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WEIGHTED ANALYTICITY OF HARTREE-FOCK EIGENFUNCTIONS

YVON MADAY^{†,*} AND CARLO MARCATI[¢]

ABSTRACT. We prove analytic-type estimates in weighted Sobolev spaces on the eigenfunctions of a class of elliptic and nonlinear eigenvalue problems with singular potentials, which includes the Hartree-Fock equations. Going beyond classical results on the analyticity of the wavefunctions away from the nuclei, we prove weighted estimates locally at each singular point, with precise control of the derivatives of all orders.

Our estimates have far-reaching consequences for the approximation of the eigenfunctions of the problems considered, and they can be used to prove a priori estimates on the numerical solution of such eigenvalue problems.

1. INTRODUCTION

The Hartree-Fock equations are one of the most studied and used models in *ab initio* quantum chemistry in order to approximate the behavior of many-body quantum system [SO12]. Due to their (relative) simplicity, they constitute a starting point both for the analysis and for the computation of the state of many complex systems. The precise characterization of their solutions is therefore a subject of great theoretical and practical interest.

In this paper, we prove analytic-type estimates in weighted Sobolev spaces on the wave functions of a class of elliptic, nonlinear systems, which includes the Hartree-Fock model. Specifically, we consider operators that contain potentials that are singular (divergent) at a set of isolated points (physically, the locations of the nuclei) in \mathbb{R}^d , $d \in \{2,3\}$, but that are regular otherwise. Due to the presence of these singularities, the eigenfunctions will not, in general, be regular in classical Sobolev spaces and are well known [Kat57] to exhibit cusps at the point singularities. The regularity of functions with point singularities is better described in the context of weighted Sobolev spaces, in which higher order derivatives are multiplied by a weight representing the distance from the singularity. In these spaces, under some assumptions on the potential, we can therefore derive analytic-type bounds on the growth of the norms of the eigenfunctions of the nonlinear elliptic systems under consideration. Essentially, we refine the known result on analyticity of the wavefunctions away from the nuclei (see, e.g., [FHHØ02, Lew04]) and show how the radius of convergence of Taylor series associated to the wavefunction decreases to zero in the vicinity of the singular points.

The theory of weighted Sobolev spaces of the kind we consider here has its roots in the analysis of elliptic problems in non smooth domains and was initiated in the second half of the twentieth century [Kon67]. Analytic regularity of solutions to linear elliptic systems in polygons and polyhedra has been analyzed, e.g, in [GS06, CDN12]. Concerning nonlinear problems, we mention our work on nonlinear Schrödinger equations [MM19a] and on the Navier-Stokes

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equation in plane polygons [MS20]. For a general theory of elliptic regularity in weighted spaces, we refer the reader to, e.g., [Gri85, KMR97, KMR01, MR10], and the recent work [DHSS19]. Here, we try to make our exposition as independent as possible from the usual notation of weighted, Kondratev-type Sobolev spaces and introduce them only in the appendix. The theory of regularity in those spaces is, nonetheless, ultimately central to the derivation of our estimates.

The techniques used in the present paper are heavily inspired by those used in [DFØS12] to prove analyticity away from the nuclei of the solution to the relativistic Hartree-Fock equations. Here, we transport those techniques in a weighted framework, and use them to estimate higher order norms of the nonlinear terms. The analysis of linear, many-body Schrödinger-type operators has been carried out, among others, in [ACN12, FØ18] in a functional setting very similar to the one considered here. An asymptotic analysis at the nuclei for the Hartree-Fock equation with Coulomb potential is carried out, with different tools, in [FSS08]; the electron-electron singularities emerging in many-body models are analyzed in [FH11, FHS15]. Here, we only consider two and three dimensional nonlinear models with isolated point singularities; we furthermore take into account a wider class of potentials than Coulomb ones, as we allow for more general weighted analytic potentials. The technique used in this paper can also be rather directly extended to deal with the nonlinear part of other types of operators, once the behavior of the linear part of the operator is well understood: see, for example, the application to Navier-Stokes equations in [MS20].

We will discuss, in the next subsection, some of the consequences of the weighted analytic regularity of the eigenfunctions, in particular from the point of view of their numerical approximation, through linear and nonlinear techniques. Then, after having clarified our notation, we shortly introduce the Hartree-Fock equations and the more general nonlinear elliptic system, in Section 2. In the following Section 3, specifically in Theorem 1, we introduce the main result of this paper, and most of the section will be devoted to its proof. We conclude by introducing, for the sake of completeness, the definition of weighted, homogeneous and non homogeneous, Sobolev spaces and some technical results, in Appendix A.

1.1. **Consequences of weighted analytic regularity.** The weighted analytic regularity of the solutions to Hartree-Fock and more general elliptic problems has important and far-reaching consequences for the numerical solution of those problems. We can, indeed, obtain exponential rates of convergence of solutions obtained via numerical methods based on finite elements, see [SSW13b, SSW13a] for a general approximation theory and [MM19b, MM19a, HSW19] for applications to linear and nonlinear eigenvalue problems, and on virtual elements [ČGM⁺20]. In addition, nonlinear approximation techniques based on tensor compression and on the solution of partial differential equation in tensor-formatted form also provide exponentially convergent solutions to problems with weighted analytic solutions [MRS19]. Similarly, for such functions, neural networks with ReLU activation function can be constructed so that their size is bounded polylogarithmically with respect to the error (or, equivalently, the error converges exponentially with respect to the size) [MPOS20]. The present analytic-type regularity results, therefore, allow for an *a priori* analysis of multiple numerical methods which have proven and will probably prove useful for applications.

1.2. Notation. Let the space dimension be $d \in \{2, 3\}$. We denote by \mathbb{N} the set of positive integers, with $\mathbb{N}_0 = \{0\} \cup \mathbb{N}$. For $k \in \mathbb{N}$ and $1 \leq p \leq \infty$, Sobolev spaces are denoted by $W^{k,p}$, with their Hilbertian version written $H^k = W^{k,2}$. For two multi indices $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}^d$ and $\beta = (\beta_1, \ldots, \beta_d) \in \mathbb{N}^d$, we write $|\alpha| = \sum_i \alpha_i, \alpha! = \alpha_1! \cdots \alpha_d!, \alpha + \beta = (\alpha_1 + \beta_1, \ldots, \alpha_d + \beta_d)$, and

(1)
$$\binom{\alpha}{\beta} = \frac{\alpha!}{\beta!(\alpha-\beta)!}$$

We recall from [Kat96] that

$$\sum_{\substack{|\beta|=n\\\beta\leq\alpha}} \binom{\alpha}{\beta} = \binom{|\alpha|}{n}.$$

Let $x = (x_1, \ldots, x_d)$: we indicate by ∂_i the partial derivative with respect to x_i , and for $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$, $\partial^{\alpha} = \partial_1^{\alpha_1} \cdots \partial_d^{\alpha_d}$.

2. The Hartree-Fock equations

Let $N, N_n \in \mathbb{N}$ be the number of electrons and nuclei of a system, let \mathfrak{c}_i , $i = 1, ..., N_n$ be isolated points in \mathbb{R}^3 representing the positions of the nuclei, and let $Z_i > 0$ be the charges of the nuclei, for all $i = 1, ..., N_n$. the Hartree-Fock problem consists in finding the smallest eigenvalues λ_i and associated orthonormal eigenfunctions φ_i , i = 1, ..., N of the equations

(2)
$$-\frac{1}{2}\Delta\varphi_{\iota} + V_{C}\varphi_{\iota} + \left(\rho_{\Phi} \star \frac{1}{|\cdot|}\right)\varphi_{\iota} - \int_{\mathbb{R}^{3}} \frac{\tau_{\Phi}(\cdot, y)}{|\cdot - y|}\varphi_{\iota}(y)dy = \lambda_{\iota}\varphi_{\iota} \qquad \iota = 1, \dots, N \qquad \text{in } \mathbb{R}^{3}$$

where V_C is the potential

$$V_C(x) = -\sum_{i=1}^{N_n} \frac{Z_i}{|x - \mathfrak{c}_i|},$$

and

$$\tau_{\Phi}(x,y) = \sum_{\iota=1}^{N} \varphi_{\iota}(x) \varphi_{\iota}(y), \qquad \rho_{\Phi}(x) = \tau_{\Phi}(x,x).$$

The analyticity of the wave functions away from the positions of the nuclei (i.e., the singularities of V) is classical, see, e.g., [FHHØ02, Lew04]. In this setting we consider instead the parts of the domain containing the nuclei, in order to deduce the weighted estimates.

