(\frac{B}{\epsilon} \right)^{m+2\theta-2} \left(\frac{m+1/4}{j-k+1/4} \right)^{m+2\theta-2}. \quad (120)$$

We now estimate the last term in (118). Let $\delta = m - 2\lfloor \frac{m}{2} \rfloor \in \{0, 1\}$ (depending on whether m is even or odd). Then, using (116) and Lemma 5.2, we get that

$$\left(\prod_{\ell=1}^{\lfloor \frac{m}{2} \rfloor} \frac{16K_3}{\tilde{\epsilon}_\ell^2} \right) \| D^{\mu_{m-2\lfloor \frac{m}{2} \rfloor}} U_{a,b} \|_{L^{3p/2}(\omega_{\tilde{\epsilon}_{\lfloor \frac{m}{2} \rfloor}(m-2\lfloor \frac{m}{2} \rfloor+1)})}$$
$$\le 4\pi K_3 (C^2 + 2C_1/R^2) \left(\frac{\sqrt{16K_3}}{\epsilon} \right)^m \left(\frac{m-1+1/4}{j-k+1/4} \right)^m \left(\frac{\epsilon(j-k+1/4)}{m-1+1/4} \right)^\delta$$
$$\le 4\pi K_3 (1 + 2C_1/R^2) C^2 \left(\frac{\sqrt{B}}{\epsilon} \right)^m \left(\frac{m+1/4}{j-k+1/4} \right)^m. \quad (121)$$

Here we also used that $m \ge 3$ and $K_3 \ge 1$ (see Corollary D.4), that $C > 1$ and $B > 16K_3$ (see Remark 2.2), and that $\epsilon(j-k+1/4) \le 1$.

Combining (118), (120), and (121) finishes the proof of (111) in the case $m = |\mu| \ge 3$.

This finishes the proof of Lemma 5.3. $\qquad \square$

Appendix A: Multiindices and Stirling's formula

For $\sigma = (\sigma_1, \sigma_2, \sigma_3) \in \mathbb{N}_0^3$ we let $|\sigma| := \sigma_1 + \sigma_2 + \sigma_3$, and

$$D^\sigma := D_1^{\sigma_1} D_2^{\sigma_2} D_3^{\sigma_3}, \quad D_\nu := -\mathrm{i} \frac{\partial}{\partial x_\nu} =: -\mathrm{i} \partial_\nu, \quad \nu = 1, 2, 3. \quad (\text{A.1})$$

This way,

$$\partial^\sigma := \frac{\partial^{|\sigma|}}{\partial \boldsymbol{x}^\sigma} := \frac{\partial^{|\sigma|}}{\partial x_1^{\sigma_1} x_2^{\sigma_2} x_3^{\sigma_3}} = (-\mathrm{i})^{|\sigma|} D^\sigma.$$

We let $\sigma! := \sigma_1! \sigma_2! \sigma_3!$, and, for $n \in \mathbb{N}_0$,

$$\binom{n}{\sigma} := \frac{n!}{\sigma!} = \frac{n!}{\sigma_1! \sigma_2! \sigma_3!}. \quad (\text{A.2})$$

With this notation we have the multinomial formula, for $\boldsymbol{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ and $n \in \mathbb{N}_0$,

$$(x_1 + x_2 + x_3)^n = \sum_{\substack{\mu \in \mathbb{N}_0^3 \\ |\mu|=n}} \binom{n}{\mu} \boldsymbol{x}^\mu. \quad (\text{A.3})$$

Here, $x^\mu := x_1^{\mu_1} x_2^{\mu_2} x_3^{\mu_3}$. It follows that

$$|\sigma|! \le 3^{|\sigma|} \sigma! \quad \text{for all } \sigma \in \mathbb{N}_0^3, \tag{A.4}$$

since, using (A.2), that $(1, 1, 1)^\mu = 1$ for all $\mu \in \mathbb{N}_0^3$, and (A.3),

$$\frac{|\sigma|!}{\sigma!} = \binom{|\sigma|}{\sigma} \le \sum_{\substack{\mu \in \mathbb{N}_0^3 \\ |\mu| = |\sigma|}} \binom{|\sigma|}{\mu} (1, 1, 1)^\mu = (1 + 1 + 1)^{|\sigma|} = 3^{|\sigma|}.$$

We also define

$$\binom{\sigma}{\mu} := \frac{\sigma!}{\mu! \, (\sigma - \mu)!} \tag{A.5}$$

for $\sigma, \mu \in \mathbb{N}_0^3$ with $\mu \le \sigma$, that is, $\mu_\nu \le \sigma_\nu$, $\nu = 1, 2, 3$. Note that for all $\sigma \in \mathbb{N}_0^3$ and $k \in \mathbb{N}_0$ (see [Kato 1996, Proposition 2.1]),

$$\sum_{\mu \le \sigma, |\mu| = k} \binom{\sigma}{\mu} = \binom{|\sigma|}{k}. \tag{A.6}$$

Finally, by [Abramowitz and Stegun 1992, 6.1.38], we have the following generalization of Stirling's formula: For $m \in \mathbb{N}$,

$$m! = \sqrt{2\pi} \, m^{m+\frac{1}{2}} \exp\left(-m + \frac{\vartheta}{12m}\right) \quad \text{for some } \vartheta = \vartheta(m) \in (0, 1), \tag{A.7}$$

and so for $n, m \in \mathbb{N}$, $m < n$,

$$\binom{n}{m} = \frac{1}{\sqrt{2\pi}} \frac{n^{n+1/2}}{m^{m+1/2}(n-m)^{n-m+1/2}} \exp\left(\frac{\vartheta(n)}{12n} - \frac{\vartheta(m)}{12m} - \frac{\vartheta(n-m)}{12(n-m)}\right)$$

$$\le \frac{e^{1/12}}{\sqrt{2\pi}} \frac{n^{n+1/2}}{m^{m+1/2}(n-m)^{n-m+1/2}}. \tag{A.8}$$

Appendix B: Choice of the localization

Recall that, for $x_0 \in \mathbb{R}^3 \setminus \{0\}$ and $R = \min\{1, |x_0|/4\}$, we have defined $\omega = B_R(x_0)$, $\omega_\delta = B_{R-\delta}(x_0)$, and that $\epsilon > 0$ is such that $\epsilon(j + 1) \le R/2$. Also, recall (see (44)) that we have chosen a function Φ (depending on j) satisfying

$$\Phi \in C_0^\infty(\omega_{\epsilon(j+3/4)}), \quad 0 \le \Phi \le 1, \quad \text{with } \Phi \equiv 1 \text{ on } \omega_{\epsilon(j+1)}. \tag{B.1}$$