Let now $V : \mathbb{R}^d \to \mathbb{R}$ be a potential to be specified later; we consider the nonlinear elliptic system given by

(3)
$$(-\Delta + V) \varphi_{\iota} + \sum_{\sigma, a, b=1}^{N} c_{ab}^{\iota\sigma} u_{ab} \varphi_{\sigma} = \lambda_{\iota} \varphi_{\iota} \qquad \iota = 1, \dots, N$$
$$-\Delta u_{ab} = 4\pi \varphi_{a} \varphi_{b} \quad a, b = 1, \dots, N.$$

with $c_{ab}^{\iota\sigma} \in \mathbb{R}$ for all $\iota, \sigma, a, b = 1, ..., N$ and $\lambda_{\iota} \in \mathbb{R}$ for all $\iota = 1, ..., N$. The Hartree-Fock equations can be rewritten under the form (3), with $V = V_C$. The nonlinear elliptic eigenvalue problem (3) is the one we will analyze in the following.

3. Weighted analyticity of eigenfunctions

In this section, we present and prove our regularity result. We will widen our scope from the Hartree-Fock equations and analyze the behavior of the eigenfunctions near the singular points of the potential for solutions to (3) in a *d*-dimensional domain for d = 2, 3. Our results, furthermore, will hold for a class of weighted analytic potential, including Coulomb potentials. Given a set of isolated points \mathfrak{C} in \mathbb{R}^d such that there exists D > 0 such that

(4)
$$|\mathfrak{c}_i - \mathfrak{c}_j| \ge 4D > 0 \quad \forall \mathfrak{c}_i, \mathfrak{c}_j \in \mathfrak{C},$$

we introduce the weight function $r : \mathbb{R}^d \to \mathbb{R}$ such that

(5)
$$r(x) = |x - \mathfrak{c}| \text{ in } B_D(\mathfrak{c}), \text{ for all } \mathfrak{c} \in \mathfrak{C}, \qquad r(x) \equiv 1 \text{ in } \left(\bigcup_{\mathfrak{c} \in \mathfrak{C}} B_{2D}(\mathfrak{c})\right)^C,$$

and *r* is smooth in $\mathbb{R}^d \setminus \mathfrak{C}$. The dependence of *r* in *x* will be mostly omitted.

Theorem 1. Let $\varepsilon \in (0,1)$, $d \in \{2,3\}$, r be defined as in (5) for a collection of isolated points $\mathfrak{C} \subset \mathbb{R}^d$ such that (4) holds and let V be such that

(6)
$$||r^{2-\varepsilon+|\alpha|}\partial^{\alpha}V||_{L^{\infty}(\mathbb{R}^d)} \leq C_V A_V^{|\alpha|}|\alpha|!, \quad \text{for all } \alpha \in \mathbb{N}_0^d,$$

and that there exists a unique solution $\Phi = \{\varphi_{\iota}\}_{\iota=1}^{N} \in (H^{1}(\mathbb{R}^{d}))^{N}$ to (3). Then, for any $\eta < \varepsilon$ there exist A > 0 such that

(7)
$$|\partial^{\alpha}\varphi_{\iota}(x)| \leq r(x)^{\min(\eta-|\alpha|,0)} A^{|\alpha|+1} |\alpha|!, \qquad \iota = 1, \dots, N,$$

for all $x \in \bigcup_{\mathfrak{c} \in \mathfrak{C}} B_D(\mathfrak{c})$ and $\alpha \in \mathbb{N}_0^d$.

From Theorem 1 and classical results on the analyticity of the Hartree-Fock wavefunctions away from the singular points [Lew04], we directly obtain the following estimate on the wavefunctions of (2). Note that (6) holds for V_C for any $\varepsilon < 1$.

Corollary 1. Let Z_i be such that there exist a unique solution $\Phi = \{\varphi_i\}_{i=1}^N \in (H^1(\mathbb{R}^3))^N$ to the Hartree-Fock problem (2), with negative eigenvalues. Then, for any $\eta < 1$ there exists A > 0 such that

$$|\partial^{\alpha}\varphi_{\iota}(x)| \leq r(x)^{\min(\eta-|\alpha|,0)} A^{|\alpha|+1} |\alpha|!, \qquad \iota = 1, \dots, N,$$

for all $x \in \mathbb{R}^3$ and $\alpha \in \mathbb{N}_0^3$.

Remark 1. The result of Corollary 1 can also be obtained via the arguments in [FSS08] or in [FHHØ09]. Nonetheless, the result in Theorem 1 allows for a more general class of singular potentials, and the techniques used in the proof are of independent interest, as they can be extended rather straightforwardly to other nonlinear, elliptic systems.

The rest of this manuscript will be devoted to the proof of Theorem 1.

3.1. **Proof of Theorem 1.** Hereafter, we suppose that the potential *V* has only one singularity, i.e, $\mathfrak{C} = {\mathfrak{c}}$, set $R \leq 1$ and place ourselves in a ball $B_R = B_R(\mathfrak{c})$ centered in \mathfrak{c} , with $r(x) = |x - \mathfrak{c}|$ in B_R . The generalization to the case where *V* has a set of isolated singularities is straightforward. Let us formulate the induction assumption that will be used in the sequel.

Induction Assumption. Let $\Phi = \{\varphi_{\iota}\}_{\iota=1}^{N}$, $2 \leq p < \infty$, $\gamma \in \mathbb{R}$, $k \in \mathbb{N}$, and C_{Φ} , $A_{\Phi} > 0$. We say that $H_{\Phi}(p, \gamma, k, C_{\Phi}, A_{\Phi})$ holds if for all $\iota = 1, \ldots, N$, $\varphi_{\iota} \in H^{1}(B_{R}) \cap L^{\infty}(B_{R})$, $C_{\Phi} \geq \|\varphi_{\iota}\|_{L^{\infty}(B_{R})}$, and

(8)
$$\sum_{|\alpha|=j} \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi_{\iota}\|_{L^{p}(B_{R-k\rho})} \leq C_{\Phi} A^{j}_{\Phi}(k\rho)^{-j} j^{j}$$

for all $j \in \mathbb{N}$ such that $1 \leq j \leq k$ and $\rho \in (0, R/(2k)]$.

We introduce some lemmas where—under the induction assumption—we estimate the norms of φ_i (Lemma 2), of products $\varphi_a \varphi_b$ (Lemma 3), of u_{ab} (Lemma 4), of the product $u_{ab}\varphi_i$ (Lemma 5), and of $V\varphi_i$ (Lemma 6).

Lemma 2 (Bounds on L^{3p} norms of eigenfunctions). Let $p \ge 2d/3$, $0 < \gamma - d/p < \min(\varepsilon, 2)$. There exists $C_{\text{interp}} > 0$ such that, for all $C_{\Phi}, A_{\Phi} \ge 1$, for all $k \in \mathbb{N}, k \ge 2$, if $H_{\Phi}(p, \gamma, k, C_{\Phi}, A_{\Phi})$ holds, (9) $\sum_{k=1}^{2-\gamma} \frac{2-\gamma}{2} + |\alpha| 2\alpha$, $||\alpha| = 1$, $|\alpha| = 1$, $|\alpha|$

$$\sum_{|\alpha|=j} \|r^{\frac{2-\gamma}{3}+|\alpha|}\partial^{\alpha}\varphi_{\iota}\|_{L^{3p}(B_{R-k\rho})} \leq (d+1)C_{\text{interp}}e^{\vartheta}C_{\Phi}A_{\Phi}^{j+\vartheta}(k\rho)^{-j-\vartheta}j^{j}(j+1)^{\vartheta}, \qquad \iota=1,\ldots,N,$$

for all $1 \leq j \leq k-1$, for all $\rho \in (0, R/(2k)]$, and with $\vartheta = \frac{2}{3}\frac{d}{p}$.

Proof. For any $\iota \in \{1, ..., N\}$, denote $\varphi = \varphi_{\iota}$. First, we use equation (45) of Lemma 9 in the Appendix in order to go back to integrals in L^p : for any $j \in \{1, ..., k-1\}$ and for any $|\alpha| = j$,

$$\|r^{\frac{2-\gamma}{3}+|\alpha|}\partial^{\alpha}\varphi\|_{L^{3p}(B_{R-k\rho})} \leq C_{\text{interp}}\|r^{|\alpha|-\gamma}\partial^{\alpha}\varphi\|_{L^{p}(B_{R-k\rho})}^{1-\vartheta} \left\{ (|\alpha|+1)^{\vartheta}\|r^{|\alpha|-\gamma}\partial^{\alpha}\varphi\|_{L^{p}(B_{R-k\rho})}^{\vartheta} + \sum_{i=1}^{d}\|r^{|\alpha|+1-\gamma}\partial^{\alpha}\partial_{i}\varphi\|_{L^{p}(B_{R-k\rho})}^{\vartheta} \right\}.$$

By the Cauchy-Schwarz inequality,

$$\sum_{|\alpha|=j} \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi\|_{L^{p}(B_{R-k\rho})}^{1-\vartheta} (|\alpha|+1)^{\vartheta} \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi\|_{L^{p}(B_{R-k\rho})}^{\vartheta}$$

$$\leq \left(\sum_{|\alpha|=j} \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi\|_{L^{p}(B_{R-k\rho})}\right)^{1-\vartheta} \left(\sum_{|\alpha|=j} (|\alpha|+1) \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi\|_{L^{p}(B_{R-k\rho})}\right)^{\vartheta}$$

and,

$$\sum_{|\alpha|=j} \left(\|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi\|^{1-\vartheta}_{L^{p}(B_{R-k\rho})} \sum_{i=1}^{d} \|r^{|\alpha|+1-\gamma} \partial^{\alpha} \partial_{i} \varphi\|^{\vartheta}_{L^{p}(B_{R-k\rho})} \right)$$
$$\leq \sum_{i=1}^{d} \left(\sum_{|\alpha|=j} \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi\|_{L^{p}(B_{R-k\rho})} \right)^{1-\vartheta} \left(\sum_{|\alpha|=j} \|r^{|\alpha|+1-\gamma} \partial^{\alpha} \partial_{i} \varphi\|_{L^{p}(B_{R-k\rho})} \right)^{\vartheta}$$

Then, hypothesis (8) implies

$$\left(\sum_{|\alpha|=j} \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi\|_{L^{p}(B_{R-k\rho})}\right)^{1-\vartheta} \leq C_{\Phi}^{1-\vartheta} A_{\Phi}^{j(1-\vartheta)} \rho^{-j(1-\vartheta)} \left(\frac{j}{k}\right)^{j(1-\vartheta)}$$

and

$$\begin{split} (j+1)^{\vartheta} \left(\sum_{|\alpha|=j} \|r^{j-\gamma} \partial^{\alpha} \varphi\|_{L^{p}(B_{R-k\rho})} \right)^{\vartheta} + \sum_{i=1}^{d} \left(\sum_{|\alpha|=j} \|r^{j+1-\gamma} \partial^{\alpha} \partial_{i} \varphi\|_{L^{p}(B_{R-k\rho})} \right)^{\vartheta} \\ & \leq C_{\Phi}^{\vartheta}(j+1)^{\vartheta} A_{\Phi}^{j\vartheta} \rho^{-j\vartheta} \left(\frac{j}{k} \right)^{j\vartheta} + dC_{\Phi}^{\vartheta} A_{\Phi}^{(j+1)\vartheta} \rho^{-(j+1)\vartheta} \left(\frac{j+1}{k} \right)^{(j+1)\vartheta}. \end{split}$$

Therefore, multiplying the right hand sides of the two last inequalities,

$$\sum_{|\alpha|=j} \|r^{\frac{2-\gamma}{3}+|\alpha|}\partial^{\alpha}u\|_{L^{3p}(B_{R-k\rho})} \leq (d+1)C_{\text{interp}}C_{\Phi}A_{\Phi}^{j+\vartheta}(k\rho)^{-j-\vartheta}j^{j(1-\vartheta)}(j+1)^{(j+1)\vartheta}.$$

We finally need to bound the last two terms in the multiplication above:

$$j^{j(1-\vartheta)}(j+1)^{(j+1)\vartheta} = j^j(j+1)^\vartheta \left(1+\frac{1}{j}\right)^{\vartheta j} \le j^j(j+1)^\vartheta e^\vartheta.$$

Lemma 3 (Bounds on norms of products of eigenfunctions). Let $p \ge 2d/3$, $0 < \gamma - d/p < \min(\varepsilon, 2)$ and C_{Φ} , $A_{\Phi} \ge 1$. Let also $\vartheta = \frac{2}{3}\frac{d}{p}$ and

(10)
$$C_1 = \frac{(d+1)^2}{2} C_{\text{interp}}^2 e^{2\vartheta + 1} C_{\Phi}^2 + 2(d+1)(4\pi)^{1/2d} C_{\text{interp}} e^{\vartheta} C_{\Phi}^2.$$

For all $k \in \mathbb{N}$, $k \ge 2$, if $H_{\Phi}(p, \gamma, k, C_{\Phi}, A_{\Phi})$ holds, then

(11)
$$\sum_{|\alpha|=j} \|r^{\frac{2}{3}(2-\gamma)+|\alpha|}\partial^{\alpha}(\varphi_{\iota}\varphi_{\kappa})\|_{L^{3p/2}(B_{R-k\rho})} \leq C_{1}A_{\Phi}^{j+2\vartheta}\rho^{-j-2\vartheta}\left(\frac{j}{k}\right)^{j}j^{1/2}, \quad \iota,\kappa=1,\ldots,N,$$

for all $1 \le j \le k - 1$ *and* $\rho \in (0, R/(2k)]$ *.*

Proof. Denote $\varphi = \varphi_{\iota}$ and $\psi = \varphi_{\kappa}$. By Leibniz's rule and the Cauchy-Schwarz inequality,

$$(12) \|r^{\frac{2}{3}(2-\gamma)+|\alpha|}\partial^{\alpha}(\varphi\psi)\|_{L^{3p/2}(B_{R-k\rho})} \\ \leq \sum_{0<\beta<\alpha} \binom{\alpha}{\beta} \|r^{\frac{2-\gamma}{3}+|\beta|}\partial^{\beta}\varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2-\gamma}{3}+|\alpha|-|\beta|}\partial^{\alpha-\beta}\psi\|_{L^{3p}(B_{R-k\rho})} \\ + \|r^{\frac{2}{3}(2-\gamma)+|\alpha|}\partial^{\alpha}\varphi\|_{L^{3p/2}(B_{R-k\rho})} \|\psi\|_{L^{\infty}(B_{R-k\rho})} \\ + \|r^{\frac{2}{3}(2-\gamma)+|\alpha|}\partial^{\alpha}\psi\|_{L^{3p/2}(B_{R-k\rho})} \|\varphi\|_{L^{\infty}(B_{R-k\rho})}$$

Consider the sum over $0 < \beta < \alpha$. By manipulation on the sums and using (1),

$$\begin{split} \sum_{|\alpha|=j} \sum_{0 < \beta < \alpha} \binom{\alpha}{\beta} \|r^{\frac{2-\gamma}{3} + |\beta|} \partial^{\beta} \varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2-\gamma}{3} + |\alpha| - |\beta|} \partial^{\alpha-\beta} \psi\|_{L^{3p}(B_{R-k\rho})} \\ &= \sum_{i=1}^{j-1} \sum_{|\beta|=i} \sum_{\substack{|\alpha|=j\\ \alpha > \beta}} \binom{\alpha}{\beta} \|r^{\frac{2-\gamma}{3} + |\beta|} \partial^{\beta} \varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2-\gamma}{3} + |\alpha| - |\beta|} \partial^{\alpha-\beta} \psi\|_{L^{3p}(B_{R-k\rho})} \\ &\leq \sum_{i=1}^{j-1} \binom{j}{i} \sum_{|\beta|=i} \sum_{\substack{|\alpha|=j\\ \alpha > \beta}} \|r^{\frac{2-\gamma}{3} + |\beta|} \partial^{\beta} \varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2-\gamma}{3} + |\alpha| - |\beta|} \partial^{\alpha-\beta} \psi\|_{L^{3p}(B_{R-k\rho})} \\ &= \sum_{i=1}^{j-1} \binom{j}{i} \sum_{|\beta|=i} \sum_{\substack{|\alpha|=j\\ \alpha > \beta}} \|r^{\frac{2-\gamma}{3} + |\beta|} \partial^{\beta} \varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2-\gamma}{3} + |\beta|} \partial^{\xi} \psi\|_{L^{3p}(B_{R-k\rho})} \end{split}$$

Hence, using Lemma 2 and Stirling's inequality on the last line above gives

$$\begin{split} \sum_{|\alpha|=j} \sum_{0<\beta<\alpha} \binom{\alpha}{\beta} \|r^{\frac{2-\gamma}{3}+|\beta|} \partial^{\beta}\varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2-\gamma}{3}+|\alpha|-|\beta|} \partial^{\alpha-\beta}\psi\|_{L^{3p}(B_{R-k\rho})} \\ &\leq (d+1)^{2} C_{\text{interp}}^{2} e^{2\vartheta} C_{\Phi}^{2} A_{\Phi}^{j+2\vartheta}(k\rho)^{-j-2\vartheta} \sum_{i=1}^{j-1} \binom{j}{i} i^{i} (j-i)^{j-i} (i+1)^{\vartheta} (j-i+1)^{\vartheta} \\ &\leq (d+1)^{2} C_{\text{interp}}^{2} e^{2\vartheta} C_{\Phi}^{2} \frac{1}{2\pi} A_{\Phi}^{j+2\vartheta}(k\rho)^{-j-2\vartheta} e^{j} \sum_{i=1}^{j-1} \binom{j}{i} i! (j-i)! (i+1)^{\vartheta} (j-i+1)^{\vartheta} \frac{1}{\sqrt{i(j-i)}} \end{split}$$