For $j \in \mathbb{N}$ we choose functions $\{\chi_k\}_{k=0}^j$, and $\{\eta_k\}_{k=0}^j$ (all depending on j) with the following properties (for an illustration, see Figures 1 and 2). The functions $\{\chi_k\}_{k=0}^j$ are such that

$$\chi_0 \in C_0^\infty(\omega_{\epsilon(j+1/4)}) \quad \text{with} \quad \chi_0 \equiv 1 \quad \text{on } \omega_{\epsilon(j+1/2)},$$

and, for $k = 1, \ldots, j$,

$$\chi_k \in C_0^\infty(\omega_{\epsilon(j-k+1/4)}) \text{ with } \begin{cases} \chi_k \equiv 1 & \text{on } \omega_{\epsilon(j-k+1/2)} \setminus \omega_{\epsilon(j-k+1+1/4)}, \\ \chi_k \equiv 0 & \text{on } \mathbb{R}^3 \setminus (\omega_{\epsilon(j-k+1/4)} \setminus \omega_{\epsilon(j-k+1+1/2)}). \end{cases}$$
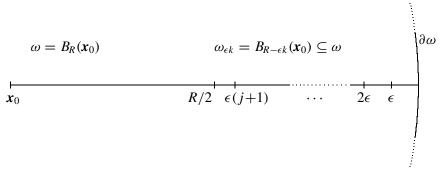
Figure 1. The geometry of $\omega = B_R(\boldsymbol{x}_0)$ and the $\omega_{\epsilon k} = B_{R-\epsilon k}(\boldsymbol{x}_0)$.
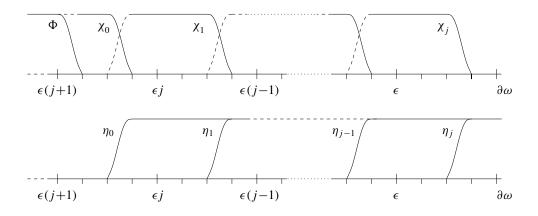
Figure 2. The localization functions.

Finally, the functions $\{\eta_k\}_{k=0}^j$ are such that for $k = 0, \ldots, j$,

$$\eta_k \in C^\infty(\mathbb{R}^3) \quad \text{with} \quad \begin{cases} \eta_k \equiv 1 & \text{on} \quad \mathbb{R}^3 \setminus \omega_{\epsilon(j-k+1/4)}, \\ \eta_k \equiv 0 & \text{on} \quad \omega_{\epsilon(j-k+1/2)}. \end{cases}$$

Moreover we ask that

$$\begin{aligned} \chi_0 + \eta_0 &\equiv 1 && \text{on} \quad \mathbb{R}^3, \\ \chi_k + \eta_k &\equiv 1 && \text{on} \quad \mathbb{R}^3 \setminus \omega_{\epsilon(j-k+1+1/4)} \quad \text{for } k = 1, \ldots, j, \\ \eta_k &\equiv \chi_{k+1} + \eta_{k+1} && \text{on} \quad \mathbb{R}^3 \text{ for } k = 0, \ldots, j-1. \end{aligned} \tag{B.2}$$

Furthermore, we choose these localization functions such that, for a constant $C_* > 0$ (independent of ϵ, k, j, β) and for all $\beta \in \mathbb{N}_0^3$ with $|\beta| = 1$, we have that

$$|D^\beta \chi_k(\boldsymbol{x})| \leq \frac{C_*}{\epsilon} \quad \text{and} \quad |D^\beta \eta_k(\boldsymbol{x})| \leq \frac{C_*}{\epsilon}, \tag{B.3}$$

for $k = 0, \ldots, j$, and all $\boldsymbol{x} \in \mathbb{R}^3$.

The next lemma shows how to use these localization functions.

Lemma B.1. *For $j \in \mathbb{N}$ fixed, choose functions $\{\chi_k\}_{k=0}^j$, and $\{\eta_k\}_{k=0}^j$ as above, and let $\sigma \in \mathbb{N}_0^3$ with $|\sigma| = j$. For $\ell \in \mathbb{N}$ with $\ell \le j$, choose multiindices $\{\beta_k\}_{k=0}^\ell$ such that*

$$|\beta_k| = k \ \text{for } k = 0, \dots, \ell, \quad \beta_{k-1} < \beta_k \ \text{for } k = 1, \dots, \ell, \ \text{and} \ \beta_\ell \le \sigma.$$

Then for all $g \in \mathscr{S}'(\mathbb{R}^3)$,

$$D^\sigma g = \sum_{k=0}^\ell D^{\beta_k} \chi_k D^{\sigma - \beta_k} g + \sum_{k=0}^{\ell-1} D^{\beta_k} [\eta_k, D^{\mu_k}] D^{\sigma - \beta_{k+1}} g + D^{\beta_\ell} \eta_\ell D^{\sigma - \beta_\ell} g, \tag{B.4}$$

with $\mu_k = \beta_{k+1} - \beta_k$ for $k = 0, \dots, \ell - 1$ (hence, $|\mu_k| = 1$).

Proof. We use induction on ℓ from $\ell = 1$ to $\ell = j$. We start by proving the claim for $\ell = 1$. By using property (B.2) of the localization functions and that $\beta_1 = \beta_0 + \mu_0 = \mu_0$ (since $\beta_0 = 0$) we find that

$$D^\sigma g = \chi_0 D^\sigma g + \eta_0 D^\sigma g = \chi_0 D^\sigma g + \eta_0 D^{\sigma - \beta_1 + \mu_0} g. \tag{B.5}$$

The first term on the right side of (B.5) is the term corresponding to $k = 0$ in the first sum in (B.4). In the second term in (B.5), commuting the derivative through η_0, we find that

$$\eta_0 D^{\sigma - \beta_1 + \mu_0} g = D^{\mu_0} \eta_0 D^{\sigma - \beta_1} g + [\eta_0, D^{\mu_0}] D^{\sigma - \beta_1} g.$$

Since $\eta_0 = \chi_1 + \eta_1$ by property (B.2), this implies that

$$\eta_0 D^{\sigma - \beta_1 + \mu_0} g = D^{\beta_1} \chi_1 D^{\sigma - \beta_1} g + D^{\beta_1} \eta_1 D^{\sigma - \beta_1} g + [\eta_0, D^{\mu_0}] D^{\sigma - \beta_1} g. \tag{B.6}$$

The identity (B.4) for $\ell = 1$ follows from (B.5) and (B.6).