Now, for any i = 1, ..., j - 1 and since $j \le k - 1$, there holds $(i + 1)^{\vartheta}(j - i + 1)^{\vartheta} \le k^{2\vartheta}$. In addition as already used in [DFØS12], by comparing the Riemann sum with the integral,

$$\sum_{i=1}^{j-1} \frac{1}{\sqrt{i(j-i)}} \le \int_0^j \frac{1}{\sqrt{i(j-i)}} di = \pi,$$

hence

$$\begin{aligned} (d+1)^2 C_{\text{interp}}^2 e^{2\vartheta} C_{\Phi}^2 \frac{1}{2\pi} A_{\Phi}^{j+2\vartheta}(k\rho)^{-j-2\vartheta} e^j \sum_{i=1}^{j-1} \binom{j}{i} i! (j-i)! (i+1)^\vartheta (j-i+1)^\vartheta \frac{1}{\sqrt{i(j-i)}} \\ & \leq \frac{(d+1)^2}{2} C_{\text{interp}}^2 e^{2\vartheta} C_{\Phi}^2 A_{\Phi}^{j+2\vartheta} \rho^{-j-2\vartheta} k^{-j} e^j j! \end{aligned}$$

Using again Stirling's inequality,

$$\begin{split} \sum_{|\alpha|=j} \sum_{0<\beta<\alpha} \binom{\alpha}{\beta} \|r^{\frac{2-\gamma}{3}+|\beta|} \partial^{\beta}\varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2-\gamma}{3}+|\alpha|-|\beta|} \partial^{\alpha-\beta}\psi\|_{L^{3p}(B_{R-k\rho})} \\ &\leq \frac{(d+1)^2}{2} C_{\text{interp}}^2 e^{2\vartheta+1} C_{\Phi}^2 A_{\Phi}^{j+2\vartheta} \rho^{-j-2\vartheta} k^{-j} j^j \sqrt{j}. \end{split}$$

The two remaining terms at the right hand side of (12) are controlled using Lemma 2 and the boundedness of the functions in Φ . Indeed

$$\begin{aligned} \|r^{\frac{2}{3}(2-\gamma)+|\alpha|}\partial^{\alpha}\varphi\|_{L^{3p/2}(B_{R-k\rho})} &\leq \|r^{\frac{2-\gamma}{3}}\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2-\gamma}{3}+|\alpha|}\partial^{\alpha}\varphi\|_{L^{3p}(B_{R-k\rho})} \\ &\leq (4\pi)^{1/3p}R^{\frac{2-(\gamma-d/p)}{3}} \|r^{\frac{2-\gamma}{3}+|\alpha|}\partial^{\alpha}\varphi\|_{L^{3p}(B_{R-k\rho})} \\ &\leq (4\pi)^{1/3p}(d+1)C_{\text{interp}}e^{\vartheta}C_{\Phi}A_{\Phi}^{j+\vartheta}(k\rho)^{-j-\vartheta}j^{j}(j+1)^{\vartheta} \end{aligned}$$

where we have used Lemma 2, the fact that $\gamma - d/p < 2$, and $R \leq 1$. Then, since $\|\psi\|_{L^{\infty}(B_{R-k\rho})} \leq 1$ C_{Φ} by hypothesis and $p \geq 2d/3$

$$\|r^{\frac{2}{3}(2-\gamma)+|\alpha|}\partial^{\alpha}\varphi\|_{L^{3p/2}(B_{R-k\rho})}\|\psi\|_{L^{\infty}(B_{R-k\rho})} \leq (4\pi)^{1/2d}(d+1)C_{\text{interp}}e^{\vartheta}C_{\Phi}^{2}A_{\Phi}^{j+\vartheta}(k\rho)^{-j-\vartheta}j^{j}(j+1)^{\vartheta}.$$

The same holds for the last term of (12), thus concluding the proof.

The same holds for the last term of (12), thus concluding the proof.

Lemma 4 (Bounds on norms of the potentials u_{ab}). Let $\Phi = \{\varphi_1, \ldots, \varphi_N\}$ and let u_{ab} , a, b = $1, \ldots, N$ be the solution in \mathbb{R}^d , d = 2, 3, to

(13)
$$-\Delta u_{ab} = 4\pi\varphi_a\varphi_b.$$

Let also $p \ge 2d/3$, $0 < \gamma - d/p < \min(\varepsilon, 2)$, and $C_{\Phi}, A_{\Phi} \ge 1$ such that

(14)
$$C_{\Phi} \ge \max_{a,b=1,\dots,N} \|u_{ab}\|_{L^{\infty}(\mathbb{R}^d)}, \qquad A_{\Phi} \ge 4\pi C_{\operatorname{reg},\frac{3p}{2}} \frac{1+\sqrt{5}}{2}.$$

There exists $C_{2,p} > 0$ independent of A_{Φ} such that, for all $k \in \mathbb{N}$, $k \ge 2$, if $H_{\Phi}(p, \gamma, k, C_{\Phi}, A_{\Phi})$ holds, then

(15)
$$\sum_{|\alpha|=j} \|r^{j-\tilde{\gamma}}\partial^{\alpha}u_{ab}\|_{L^{3p/2}(B_{R-k\rho})} \le C_{2,p}A_{\Phi}^{j+2\vartheta}\rho^{-j-2\vartheta}\left(\frac{j}{k}\right)^{j}$$

for all integers $1 \le j \le k$ and all $\rho \in (0, R/(2k)]$, and where $\tilde{\gamma} = \frac{2}{3}(\gamma - 2)$ and $\vartheta = \frac{2}{3}\frac{d}{p}$.

Proof. Suppose $j \ge 3$. We start by considering j + 1 concentric balls

$$B_i = B_{R-k\frac{j-i}{j}\rho}, \quad i = 0, \dots, j,$$

see Figure 1. Clearly, $B_{R-k\rho} = \widetilde{B}_0 \subset \widetilde{B}_1 \subset \cdots \subset \widetilde{B}_j = B_R$. Now, for all $i = 0, \ldots, j-2$, using



FIGURE 1. Concentric balls B_i .

Proposition 7 in the Appendix (with *k* replaced by j - i - 1, *j* replaced by j - i - 1, ρ replaced by $\frac{k}{j}\rho$ and γ replaced by $\tilde{\gamma}$) and equation (13) we find (16)

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$$\sum_{|\alpha|=j-i} \|r^{-\tilde{\gamma}+|\alpha|} \partial^{\alpha} u_{ab}\|_{L^{3p/2}(\tilde{B}_{i})} \leq C_{\operatorname{reg},\frac{3p}{2}} \left(4\pi \sum_{|\alpha|=j-i-2} \|r^{-\tilde{\gamma}+2+|\alpha|} \partial^{\alpha} (\varphi_{a}\varphi_{b})\|_{L^{3p/2}(\tilde{B}_{i+1})} + \left(\rho \frac{k}{j}\right)^{-1} \sum_{|\alpha|=j-i-1} \|r^{-\tilde{\gamma}+|\alpha|} \partial^{\alpha} u_{ab}\|_{L^{3p/2}(\tilde{B}_{i+1})} + \left(\rho \frac{k}{j}\right)^{-2} \sum_{|\alpha|=j-i-2} \|r^{-\tilde{\gamma}+|\alpha|} \partial^{\alpha} u_{ab}\|_{L^{3p/2}(\tilde{B}_{i+1})} \right).$$

We also write

$$s_i = C_{\operatorname{reg},\frac{3p}{2}}^i \left(\frac{k}{j}\rho\right)^{-i} \sum_{|\alpha|=j-i} \|r^{-\tilde{\gamma}+|\alpha|}\partial^{\alpha}u_{ab}\|_{L^{3p/2}(\widetilde{B}_i)} \qquad i=0,\ldots,j$$

and

$$t_{i} = (4\pi C_{\text{reg},\frac{3p}{2}})^{i+1} \left(\frac{k}{j}\rho\right)^{-i} \sum_{|\alpha|=j-i-2} \|r^{-\tilde{\gamma}+2+|\alpha|}\partial^{\alpha}(\varphi_{a}\varphi_{b})\|_{L^{3p/2}(\widetilde{B}_{i+1})} \qquad i=0,\ldots,j-2.$$