We now assume that (B.4) holds for $\ell - 1$ for some $\ell \ge 2$, i.e.,

$$D^\sigma g = \sum_{k=0}^{\ell-1} D^{\beta_k} \chi_k D^{\sigma - \beta_k} g + \sum_{k=0}^{\ell-2} D^{\beta_k} [\eta_k, D^{\mu_k}] D^{\sigma - \beta_{k+1}} g + D^{\beta_{\ell-1}} \eta_{\ell-1} D^{\sigma - \beta_{\ell-1}} g, \tag{B.7}$$

and prove it then holds for ℓ. Since $\beta_{\ell-1} = \beta_\ell - \mu_{\ell-1}$ we can rewrite the last term on the right side of (B.7) as

$$D^{\beta_{\ell-1}} \eta_{\ell-1} D^{\sigma - \beta_{\ell-1}} g = D^{\beta_{\ell-1}} \eta_{\ell-1} D^{\sigma - \beta_\ell + \mu_{\ell-1}} g.$$

Again, commuting the $\mu_{\ell-1}$-derivative through $\eta_{\ell-1}$ this implies that

$$
\begin{aligned}
D^{\beta_{\ell-1}} \eta_{\ell-1} D^{\sigma - \beta_{\ell-1}} g &= D^{\beta_{\ell-1} + \mu_{\ell-1}} \eta_{\ell-1} D^{\sigma - \beta_\ell} g + D^{\beta_{\ell-1}} [\eta_{\ell-1}, D^{\mu_{\ell-1}}] D^{\sigma - \beta_\ell} g \\
&= D^{\beta_\ell} (\eta_\ell + \chi_\ell) D^{\sigma - \beta_\ell} g + D^{\beta_{\ell-1}} [\eta_{\ell-1}, D^{\mu_{\ell-1}}] D^{\sigma - \beta_\ell} g, \tag{B.8}
\end{aligned}
$$

using (B.2). Collecting together (B.7) and (B.8) proves that (B.4) holds for ℓ.

The claim of the lemma then follows by induction. $\qquad\square$

Appendix C: Norms of some operators on $L^p(\mathbb{R}^3)$

In this section we prove two lemmas on bounds on certain operators involving the operator $E(\boldsymbol{p}) = \sqrt{-\Delta + \alpha^{-2}}$.

Lemma C.1. *Let the operators $S_\nu = E(\boldsymbol{p})^{-1}D_\nu$, $\nu \in \{1, 2, 3\}$, be defined for $f \in \mathscr{S}(\mathbb{R}^3)$ by*

$$(S_\nu f)(\boldsymbol{x}) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{i\boldsymbol{x}\cdot\boldsymbol{p}} E(\boldsymbol{p})^{-1} p_\nu \hat{f}(\boldsymbol{p}) \, d\boldsymbol{p},$$

with $\hat{f}(\boldsymbol{p}) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{-i\boldsymbol{x}\cdot\boldsymbol{p}} f(\boldsymbol{x}) \, d\boldsymbol{x}$ the Fourier transform of f. (Here, $\boldsymbol{p} = (p_1, p_2, p_3)$.)

Then, for all $\mathfrak{p} \in (1, \infty)$, the S_ν extend to bounded operators, $S_\nu : L^{\mathfrak{p}}(\mathbb{R}^3) \to L^{\mathfrak{p}}(\mathbb{R}^3)$, $\nu \in \{1, 2, 3\}$. Clearly, $\|S_\nu\|_{\mathscr{B}_{\mathfrak{p}}} = \|S_\mu\|_{\mathscr{B}_{\mathfrak{p}}}$, $\nu \neq \mu$. We let

$$K_1 \equiv K_1(\mathfrak{p}) := \|S_1\|_{\mathscr{B}_{\mathfrak{p}}}. \tag{C.1}$$

Proof. This follows from [Sogge 1993, Theorem 0.2.6] and the *Remarks* right after it. In fact, since (by induction),

$$D_{\boldsymbol{p}}^\gamma \big(p_\nu E(\boldsymbol{p})^{-1}\big) = P_{\gamma,\nu}(\boldsymbol{p})E(\boldsymbol{p})^{-1-2|\gamma|}, \quad \gamma \in \mathbb{N}_0^3,$$

for some polynomials $P_{\gamma,\nu}$ of degree $|\gamma| + 1$, the functions $m_\nu(\boldsymbol{p}) = p_\nu E(\boldsymbol{p})^{-1}$ are smooth and satisfy the estimates

$$|D_{\boldsymbol{p}}^\gamma m_\nu(\boldsymbol{p})| \leq C_{\gamma,\nu}|\boldsymbol{p}|^{-|\gamma|}, \quad \gamma \in \mathbb{N}_0^3,$$

for some constants $C_{\gamma,\nu} > 0$, which is what is needed in the reference above. $\qquad\square$

For $\mathfrak{p}, \mathfrak{q} \in [1, \infty]$, denote by $\|\cdot\|_{\mathscr{B}_{\mathfrak{p},\mathfrak{q}}}$ the operator norm on bounded operators from $L^{\mathfrak{p}}(\mathbb{R}^3)$ to $L^{\mathfrak{q}}(\mathbb{R}^3)$.

Lemma C.2. *For all $\mathfrak{p}, \mathfrak{r} \in [1, \infty)$, $\mathfrak{q} \in (1, \infty)$, with $\mathfrak{p}^{-1} + \mathfrak{q}^{-1} + \mathfrak{r}^{-1} = 2$, all $\alpha > 0$, all $\beta \in \mathbb{N}_0^3$ (with $|\beta| > 1$ if $\mathfrak{r} = 1$), and all $\Phi, \chi \in C^\infty(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ with*

$$\mathrm{dist}(\mathrm{supp}(\chi), \mathrm{supp}(\Phi)) \geq d, \tag{C.2}$$

the operator $\Phi E(\boldsymbol{p})^{-1}D^\beta \chi$ is bounded from $L^{\mathfrak{p}}(\mathbb{R}^3)$ to $(L^{\mathfrak{q}}(\mathbb{R}^3))' = L^{\mathfrak{q}^*}(\mathbb{R}^3)$ (with $\mathfrak{q}^{-1} + \mathfrak{q}^{*-1} = 1$), and

$$\|\Phi E(\boldsymbol{p})^{-1}D^\beta \chi\|_{\mathscr{B}_{\mathfrak{p},\mathfrak{q}^*}} \leq \frac{4\sqrt{2}}{\pi}\beta!\left(\frac{8}{d}\right)^{|\beta|}d^{3/\mathfrak{r}-2}\big(\mathfrak{r}(|\beta|+2)-3\big)^{-1/\mathfrak{r}}\|\Phi\|_\infty\|\chi\|_\infty. \tag{C.3}$$

In particular, (when $\mathfrak{r} = 1$, i.e., $\mathfrak{q}^* = \mathfrak{p}$),

$$\|\Phi E(\boldsymbol{p})^{-1}D^\beta \chi\|_{\mathscr{B}_{\mathfrak{p}}} \leq \frac{32\sqrt{2}}{\pi}\frac{\beta!}{|\beta|-1}\left(\frac{8}{d}\right)^{|\beta|-1}\|\Phi\|_\infty\|\chi\|_\infty, \tag{C.4}$$

for all $\beta \in \mathbb{N}_0^3$ with $|\beta| > 1$.

Proof. We use duality. Let $f, g \in \mathscr{S}(\mathbb{R}^3)$. Note that, since $\Phi f, D^\beta(\chi g) \in L^2(\mathbb{R}^3)$, the spectral theorem, and the formula

$$\frac{1}{\sqrt{x}} = \frac{1}{\pi}\int_0^\infty \frac{1}{x+t}\frac{dt}{\sqrt{t}}, \quad x > 0, \tag{C.5}$$

imply that

$$(f, \Phi E(\boldsymbol{p})^{-1} D^\beta \chi g) = \frac{1}{\pi} \int_0^\infty \frac{dt}{\sqrt{t}} \, (f, \Phi(-\Delta + \alpha^{-2} + t)^{-1} D^\beta \chi g).$$

By using the formula for the kernel of the operator $(-\Delta + \alpha^{-2} + t)^{-1}$ [Reed and Simon 1975, (IX.30)], and integrating by parts, we get

$$
\begin{aligned}
(f, \Phi E(\boldsymbol{p})^{-1} D^\beta \chi g) &= \frac{1}{\pi} \int_0^\infty \int_{\mathbb{R}^3} \overline{f(\boldsymbol{x})} \Phi(\boldsymbol{x}) \int_{\mathbb{R}^3} \frac{e^{-\sqrt{\alpha^{-2}+t}\,|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi |\boldsymbol{x}-\boldsymbol{y}|} [D^\beta(\chi g)](\boldsymbol{y}) \, d\boldsymbol{x} \, d\boldsymbol{y} \, \frac{dt}{\sqrt{t}} \\
&= \frac{(-1)^{|\beta|}}{\pi} \int_0^\infty \int_{\mathbb{R}^3} \overline{f(\boldsymbol{x})} \Phi(\boldsymbol{x}) \int_{\mathbb{R}^3} \left(D_{\boldsymbol{y}}^\beta \frac{e^{-\sqrt{\alpha^{-2}+t}\,|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi |\boldsymbol{x}-\boldsymbol{y}|} \right) \chi(\boldsymbol{y}) g(\boldsymbol{y}) \, d\boldsymbol{x} \, d\boldsymbol{y} \, \frac{dt}{\sqrt{t}}.
\end{aligned}
$$

Notice that the integrand is different from zero only for $|\boldsymbol{x} - \boldsymbol{y}| \geq d$, due to the assumption (C.2). Hence, by Fubini's theorem,

$$(f, \Phi E(\boldsymbol{p})^{-1} D^\beta \chi g) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} F(\boldsymbol{x}) H(\boldsymbol{x} - \boldsymbol{y}) G(\boldsymbol{y}) \, d\boldsymbol{x} \, d\boldsymbol{y}, \tag{C.6}$$

with $F(\boldsymbol{x}) = \overline{f(\boldsymbol{x})} \Phi(\boldsymbol{x})$, $G(\boldsymbol{y}) = \chi(\boldsymbol{y}) g(\boldsymbol{y})$, and

$$H(\boldsymbol{z}) \equiv H_{\alpha,\beta,d}(\boldsymbol{z}) = \mathbb{1}_{\{|\cdot| \geq d\}}(\boldsymbol{z}) \frac{(-1)^{|\beta|}}{\pi} \int_0^\infty \left(D_{\boldsymbol{z}}^\beta \frac{e^{-\sqrt{\alpha^{-2}+t}\,|\boldsymbol{z}|}}{4\pi |\boldsymbol{z}|} \right) \frac{dt}{\sqrt{t}}.$$

Now, by (C.8) in Lemma C.3 below, uniformly for $\alpha > 0$,

$$|H(\boldsymbol{z})| \leq \mathbb{1}_{\{|\cdot| \geq d\}}(\boldsymbol{z}) \frac{\sqrt{2}}{4\pi^2} \frac{\beta!}{|\boldsymbol{z}|} \left(\frac{8}{|\boldsymbol{z}|} \right)^{|\beta|} \int_0^\infty e^{-\sqrt{t}|\boldsymbol{z}|/2} \frac{dt}{\sqrt{t}} = \mathbb{1}_{\{|\cdot| \geq d\}}(\boldsymbol{z}) \frac{\sqrt{2}}{\pi^2} \frac{\beta!}{|\boldsymbol{z}|^2} \left(\frac{8}{|\boldsymbol{z}|} \right)^{|\beta|},$$

and so, for all $\alpha > 0$, $\mathfrak{r} \in [1, \infty)$, and all $\beta \in \mathbb{N}_0^3$ (with $|\beta| > 1$ if $\mathfrak{r} = 1$),

$$
\begin{aligned}
\|H\|_{\mathfrak{r}} &\leq (4\pi)^{1/\mathfrak{r}} \frac{\sqrt{2}}{\pi^2} \beta! \, 8^{|\beta|} \left(\int_d^\infty \left(|\boldsymbol{z}|^{-|\beta|-2} \right)^r |\boldsymbol{z}|^2 \, d|\boldsymbol{z}| \right)^{1/\mathfrak{r}} \\
&= (4\pi)^{1/\mathfrak{r}} \frac{\sqrt{2}}{\pi^2} \beta! \left(\frac{8}{d} \right)^{|\beta|} d^{3/\mathfrak{r}-2} \left(\mathfrak{r}(|\beta| + 2) - 3 \right)^{-1/\mathfrak{r}}.
\end{aligned}
$$