Then, since $C_{\text{reg},\frac{3p}{2}} \ge 1$ and $\widetilde{B}_{i+1} \subset \widetilde{B}_{i+2}$, equation (16) implies

$$s_i \le t_i + s_{i+1} + s_{i+2}.$$

Let now F_i denote the *i*th Fibonacci number (with $F_0 = F_1 = 1$). Iterating on the above, one obtains

$$s_0 \le \sum_{i=0}^{j-2} F_i t_i + F_{j-1} s_{j-1} + F_{j-2} s_j.$$

Denoting $\mathfrak{f} = \frac{1+\sqrt{5}}{2}$ and remarking that $F_i \leq \mathfrak{f}^i$, (17)

$$\begin{split} \sum_{|\alpha|=j} \|r^{-\tilde{\gamma}+|\alpha|} \partial^{\alpha} u_{ab}\|_{L^{3p/2}(\tilde{B}_{0})} &\leq \sum_{i=0}^{j-2} (4\pi C_{\operatorname{reg},\frac{3p}{2}} \mathfrak{f})^{i+1} \left(\frac{k}{j}\rho\right)^{-i} \sum_{|\alpha|=j-i-2} \|r^{-\tilde{\gamma}+2+|\alpha|} \partial^{\alpha} (\varphi_{a}\varphi_{b})\|_{L^{3p/2}(\tilde{B}_{i+1})} \\ &+ \sum_{|\alpha|=0,1} (C_{\operatorname{reg},\frac{3p}{2}} \mathfrak{f})^{j-|\alpha|} \left(\frac{k}{j}\rho\right)^{-j+|\alpha|} \|r^{-\tilde{\gamma}+|\alpha|} \partial^{\alpha} u_{ab}\|_{L^{3p/2}(\tilde{B}_{j-|\alpha|})}. \end{split}$$

We consider the first term at the right hand side of the above equation: φ_a and φ_b satisfy the hypotheses of Lemma 3 (with $\tilde{\rho} = \frac{j-i-1}{j}\rho$), thus, when $0 \le i \le j-3$

$$\sum_{|\alpha|=j-i-2} \|r^{-\tilde{\gamma}+2+|\alpha|} \partial^{\alpha}(\varphi_{a}\varphi_{b})\|_{L^{3p/2}(\tilde{B}_{i+1})}$$

$$\leq \|r^{2}\|_{L^{\infty}(B_{R})} \sum_{|\beta|=j-i-2} \|r^{|\beta|-\tilde{\gamma}} \partial^{\beta}(\varphi_{a}\varphi_{b})\|_{L^{3p/2}(\tilde{B}_{i+1})}$$

$$\leq 4\pi C_{1} A_{\Phi}^{j-i-2+2\vartheta} k^{-j+i+2} \left(\frac{j-i-1}{j}\rho\right)^{-j+i+2-2\vartheta} (j-i-2)^{j-i-2} (j-i-2)^{1/2}.$$

When i = j - 2 in the sum above, instead, we have the term

(18)
$$\frac{\|r^{-\tilde{\gamma}+2}\varphi_a\varphi_b\|_{L^{3p/2}(\tilde{B}_{i+1})} \le \|\varphi_a\varphi_b\|_{L^{\infty}(B_R)}\|r^{-\tilde{\gamma}+2}\|_{L^{3p/2}(\tilde{B}_{i+1})} \le R^{-\tilde{\gamma}+2+\vartheta}4\pi C_{\Phi}^2 \le R^2 4\pi C_{\Phi}^2}{\le 4\pi C_{\Phi}^2},$$

where we have used that $\tilde{\gamma} \leq \vartheta$ and R < 1. Hence, since $A_{\Phi} \geq 4\pi C_{\text{reg},\frac{3p}{2}}\mathfrak{f}$ and indicating by $\zeta(\cdot)$ the Riemann zeta function,

$$(19) \qquad \sum_{i=0}^{j-3} (4\pi C_{\operatorname{reg},\frac{3p}{2}} \mathfrak{f})^{i+1} \left(\frac{k}{j}\rho\right)^{-i} \sum_{|\alpha|=j-i-2} \|r^{-\tilde{\gamma}+2+|\alpha|} \partial^{\alpha}(\varphi_{a}\varphi_{b})\|_{L^{3p/2}(\widetilde{B}_{i+1})} \\ \leq 4\pi C_{1} A_{\Phi}^{j-1+2\vartheta} \rho^{-j+2-2\vartheta} k^{-j+2} j^{j} \sum_{i=0}^{j-3} j^{2\vartheta-2} \left(\frac{j-i-2}{j-i-1}\right)^{j-i-2} (j-i-1)^{-2\vartheta} (j-i-2)^{1/2} \\ \leq 4\pi C_{1} A_{\Phi}^{j-1+2\vartheta} \rho^{-j+2-2\vartheta} k^{-j+2} j^{j} \sum_{i=0}^{j-3} \left(\frac{j-i-2}{j-i-1}\right)^{j-i} \left(\frac{j-i-1}{j}\right)^{2-2\vartheta} (j-i-2)^{-3/2} \\ \leq \pi C_{1} \zeta(3/2) A_{\Phi}^{j+2\vartheta} \rho^{-j-2\vartheta} k^{-j} j^{j},$$

where we have also used the facts that $k\rho \leq \frac{1}{2}$, and $\vartheta \leq 1$.

We still need to bound the second term at the right hand side of (17). There holds

(20)
$$\|r^{-\tilde{\gamma}}u_{ab}\|_{L^{3p/2}(\tilde{B}_{j})} \leq \|r^{-\tilde{\gamma}}\|_{L^{3p/2}(B_{R})} \|u_{ab}\|_{L^{\infty}(B_{R})} \leq 4\pi C_{\Phi}$$

by hypothesis (14). Furthermore, note that by the hypotheses on γ and p, we have $1 - \tilde{\gamma} \ge 0$. By classical elliptic regularity in Sobolev spaces [DFØS12, Corollary D.4], there exists a constant $C_{S,p}$ dependent only on p such that

(21)

$$\sum_{\alpha \leq 2} \|\partial^{\alpha} u_{ab}\|_{L^{3p/2}(\widetilde{B}_{j-1})} \leq C_{S,\frac{3p}{2}} \left(\|\varphi_{a}\varphi_{b}\|_{L^{3p/2}(B_{R+1})} + \|u_{ab}\|_{L^{3p/2}(B_{R+1})} \right) \\
\leq |B_{R+1}|^{2/(3p)} C_{S,\frac{3p}{2}} \left(\|\varphi_{a}\varphi_{b}\|_{L^{\infty}(\mathbb{R}^{d})} + \|u_{ab}\|_{L^{\infty}(\mathbb{R}^{d})} \right) \\
\leq (4\pi)^{2/(3p)} (R+1)^{\vartheta} C_{S,\frac{3p}{2}} \left(\|\varphi_{a}\varphi_{b}\|_{L^{\infty}(\mathbb{R}^{d})} + \|u_{ab}\|_{L^{\infty}(\mathbb{R}^{d})} \right) \\
\leq 16\pi C_{S,\frac{3p}{2}} C_{\Phi}^{2}$$

where we have also used $2/(3p) \leq$ 1, $R \leq$ 1, and (14). Hence,

(22)
$$\sum_{|\alpha|=1} \|r^{1-\tilde{\gamma}}\partial^{\alpha}u_{ab}\|_{L^{3p/2}(\tilde{B}_{j-1})} \le \|r^{1-\tilde{\gamma}}\|_{L^{\infty}(B_R)} \sum_{|\alpha|=1} \|\partial^{\alpha}u_{ab}\|_{L^{3p/2}(\tilde{B}_{j-1})} \le 16\pi C_{S,\frac{3p}{2}}C_{\Phi}^2.$$

Now, combining (17), (18), (19), (20), and (22), we obtain

$$\begin{split} \sum_{|\alpha|=j} \|r^{-\tilde{\gamma}+|\alpha|}\partial^{\alpha}u_{ab}\|_{L^{3p/2}(B_{R-k\rho})} \\ &\leq (4\pi C_{\Phi}^{2} + \pi C_{1}\zeta(3/2) + 16\pi C_{S,\frac{3p}{2}}C_{\Phi}^{2} + 4\pi C_{\Phi})A_{\Phi}^{j+2\vartheta}\rho^{-j-2\vartheta}k^{-j}j^{j} \end{split}$$

when $j \ge 3$. The cases j = 0, 1, 2 are easily treated using (20) and (21).