From this, (C.6), and Young's inequality [Lieb and Loss 2001, Theorem 4.2] (notice that $C_Y \leq 1$), follows that, with $\mathfrak{p}, \mathfrak{q}, \mathfrak{r} \in [1, \infty)$, $\mathfrak{p}^{-1} + \mathfrak{q}^{-1} + \mathfrak{r}^{-1} = 2$,

$$
\begin{aligned}
|(f, \Phi E(\boldsymbol{p})^{-1} D^\beta \chi g)| &\leq \|F\|_{\mathfrak{q}} \|H\|_{\mathfrak{r}} \|G\|_{\mathfrak{p}} \\
&\leq (4\pi)^{1/\mathfrak{r}} \frac{\sqrt{2}}{\pi^2} \beta! \left(\frac{8}{d} \right)^{|\beta|} d^{3/\mathfrak{r}-2} \left(\mathfrak{r}(|\beta| + 2) - 3 \right)^{-1/\mathfrak{r}} \|F\|_{\mathfrak{q}} \|G\|_{\mathfrak{p}} \\
&\leq \frac{4\sqrt{2}}{\pi} \beta! \left(\frac{8}{d} \right)^{|\beta|} d^{3/\mathfrak{r}-2} \left(\mathfrak{r}(|\beta| + 2) - 3 \right)^{-1/\mathfrak{r}} \|\Phi\|_\infty \|\chi\|_\infty \|f\|_{\mathfrak{q}} \|g\|_{\mathfrak{p}}.
\end{aligned}
$$

Since $\mathscr{S}(\mathbb{R}^3)$ is dense in both $L^{\mathfrak{p}}(\mathbb{R}^3)$ and $L^{\mathfrak{q}^*}(\mathbb{R}^3)$, this finishes the proof of the lemma. $\square$

Lemma C.3. *For all $s > 0$, $\boldsymbol{x} \in \mathbb{R}^3 \setminus \{0\}$, and $\beta \in \mathbb{N}_0^3$,*

$$\left| \partial_{\boldsymbol{x}}^{\beta} \frac{1}{|\boldsymbol{x}|} \right| \leq \frac{\sqrt{2}\beta!}{|\boldsymbol{x}|} \left(\frac{8}{|\boldsymbol{x}|} \right)^{|\beta|}, \tag{C.7}$$

$$\left| \partial_{\boldsymbol{x}}^{\beta} \frac{e^{-s|\boldsymbol{x}|}}{|\boldsymbol{x}|} \right| \leq \frac{\sqrt{2}\beta!}{|\boldsymbol{x}|} \left(\frac{8}{|\boldsymbol{x}|} \right)^{|\beta|} e^{-s|\boldsymbol{x}|/2}. \tag{C.8}$$

Proof. We will use the Cauchy inequalities [Hörmander 1973, Theorem 2.2.7]. To avoid confusion with the Euclidean norm $|\cdot|$ (in $\mathbb{R}^3$ or in $\mathbb{C}^3$), we denote by $|\cdot|_{\mathbb{C}}$ the absolute value in $\mathbb{C}$.

Let, for $\boldsymbol{w} = (w_1, w_2, w_3) \in \mathbb{C}^3$ and $r > 0$,

$$P_r^3(\boldsymbol{w}) = \{ \boldsymbol{z} \in \mathbb{C}^3 \mid |z_\nu - w_\nu|_{\mathbb{C}} < r, \ \nu = 1, 2, 3 \} \tag{C.9}$$

be the *polydisc* with *polyradius* $\boldsymbol{r} = (r, r, r)$. The Cauchy inequalities then state that if u is analytic in $P_r^3(\boldsymbol{w})$ and if $\sup_{\boldsymbol{z} \in P_r^3(\boldsymbol{w})} |u(\boldsymbol{z})|_{\mathbb{C}} \leq M$, then

$$|\partial_{\boldsymbol{z}}^{\beta} u(\boldsymbol{w})|_{\mathbb{C}} \leq M\beta! \, r^{-|\beta|} \quad \text{for all } \beta \in \mathbb{N}_0^3. \tag{C.10}$$

We take $\boldsymbol{w} = \boldsymbol{x} \in \mathbb{R}^3 \setminus \{0\} \subseteq \mathbb{C}^3$ and choose $r = |\boldsymbol{x}|/8$. We prove below that then we have (with $\boldsymbol{z}^2 := \sum_{\nu=1}^{3} z_\nu^2 \in \mathbb{C}$)

$$\operatorname{Re}(\boldsymbol{z}^2) \geq \tfrac{1}{2} |\boldsymbol{x}|^2 \quad \text{for } \boldsymbol{z} \in P_r^3(\boldsymbol{x}). \tag{C.11}$$

It follows that $\sqrt{\boldsymbol{z}^2} := \exp(\frac{1}{2} \operatorname{Log} \boldsymbol{z}^2)$ is well-defined and analytic on $P_r^3(\boldsymbol{x})$ with Log being the principal branch of the logarithm.

We will also argue below that

$$\operatorname{Re}(\sqrt{\boldsymbol{z}^2}) \geq \tfrac{1}{2} |\boldsymbol{x}| \quad \text{for } \boldsymbol{z} \in P_r^3(\boldsymbol{x}). \tag{C.12}$$

Then (by (C.11)) for all $\boldsymbol{z} \in P_r^3(\boldsymbol{x})$,

$$\left| \sqrt{\boldsymbol{z}^2} \right|_{\mathbb{C}} = \sqrt{|\boldsymbol{z}^2|_{\mathbb{C}}} \geq \sqrt{|\operatorname{Re} \boldsymbol{z}^2|} \geq |\boldsymbol{x}|/\sqrt{2}, \tag{C.13}$$

and (by (C.12)), for all $s \geq 0$ and all $\boldsymbol{z} \in P_r^3(\boldsymbol{x})$,

$$\left| \exp(-s\sqrt{\boldsymbol{z}^2}) \right|_{\mathbb{C}} = \exp(-s \operatorname{Re}(\sqrt{\boldsymbol{z}^2})) \leq \exp(-s|\boldsymbol{x}|/2). \tag{C.14}$$

Therefore, (C.7) and (C.8) follow from (C.10), (C.13), and (C.14).