Lemma 5 (Bounds on products of eigenfunctions and electronic potentials). Let $\Phi = \{\varphi_1, \ldots, \varphi_N\}$ and let u_{ab} , $a, b = 1, \ldots, N$ be solution to (13). Let furthermore $p \ge 2d/3$, $0 < \gamma - d/p < \min(\varepsilon, 2)$, and C_{Φ} , $A_{\Phi} \ge 1$ such that

(23)
$$C_{\Phi} \ge \max_{a,b=1,\dots,N} \|u_{ab}\|_{L^{\infty}(\mathbb{R}^d)}, \qquad A_{\Phi} \ge 4\pi C_{\operatorname{reg},\frac{3p}{2}} \frac{1+\sqrt{5}}{2}.$$

There exists $C_{3,p}$ independent of A_{Φ} such that, for all $k \in \mathbb{N}$, if $H_{\Phi}(p,\gamma,k,C_{\Phi},A_{\Phi})$ holds, then

(24)
$$\sum_{|\alpha|=j} \|r^{2-\gamma+j}\partial^{\alpha}(u_{ab}\varphi_{\iota})\|_{L^{p}(B_{R-k\rho})} \leq C_{3,p}A_{\Phi}^{j+3\vartheta}\rho^{-j-3\vartheta}\left(\frac{j}{k}\right)^{j}j, \qquad a, b, \iota = 1, \dots, N,$$

for all integer $1 \leq j \leq k$, all $\rho \in (0, R/(2k)]$, and where $\vartheta = \frac{2}{3} \frac{d}{p}$.

Proof. Denote $u = u_{ab}$, $\varphi = \varphi_j$. We have

(25)
$$\sum_{|\alpha|=j} \|r^{2-\gamma+|\alpha|}\partial^{\alpha}(u\varphi)\|_{L^{p}(B_{R-k\rho})}$$
$$\leq \sum_{|\alpha|=j} \sum_{\beta \leq \alpha} {\alpha \choose \beta} \|r^{\frac{2-\gamma}{3}+|\beta|}\partial^{\beta}\varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2}{3}(2-\gamma)+|\alpha|-|\beta|}\partial^{\alpha-\beta}u\|_{L^{3p/2}(B_{R-k\rho})}.$$

Using (11) we follow the same procedure as in the proof of Lemma 3. When $0 < \beta < \alpha$ in the sum above, using Lemmas 2 and 4,

$$\begin{split} \sum_{|\alpha|=j} \sum_{0<\beta<\alpha} \binom{\alpha}{\beta} \|r^{\frac{2-\gamma}{3}+|\beta|} \partial^{\beta}\varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2}{3}(2-\gamma)+|\alpha|-|\beta|} \partial^{\alpha-\beta}u\|_{L^{3p/2}(B_{R-k\rho})} \\ &\leq \sum_{i=1}^{j-1} \binom{j}{i} \sum_{|\beta|=i} \sum_{|\xi|=j-i} \|r^{\frac{2-\gamma}{3}+|\beta|} \partial^{\beta}\varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2}{3}(2-\gamma)+|\xi|} \partial^{\xi}u\|_{L^{3p}(B_{R-k\rho})} \\ &\leq (d+1)C_{\text{interp}} e^{\vartheta} C_{\Phi} C_{2,p} A_{\Phi}^{j+3\vartheta} \rho^{-j-3\vartheta} k^{-j-\vartheta} \sum_{i=1}^{j-1} \binom{j}{i} i^{i}(j-i)^{j-i}(i+1)^{\vartheta} \\ &\leq (d+1)C_{\text{interp}} e^{\vartheta} C_{\Phi} C_{2,p} \frac{1}{2\pi} A_{\Phi}^{j+3\vartheta} \rho^{-j-3\vartheta} k^{-j-\vartheta} e^{j} \sum_{i=1}^{j-1} \binom{j}{i} i!(j-i)!(i+1)^{\vartheta} \frac{1}{\sqrt{i(j-i)}}. \\ &\leq \frac{d+1}{2}C_{\text{interp}} e^{\vartheta} C_{\Phi} C_{2,p} A_{\Phi}^{j+3\vartheta} \rho^{-j-3\vartheta} k^{-j} e^{j} j!. \\ &\leq \frac{d+1}{2}C_{\text{interp}} e^{\vartheta+1} C_{\Phi} C_{2,p} A_{\Phi}^{j+3\vartheta} \rho^{-j-3\vartheta} k^{-j} j^{j+1/2}, \end{split}$$

where the last inequalities stem from the same arguments as in the proof of Lemma 3. The terms in the sum in (25) where $\beta = 0$ and $\beta = \alpha$ give a similar bound: firstly, by H_{Φ} and Lemma 4

$$\begin{split} \sum_{|\alpha|=j} \|r^{\frac{2-\gamma}{3}}\varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2}{3}(2-\gamma)+|\alpha|}\partial^{\alpha}u\|_{L^{3p/2}(B_{R-k\rho})} \\ &\leq \|r^{\frac{2-\gamma}{3}}\|_{L^{3p}(B_{R})} \|\varphi\|_{L^{\infty}(B_{R-k\rho})} \sum_{|\alpha|=j} \|r^{\frac{2}{3}(2-\gamma)+|\alpha|}\partial^{\alpha}u\|_{L^{3p/2}(B_{R-k\rho})} \\ &\leq 4\pi C_{\Phi}C_{2,p}A_{\Phi}^{j+2\vartheta}\rho^{-j-2\vartheta}j^{j}k^{-j}. \end{split}$$

In addition, by Lemma 2 and since $C_{\Phi} \geq ||u||_{L^{\infty}(\mathbb{R}^d)}$

$$\begin{split} \sum_{|\alpha|=j} \|r^{\frac{2-\gamma}{3}+|\alpha|}\partial^{\alpha}\varphi\|_{L^{3p}(B_{R-k\rho})} \|r^{\frac{2}{3}(2-\gamma)}u\|_{L^{3p/2}(B_{R-k\rho})} \\ &\leq (d+1)C_{\text{interp}}e^{\vartheta}C_{\Phi}A_{\Phi}^{j+\vartheta}(k\rho)^{-j-\vartheta}j^{j}(j+1)^{\vartheta}\|r^{\frac{2}{3}(2-\gamma)}\|_{L^{3p/2}(B_{R-k\rho})} \|u\|_{L^{\infty}(B_{R-k\rho})} \\ &\leq (d+1)4\pi C_{\text{interp}}C_{\Phi}e^{\vartheta}C_{\Phi}A_{\Phi}^{j+\vartheta}\rho^{-j-\vartheta}k^{-j}j^{j} \end{split}$$

and choosing

$$C_{3,p} = \frac{d+1}{2} C_{\text{interp}} e^{\vartheta + 1} C_{\Phi} C_{2,p} + 4\pi C_{\Phi} C_{2,p} + (d+1) 4\pi C_{\text{interp}} C_{\Phi} e^{\vartheta} C_{\Phi}$$

concludes the proof.

Lemma 6 (Bounds on products of singular potential and eigenfunction). Let $\Phi = \{\varphi_1, \ldots, \varphi_N\}$ and let $V : \mathbb{R}^d \to \mathbb{R}$ such that (6) holds. Let then $p \ge 2d/3$, $0 < \gamma - d/p < \min(\varepsilon, 2)$, and $C_{\Phi}, A_{\Phi} \ge 1$ such that

For all $k \in \mathbb{N}$, if $H_{\Phi}(p, \gamma, k, C_{\Phi}, A_{\Phi})$ holds, then

(27)
$$\sum_{|\alpha|=k-1} \|r^{2-\gamma+|\alpha|} \partial^{\alpha} (V\varphi_{\iota})\|_{L^{p}(B_{R-k\rho})} \leq C_{4} A_{\Phi}^{k-1} \rho^{-k+1} k^{-k+1} (k-1)^{k}, \qquad \iota = 1, \dots, N,$$

for all $\rho \in (0, R/(2k)]$, with $C_4 = \left(\frac{1}{2\sqrt{2\pi}}e + 4\pi e + 1\right)C_V C_{\Phi}$.