It remains to prove (C.11) and (C.12).

For $\boldsymbol{z} \in P_r^3(\boldsymbol{x})$, write $\boldsymbol{z} = \boldsymbol{x} + \boldsymbol{a} + i\boldsymbol{b}$ with $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^3$ satisfying $|z_\nu - x_\nu|_{\mathbb{C}}^2 = a_\nu^2 + b_\nu^2 \leq (|\boldsymbol{x}|/8)^2$. Then

$$\boldsymbol{z}^2 = |\boldsymbol{x} + \boldsymbol{a}|^2 - |\boldsymbol{b}|^2 + 2i(\boldsymbol{x} + \boldsymbol{a}) \cdot \boldsymbol{b},$$

so, with $\epsilon = 1/8$,

$$\operatorname{Re}(\boldsymbol{z}^2) = |\boldsymbol{x}|^2 + |\boldsymbol{a}|^2 + 2\boldsymbol{x} \cdot \boldsymbol{a} - |\boldsymbol{b}|^2$$
$$\geq (1 - \epsilon)|\boldsymbol{x}|^2 + (2 - \epsilon^{-1})|\boldsymbol{a}|^2 - (|\boldsymbol{a}|^2 + |\boldsymbol{b}|^2) \geq \tfrac{35}{64}|\boldsymbol{x}|^2 > \tfrac{1}{2}|\boldsymbol{x}|^2.$$

This establishes (C.11) .

It follows from (C.11) that, with Arg the principal branch of the argument,

$$-\frac{\pi}{4} \leq \frac{1}{2}\text{Arg}(z^2) \leq \frac{\pi}{4} \quad \text{for } z \in P_r^3(\boldsymbol{x}). \tag{C.15}$$

Furthermore (still for $z \in P_r^3(\boldsymbol{x})$), because of (C.15),

$$\text{Re}(\sqrt{z^2}) = |z^2|_{\mathbb{C}}^{1/2} \cos(\tfrac{1}{2}\text{Arg}(z^2)) \geq |z^2|_{\mathbb{C}}^{1/2}/\sqrt{2}. \tag{C.16}$$

Combining with (C.11) we get (C.12).

This finishes the proof of the lemma.   □

Appendix D: Needed results

In this section we gather some results from the literature which are needed in our proofs.

Theorem D.1 [Adams and Fournier 2003, Theorem 5.8]. *Let Ω be a domain in $\mathbb{R}^n$ satisfying the cone condition. Let $m \in \mathbb{N}$, $\mathfrak{p} \in (1, \infty)$. If $m\mathfrak{p} > n$, let $\mathfrak{p} \leq \mathfrak{q} \leq \infty$; if $m\mathfrak{p} = n$, let $\mathfrak{p} \leq \mathfrak{q} < \infty$; if $m\mathfrak{p} < n$, let $\mathfrak{p} \leq \mathfrak{q} \leq \mathfrak{p}^* = n\mathfrak{p}/(n - m\mathfrak{p})$. Then there exists a constant K depending on $m, n, \mathfrak{p}, \mathfrak{q}$ and the dimensions of the cone C providing the cone condition for Ω, such that for all $u \in W^{m,\mathfrak{p}}(\Omega)$,*

$$\|u\|_{L^{\mathfrak{q}}(\Omega)} \leq K \|u\|_{W^{m,\mathfrak{p}}(\Omega)}^{\theta} \|u\|_{L^{\mathfrak{p}}(\Omega)}^{1-\theta}, \tag{D.1}$$

where $\theta = (n/m\mathfrak{p}) - (n/m\mathfrak{q})$.

We write $K = K(m, n, \mathfrak{p}, \mathfrak{q}, \Omega)$. We always use Theorem D.1 with $n = 3$, $m = 1$, and $\mathfrak{p} = p$, $\mathfrak{q} = 3p$ for some $p > 3$. Hence $m\mathfrak{p} > n$, $\mathfrak{p} \leq \mathfrak{q} \leq \infty$, and $\theta = \theta(p) = 2/p < 1$. Moreover, we always use it with Ω being a ball, whose radius in all cases is bounded from above by 1 and from below by $R/2$ for some $R > 0$ fixed.

Let $K_0 \equiv K_0(p) \equiv K(1, 3, p, 3p, B_1(0))$ with $B_1(0) \subseteq \mathbb{R}^3$ the unit ball (which does satisfy the cone condition). Note that then, by scaling, (D.1) implies that for all $r \leq 1$ and all $\boldsymbol{x}_0 \in \mathbb{R}^3$,

$$\|u\|_{L^{3p}(B_r(\boldsymbol{x}_0))} \leq K_0 r^{-\theta} \|u\|_{W^{1,p}(B_r(\boldsymbol{x}_0))}^{\theta} \|u\|_{L^p(B_r(\boldsymbol{x}_0))}^{1-\theta}, \tag{D.2}$$

with $\theta = 2/p$.

To summarize, we therefore have:

Corollary D.2. *Let $p > 3$ and $R \in (0, 1]$. Then there exists a constant K_2, depending only on p and R, such that for all $r \in [R/2, 1]$, $\boldsymbol{x}_0 \in \mathbb{R}^3$, and all $u \in W^{1,p}(B_r(\boldsymbol{x}_0))$,*

$$\|u\|_{L^{3p}(B_r(\boldsymbol{x}_0))} \leq K_2 \|u\|_{W^{1,p}(B_r(\boldsymbol{x}_0))}^{\theta} \|u\|_{L^p(B_r(\boldsymbol{x}_0))}^{1-\theta}, \tag{D.3}$$

with $\theta = 2/p$.

Here,

$$K_2 \equiv K_2(p, R) = (2/R)^{2/p} K_0(p), \tag{D.4}$$

where $K_0(p) = K(1, 3, p, 3p, B_1(0))$ in Theorem D.1 above.

Theorem D.3 [Chen and Wu 1998, Theorem 4.2]. *Let Ω be a bounded domain in $\mathbb{R}^n$ and let $a^{ij} \in C(\overline{\Omega})$, $b^i, c \in L^\infty(\Omega)$ $i, j \in \{1, \ldots, n\}$, with $\lambda, \Lambda > 0$ such that*

$$\sum_{i,j=1}^n a^{ij} \xi_i \xi_j \geq \lambda |\xi|^2 \quad \text{for all } x \in \Omega, \ \xi \in \mathbb{R}^n, \tag{D.5}$$

$$\sum_{i,j=1}^n \|a^{ij}\|_{L^\infty(\Omega)} + \sum_{i=1}^n \|b^i\|_{L^\infty(\Omega)} + \|c\|_{L^\infty(\Omega)} \leq \Lambda. \tag{D.6}$$

Suppose $u \in W^{2,\mathfrak{p}}_{\mathrm{loc}}(\Omega)$ satisfies

$$Lu = \sum_{i,j=1}^n -a^{ij} D_i D_j u + \sum_{i=1}^n b^i D_i u + cu = f. \tag{D.7}$$

Then for any $\Omega' \Subset \Omega$,

$$\|u\|_{W^{2,\mathfrak{p}}(\Omega')} \leq C \left\{ \frac{1}{\lambda} \|f\|_{L^\mathfrak{p}(\Omega)} + \|u\|_{L^\mathfrak{p}(\Omega)} \right\}, \tag{D.8}$$

where C depends only on n, $\mathfrak{p}$, Λ/λ, $\mathrm{dist}\{\Omega', \partial\Omega\}$, and the modulus of continuity of the a^{ij}'s.

We use Theorem D.3 in the case where Ω' and Ω are concentric balls (and with $n = 3$, $\mathfrak{p} = 3p/2$, $a^{ij} = \delta_{ij}$, $b^i = c = 0$; hence $\Lambda = \lambda = 1$). Reading the proof of the theorem above with this case in mind (see [Chen and Wu 1998, Lemma 4.1] in particular), one can make the dependence on $\mathrm{dist}\{\Omega', \partial\Omega\}$ explicit. More precisely:

Corollary D.4. *For all $p > 1$ there exists a constant $K_3 = K_3(p) \geq 1$ such that*

$$\|u\|_{W^{2,3p/2}(B_r(\mathbf{x}_0))} \leq K_3 \left\{ \|\Delta u\|_{L^{3p/2}(B_{r+\delta}(\mathbf{x}_0))} + \delta^{-2} \|u\|_{L^{3p/2}(B_{r+\delta}(\mathbf{x}_0))} \right\}. \tag{D.9}$$

for all $u \in W^{2,3p/2}(B_{r+\delta}(\mathbf{x}_0))$ (with $\mathbf{x}_0 \in \mathbb{R}^3$, $r, \delta > 0$).

Theorem D.5 [Evans 1998, Theorem 5, Section 5.6.2 (Morrey's inequality)]. *Let Ω be a bounded, open subset in $\mathbb{R}^n$, $n \geq 2$, and suppose $\partial\Omega$ is C^1. Assume $n < \mathfrak{p} < \infty$, and $u \in W^{1,\mathfrak{p}}(\Omega)$. Then u has a version $u^* \in C^{0,\gamma}(\overline{\Omega})$, for $\gamma = 1 - n/\mathfrak{p}$, with the estimate*

$$\|u^*\|_{C^{0,\gamma}(\overline{\Omega})} \leq K_4 \|u\|_{W^{1,\mathfrak{p}}(\Omega)}. \tag{D.10}$$

The constant K_4 depends only on $\mathfrak{p}$, n, and Ω.

Here, u^* is a version of the given u if $u = u^*$ a.e. Above,

$$\|u\|_{C^{0,\gamma}(\overline{\Omega})} := \sup_{\mathbf{x} \in \Omega} |u(\mathbf{x})| + \sup_{\substack{\mathbf{x}, \mathbf{y} \in \Omega \\ \mathbf{x} \neq \mathbf{y}}} \frac{|u(\mathbf{x}) - u(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^\gamma}. \tag{D.11}$$

Of course, $\sup_{\mathbf{x} \in \Omega} |u(\mathbf{x})| \leq \|u\|_{C^{0,\gamma}(\overline{\Omega})}$.

Remark D.6. In [Evans 1998, p. 245] a definition of the $W^{m,\mathfrak{p}}$-norm is used which is slightly different from ours (see (18)), but which is an equivalent norm by the equivalence of norms in finite-dimensional

vector spaces. Therefore, (D.10) holds with our definition of the norm, though the constant K_4 is not the same as the one in [Evans 1998, Theorem 5, Section 5.6.2].

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References

[Abramowitz and Stegun 1992] M. Abramowitz and I. A. Stegun (editors), *Handbook of mathematical functions with formulas, graphs, and mathematical tables*, Dover, New York, 1992. MR 94b:00012 Zbl 0643.33001

[Adams and Fournier 2003] R. A. Adams and J. J. F. Fournier, *Sobolev spaces*, 2nd ed., Pure and Applied Mathematics **140**, Elsevier, Amsterdam, 2003. MR 2009e:46025 Zbl 1098.46001

[Carmona et al. 1990] R. Carmona, W. C. Masters, and B. Simon, "Relativistic Schrödinger operators: asymptotic behavior of the eigenfunctions", *J. Funct. Anal.* **91**:1 (1990), 117–142. MR 91i:35139 Zbl 0716.35006

[Chen and Wu 1998] Y.-Z. Chen and L.-C. Wu, *Second order elliptic equations and elliptic systems*, Translations of Mathematical Monographs **174**, American Mathematical Society, Providence, RI, 1998. MR 99i:35016 Zbl 0902.35003

[Dall'Acqua et al. 2008] A. Dall'Acqua, T. Østergaard Sørensen, and E. Stockmeyer, "Hartree–Fock theory for pseudorelativistic atoms", *Ann. Henri Poincaré* **9**:4 (2008), 711–742. MR 2009k:81258 Zbl 1192.81406

[Daubechies and Lieb 1983] I. Daubechies and E. H. Lieb, "One-electron relativistic molecules with Coulomb interaction", *Comm. Math. Phys.* **90**:4 (1983), 497–510. MR 85j:81007 Zbl 0946.81522