Proof. There holds

$$(28) \sum_{|\alpha|=k-1} \|r^{2-\gamma+|\alpha|}\partial^{\alpha}(V\varphi_{\iota})\|_{L^{p}(B_{R-k\rho})}$$

$$\leq \sum_{|\alpha|=k-1} \sum_{0<\beta<\alpha} \binom{\alpha}{\beta} \|r^{2-\varepsilon+|\beta|}\partial^{\beta}V\|_{L^{\infty}(B_{R-k\rho})} \|r^{\varepsilon-\gamma+|\alpha|-|\beta|}\partial^{\alpha-\beta}\varphi_{\iota}\|_{L^{p}(B_{R-k\rho})}$$

$$+ \|r^{2-\varepsilon}V\|_{L^{\infty}(B_{R-k\rho})} \sum_{|\alpha|=k-1} \|r^{\varepsilon-\gamma+|\alpha|}\partial^{\alpha}\varphi_{\iota}\|_{L^{p}(B_{R-k\rho})}$$

$$+ \sum_{|\alpha|=k-1} \|r^{2-\varepsilon+|\alpha|}\partial^{\alpha}V\|_{L^{\infty}(B_{R-k\rho})} \|r^{\varepsilon-\gamma}\varphi_{\iota}\|_{L^{p}(B_{R-k\rho})}$$

By the usual manipulations,

$$\begin{split} \sum_{|\alpha|=k-1} \sum_{0<\beta<\alpha} \binom{\alpha}{\beta} \|r^{2-\varepsilon+|\beta|} \partial^{\beta} V\|_{L^{\infty}(B_{R-k\rho})} \|r^{\varepsilon-\gamma+|\alpha|-|\beta|} \partial^{\alpha-\beta} \varphi_{\iota}\|_{L^{p}(B_{R-k\rho})} \\ &\leq C_{V} C_{\Phi} \sum_{j=1}^{k-2} \binom{k-1}{j} A_{V}^{j} A_{\Phi}^{k-1-j} j! (k-1-j)^{k-1-j} (k\rho)^{-k+1+j} \\ &\leq \frac{1}{\sqrt{2\pi}} C_{V} C_{\Phi} A_{\Phi}^{k-1} (k-1)! e^{k-1} \sum_{j=1}^{k-2} (k-1-j)^{-1/2} (k\rho)^{-k+1+j} \\ &\leq \frac{1}{\sqrt{2\pi}} C_{V} C_{\Phi} A_{\Phi}^{k-1} (k-1)! e^{k-1} (k\rho)^{-k+2} \\ &\leq \frac{1}{2\sqrt{2\pi}} eC_{V} C_{\Phi} A_{\Phi}^{k-1} (k-1)^{k-1/2} (k\rho)^{-k+1} \end{split}$$

The bound on the second to last term in (28) is straightforward, while for the last term we note that $\varepsilon - \gamma > -d/p$ thus $\|r^{\varepsilon - \gamma}\varphi_{\iota}\|_{L^p(B_R)} \leq 4\pi C_{\Phi}$ and

$$\sum_{|\alpha|=k-1} \|r^{2-\varepsilon+|\alpha|} \partial^{\alpha} V\|_{L^{\infty}(B_{R-k\rho})} \|r^{\varepsilon-\gamma} \varphi_i\|_{L^p(B_{R-k\rho})} \le 4\pi C_{\varphi} C_V A_V^{k-1}(k-1)! \le 4\pi C_{\varphi} C_V e A_V^{k-1}(k-1)^{k-1/2} e^{-k+1}.$$

Therefore,

$$\sum_{|\alpha|=k-1} \|r^{2-\gamma+|\alpha|} \partial^{\alpha} (V\varphi_{\iota})\|_{L^{p}(B_{R-k\rho})} \leq \left(\frac{1}{2\sqrt{2\pi}}e + 4\pi e + 1\right) C_{V} C_{\Phi} A_{\Phi}^{k-1} (k-1)^{k} (k\rho)^{-k+1}$$

and this concludes the proof.

Proof of Theorem 1. First, we remark that $\varphi_a, \varphi_b \in H^1(\mathbb{R}^d)$ implies $u_{ab} \in W^{2,3}(B_R)$ via the second equation of (3). Due to (6), there exists q > d/2 such that $V \in L^q(B_R)$, and, by classical elliptic regularity arguments [Sta65], $\Phi \in (L^{\infty}(B_R))^N$. Hence, for all $a, b \in \{1, \ldots, N\}$, $\varphi_a \varphi_b \in H^1(B_R) \cap L^{\infty}(B_R)$. Therefore, by (3) again, $u_{ab} \in H^3(B_R) \subset W^{1,\infty}(B_R)$ for all $1 \leq p < \infty$. This implies that $\Phi \in \left(\mathcal{J}^2_{\xi}(B_R)\right)^N$, for all $\xi - d/2 < \varepsilon$. We can conclude that, for all $a, b \in \{1, \ldots, N\}$ and all $\iota \in \{1, \ldots, \infty\}$, there holds $u_{ab}\varphi_\iota \in \mathcal{J}^2_{\gamma}(B_R)$, which in turn implies $\Phi \in \left(\mathcal{J}^4_{\xi}\right)^N$, for all $\xi - d/2 < \varepsilon$. This implies furthermore, by [MM19b, Lemma 3.1],

$$\sum_{|\alpha|=2} \|r^{2-\gamma}\partial^{\alpha}\varphi_{\iota}\|_{L^{p}(B_{R})} < \infty$$

for all p > 1, $\gamma < d/p + \varepsilon$, and $\iota = 1, ..., N$. Hence, for all $1 and <math>\gamma - d/p < \varepsilon$, there exist C, A > 0 (dependent on p and γ) such that $H_{\Phi}(p, \gamma, 2, C, A)$ holds.

Induction step. We proceed by induction and impose a restriction on p; specifically, we fix a finite p_{\star} such that

$$(29) p_{\star} \ge 2d.$$

We denote the corresponding $\vartheta_{\star} = \frac{2}{3} \frac{d}{p_{\star}}$. Let us now also fix $\gamma_{\star} \in \mathbb{R}$ such that $0 < \gamma_{\star} - d/p_{\star} < \min(\varepsilon, 2)$. Let then $C_{\Phi}, A_{\Phi} \ge 1$ such that $H_{\Phi}(p_{\star}, \gamma_{\star}, 2, C_{\Phi}, A_{\Phi})$ holds, and that (30)

$$C_{\Phi} \ge \max_{a,b=1,...,N} \|u_{ab}\|_{L^{\infty}(\mathbb{R}^{d})}$$

$$A_{\Phi} \ge \max\left(A_{V}, 4\pi C_{\operatorname{reg},\frac{3p_{\star}}{2}} \frac{1+\sqrt{5}}{2}, C_{\operatorname{reg},p_{\star}}\left(C_{4}+N^{3}\max_{a,b,\sigma,\iota}|c_{ab}^{\iota\sigma}|C_{3,p_{\star}}+(N\max_{\iota}|\lambda_{\iota}|+2)C_{\Phi}\right)\right)$$

Note that such constants fulfill the hypotheses of Lemmas 2 to 6. Suppose now that the induction hypothesis $H_{\Phi}(p_{\star}, \gamma_{\star}, k, C_{\Phi}, A_{\Phi})$ holds for a $k \in \mathbb{N}$, $k \geq 2$: we will show that $H_{\Phi}(p_{\star}, \gamma_{\star}, k + 1, C_{\Phi}, A_{\Phi})$ holds.

We start by remarking that, for all $\rho \in (0, R/(2(k+1))]$, there exists $\tilde{\rho} = \frac{k+1}{k}\rho$, so that, by induction hypothesis, for all j = 1, ..., k and all $\iota = 1, ..., N$.

$$\sum_{|\alpha|=j} \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi_{\iota}\|_{L^{p}(B_{R-(k+1)\rho})} = \sum_{|\alpha|=j} \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi_{\iota}\|_{L^{p}(B_{R-k\bar{\rho}})} \leq C_{\Phi} A^{j}_{\Phi}(k\bar{\rho})^{-j} j^{j}$$
$$= C_{\Phi} A^{j}_{\Phi}((k+1)\rho)^{-j} j^{j}.$$

We still have to show that

(31)
$$\sum_{|\alpha|=k+1} \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi_{\iota}\|_{L^{p}(B_{R-(k+1)\rho})} \leq C_{\Phi} A_{\Phi}^{k+1} \rho^{-(k+1)}, \qquad \iota = 1, \dots, N.$$

From (3) and (40), for all $\iota = 1, ..., N$,

$$(32) \qquad \sum_{|\alpha|=k+1} \|r^{k+1-\gamma}\partial^{\alpha}\varphi_{\iota}\|_{L^{p_{\star}}(B_{R-(k+1)\rho})}$$

$$\leq C_{\operatorname{reg},p_{\star}}\left(\sum_{|\alpha|=k-1} \|r^{k+1-\gamma}\partial^{\alpha}\left(V\varphi_{\iota}+\sum_{\sigma=1}^{N}\sum_{a< b}c_{ab}^{\iota\sigma}u_{ab}\varphi_{\sigma}-\lambda_{\iota}\varphi_{\iota}\right)\|_{L^{p_{\star}}(B_{R-k\rho})}$$

$$+\sum_{|\alpha|=k-1,k}\rho^{|\alpha|-k-1}\|r^{|\alpha|-\gamma}\partial^{\alpha}\varphi_{\iota}\|_{L^{p_{\star}}(B_{R-|\alpha|\rho})}\right).$$