[Enstedt and Melgaard 2009] M. Enstedt and M. Melgaard, "Existence of infinitely many distinct solutions to the quasirelativistic Hartree–Fock equations", *Int. J. Math. Math. Sci.* **2009** (2009), Art. ID 651871. MR 2011d:81094 Zbl 1181.35288

[Evans 1998] L. C. Evans, *Partial differential equations*, Graduate Studies in Mathematics **19**, American Mathematical Society, Providence, RI, 1998. MR 99e:35001 Zbl 0902.35002

[Fefferman and de la Llave 1986] C. Fefferman and R. de la Llave, "Relativistic stability of matter, I", *Rev. Mat. Iberoamericana* **2**:1-2 (1986), 119–213. MR 88g:81155 Zbl 0602.58015

[Fournais et al. 2009] S. Fournais, M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, and T. Østergaard Sørensen, "Analytic structure of solutions to multiconfiguration equations", *J. Phys. A* **42**:31 (2009), Paper #315208. MR 2010m:81398 Zbl 1181.35282

[Frank and Lenzmann 2010] R. L. Frank and E. Lenzmann, "On ground states for the L^2-critical boson star equation", preprint, 2010. arXiv 0910.2721v2

[Friedman 1958] A. Friedman, "On the regularity of the solutions of non-linear elliptic and parabolic systems of partial differential equations", *J. Math. Mech.* **7** (1958), 43–59. MR 22 #9739 Zbl 0078.27702

[Friesecke 2003] G. Friesecke, "On the infinitude of non-zero eigenvalues of the single-electron density matrix for atoms and molecules", *R. Soc. Lond. Proc. Ser. A Math. Phys. Eng. Sci.* **459**:2029 (2003), 47–52. MR 2004g:81049 Zbl 1046.81029

[Hashimoto 2006] Y. Hashimoto, "A remark on the analyticity of the solutions for non-linear elliptic partial differential equations", *Tokyo J. Math.* **29**:2 (2006), 271–281. MR 2007m:35065 Zbl 1213.35214

[Herbst 1977] I. W. Herbst, "Spectral theory of the operator $(p^2 + m^2)^{1/2} - Ze^2/r$", *Comm. Math. Phys.* **53**:3 (1977), 285–294. MR 55 #9790 Zbl 0375.35047

[Hörmander 1969] L. Hörmander, *Linear partial differential operators*, Die Grundlehren der mathematischen Wissenschaften **116**, Springer, New York, 1969. MR 40 #1687 Zbl 0175.39201

[Hörmander 1973] L. Hörmander, *An introduction to complex analysis in several variables*, North-Holland Mathematical Library **7**, North-Holland, Amsterdam, 1973. MR 49 #9246 Zbl 0271.32001

[Kato 1995] T. Kato, *Perturbation theory for linear operators*, Springer, Berlin, 1995. MR 96a:47025 Zbl 0836.47009

[Kato 1996] K. Kato, "New idea for proof of analyticity of solutions to analytic nonlinear elliptic equations", *SUT J. Math.* **32**:2 (1996), 157–161. MR 97k:35064 Zbl 0894.35036

[Krantz and Parks 2002] S. G. Krantz and H. R. Parks, *A primer of real analytic functions*, 2nd ed., Birkhäuser, Boston, 2002. MR 2003f:26045 Zbl 1015.26030

[Lewin 2004a] M. Lewin, *Quelques modèles non linéaires en mécanique quantique (Some nonlinear models in quantum mechanics)*, thesis, Université Paris Dauphine, 21 June 2004, Available at http://tel.archives-ouvertes.fr/tel-00006306.

[Lewin 2004b] M. Lewin, "Solutions of the multiconfiguration equations in quantum chemistry", *Arch. Ration. Mech. Anal.* **171**:1 (2004), 83–114. MR 2005e:81269 Zbl 1063.81102

[Lewis et al. 1997] R. T. Lewis, H. Siedentop, and S. A. Vugalter, "The essential spectrum of relativistic multi-particle operators", *Ann. Inst. H. Poincaré Phys. Théor.* **67**:1 (1997), 1–28. MR 98i:81046 Zbl 0886.35126

[Lieb and Loss 2001] E. H. Lieb and M. Loss, *Analysis*, 2nd ed., Graduate Studies in Mathematics **14**, American Mathematical Society, Providence, RI, 2001. MR 2001i:00001 Zbl 0966.26002

[Lieb and Yau 1988] E. H. Lieb and H.-T. Yau, "The stability and instability of relativistic matter", *Comm. Math. Phys.* **118**:2 (1988), 177–213. MR 90c:81251 Zbl 0686.35099

[Morrey 2008] C. B. Morrey, Jr., *Multiple integrals in the calculus of variations*, Springer, Berlin, 2008. MR 2492985 Zbl 1213.49002

[Morrey and Nirenberg 1957] C. B. Morrey, Jr. and L. Nirenberg, "On the analyticity of the solutions of linear elliptic systems of partial differential equations", *Comm. Pure Appl. Math.* **10** (1957), 271–290. MR 19,654b Zbl 0082.09402

[Nardini 1986] F. Nardini, "Exponential decay for the eigenfunctions of the two-body relativistic Hamiltonian", *J. Analyse Math.* **47** (1986), 87–109. MR 88c:81017 Zbl 0626.35075

[Reed and Simon 1975] M. Reed and B. Simon, *Methods of modern mathematical physics, II: Fourier analysis, self-adjointness*, Academic Press, New York, 1975. MR 58 #12429b Zbl 0308.47002

[Sogge 1993] C. D. Sogge, *Fourier integrals in classical analysis*, Cambridge Tracts in Mathematics **105**, Cambridge University Press, Cambridge, 1993. MR 94c:35178 Zbl 0783.35001

[Weder 1975] R. A. Weder, "Spectral analysis of pseudodifferential operators", *J. Funct. Anal.* **20**:4 (1975), 319–337. MR 53 #6366 Zbl 0317.47035

[Zhislin and Vugalter 2002] G. M. Zhislin and S. A. Vugalter, "On the discrete spectrum of Hamiltonians for pseudo-relativistic electrons", *Izv. Ross. Akad. Nauk Ser. Mat.* **66**:1 (2002), 71–102. In Russian; translated in *Izv. Math.* **66**:1 (2002), 71–102. MR 2003e:81055 Zbl 1039.81022

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