Due to Lemma 6,

(33)
$$\sum_{|\alpha|=k-1} \|r^{k+1-\gamma}\partial^{\alpha} (V\varphi_{\iota})\|_{L^{p_{\star}}(B_{R-k\rho})} \le C_4 A_{\Phi}^{k-1} \rho^{-k+1} k^{-k+1} (k-1)^k \le C_4 A_{\Phi}^{k-1} \rho^{-k},$$

where we have used $k \leq 1/\rho$ Furthermore, from Lemma 5,

$$(34) \quad \sum_{\sigma=1}^{N} \sum_{a < b} |c_{ab}^{\iota\sigma}| \sum_{|\alpha|=k-1} \|r^{2-\gamma+|\alpha|} \partial^{\alpha} (u_{ab} \varphi_{\sigma})\|_{L^{p}(B_{R-k\rho})} \\ \leq N^{3} \max_{a,b,\iota,\sigma} |c_{ab}^{\iota\sigma}| C_{3,p_{\star}} A_{\Phi}^{k-1+3\vartheta_{\star}} \rho^{-k+1-3\vartheta_{\star}} (k-1)^{k-1} k^{-k+1} (k-1) \\ \leq N^{3} \max_{a,b,\iota,\sigma} |c_{ab}^{\iota\sigma}| C_{3,p_{\star}} A_{\Phi}^{k-1+3\vartheta_{\star}} \rho^{-k+1-3\vartheta_{\star}} (k-1) \\ \leq N^{3} \max_{a,b,\iota,\sigma} |c_{ab}^{\iota\sigma}| C_{3,p_{\star}} A_{\Phi}^{k-1+3\vartheta_{\star}} \rho^{-k-3\vartheta_{\star}} \\ \leq N^{3} \max_{a,b,\iota,\sigma} |c_{ab}^{\iota\sigma}| C_{3,p_{\star}} A_{\Phi}^{k} \rho^{-k-1},$$

where we have used, in the last two inequalities, the facts that $k-1 \le 1/\rho$ and that $3\vartheta_{\star} = 2d/p_{\star} \le 1$ due to (29).

Finally, from the induction hypothesis,

(35)
$$\sum_{|\alpha|=k-1}\sum_{\sigma=1}^{N}|\lambda_{\iota,\sigma}|\|r^{k+1-\gamma_{\star}}\partial^{\alpha}\varphi_{\sigma}\|_{L^{p_{\star}}(B_{R-k\rho})} \leq N\max_{\iota}|\lambda_{\iota}|C_{\Phi}A_{\Phi}^{k-1}\rho^{-k+1}$$

and

(36)
$$\sum_{|\alpha|=k-1,k} \rho^{|\alpha|-k-1} \|r^{|\alpha|-\gamma} \partial^{\alpha} \varphi_{\iota}\|_{L^{p_{\star}}(B_{R-k\rho})} \le C_{\Phi} A_{\Phi}^{k-1} \rho^{-k-1} + C_{\Phi} A_{\Phi}^{k} \rho^{-k-1}$$

From (32), using the triangular inequality, and inequalities (33), (34), (35), and (36), we obtain

$$\sum_{|\alpha|=k+1} \|r^{k+1-\gamma}\partial^{\alpha}\varphi_{\iota}\|_{L^{p_{\star}}(B_{R-(k+1)\rho})}$$

$$\leq C_{\operatorname{reg},p_{\star}}\left(C_{4}+N^{3}\max_{a,b,\sigma,\iota}|c_{ab}^{\iota\sigma}|C_{3,p_{\star}}+(N\max_{\iota}|\lambda_{\iota}|+2)C_{\Phi}\right)A_{\Phi}^{k}\rho^{-k-1}.$$

Therefore, (31) holds thanks to (30), i.e.,

$$H_{\Phi}(p_{\star}, \gamma_{\star}, k+1, C_{\Phi}, A_{\Phi})$$

holds. Therefore, by induction, $H_{\Phi}(p_{\star}, \gamma_{\star}, k, C_{\Phi}, A_{\Phi})$ holds for all $k \in \mathbb{N}$.

Analytic estimates in the L^{∞} norm. By Lemma 10 and since we have shown that (8) holds for all $k \in \mathbb{N}$,

$$\|r^{-\eta+|\alpha|}\partial^{\alpha}\varphi_{\iota}\|_{L^{\infty}(B_{R-k\rho})} \leq C_{\Phi}|\alpha|^{2}A_{\Phi}^{|\alpha|}(k\rho)^{-|\alpha|}|\alpha|^{|\alpha|},$$

for all $|\alpha| \in \mathbb{N}$ and $\rho \in (0, R/(2k)]$. Therefore, due to Stirling's inequality and since $R - k\rho \ge R/2$, for all $0 < \eta < \varepsilon$ there exist constants $\widetilde{C}, \widetilde{A} > 0$ such that

(37)
$$\|r^{-\eta+|\alpha|}\partial^{\alpha}\varphi_{i}\|_{L^{\infty}(B_{R/2}(\mathfrak{c}))} \leq \widetilde{C}\widetilde{A}^{|\alpha|}|\alpha|!.$$

Appendix A. Technical tools in weighted spaces

The results presented in this paper rely heavily on the theory of Kondrat'ev-type weighted Sobolev spaces, that we introduce here. We also recall—mostly from [MM19a], for self-containedness a series of technical results that are ultimately necessary for the proof of Theorem 1.

We denote by $\Omega \subset \mathbb{R}^d$, d = 2, 3, a bounded domain with smooth boundary and consider the case of a single singular point $\mathfrak{c} \in \Omega$ lying in the interior of the domain. The generalization to the case of multiple singular points is straightforward. We denote by $r(x) = |x - \mathfrak{c}|$ the distance of a point $x \in \mathbb{R}^d$ from the singular point. In the whole appendix, we denote by $B_R = B_R(\mathfrak{c})$ *d*-dimensional balls centered in \mathfrak{c} of radius R > 0. Finally, for $k \in \mathbb{N}_0$ and $1 \le p \le \infty$, we denote by $W^{k,p}(\Omega)$ the classical $L^p(\Omega)$ -based Sobolev spaces of order k.

A.1. Weighted Sobolev spaces. For integer $k \in \mathbb{N}_0$, a real weight exponent $\gamma \in \mathbb{R}$, and summability exponent $1 \le p < \infty$, we introduce the *homogeneous weighted Sobolev spaces* $\mathcal{K}_{\gamma}^{k,p}(\Omega)$. Given the seminorm

(38)
$$|w|_{\mathcal{K}^{k,p}_{\gamma}(\Omega)} = \left(\sum_{|\alpha|=k} \|r^{|\alpha|-\gamma} \partial^{\alpha} w\|_{L^{p}(\Omega)}^{p}\right)^{1/p},$$

so that the spaces $\mathcal{K}^{k,p}_{\gamma}(\Omega)$ are normed by

$$\|w\|_{\mathcal{K}^{k,p}_{\gamma}(\Omega)} = \left(\sum_{j=0}^{k} |w|^p_{\mathcal{K}^{j,p}_{\gamma}(\Omega)}\right)^{1/p}.$$

We denote the weighted Kondrat'ev type spaces of infinite regularity by

$$\mathcal{K}^{\infty,p}_{\gamma}(\Omega) = \bigcap_{k \in \mathbb{N}} \mathcal{K}^{k,p}_{\gamma}(\Omega).$$

Furthermore, for constants C, A > 0 we introduce the *homogeneous weighted analytic-type* class

$$\mathcal{K}^{\varpi,p}_{\gamma}(\Omega;A) = \left\{ v \in \mathcal{K}^{\infty,p}_{\gamma}(\Omega) : |v|_{\mathcal{K}^{k,p}_{\gamma}(\Omega)} \le A^{k+!}k!, \text{ for all } k \in \mathbb{N}_0 \right\}.$$

Consider a continuous function u: we remark that, if $\gamma > d/p$, then $u \in \mathcal{K}^{0,p}_{\gamma}(\Omega)$ only if $u(\mathfrak{c}) = 0$. This condition is clearly not fulfilled by solutions to (2), which are, in general, nonzero at the singular point of the potential. For this reason, our focus will be mostly on *non-homogeneous* weighted Sobolev spaces The *non-homogeneous analytic classes* are given by

(39)
$$\mathcal{J}_{\gamma}^{\varpi,p}(\Omega;A) = \left\{ v \in W^{\lfloor \gamma - d/p \rfloor, p}(\Omega) : |v|_{\mathcal{K}_{\gamma}^{k,p}(\Omega)} \le A^{k+1}k!, \text{ for all } k \in \mathbb{N}_0 : k > \gamma - d/p \right\}.$$

For a detailed analysis of the relationship between homogeneous and non homogeneous spaces, we refer the reader to [KMR97] and [CDN10].

Remark 2. Using definition (39), the thesis of Theorem 1 can be restated as: for all $\eta < \varepsilon$, there exists A > 0 such that

$$\varphi_{\iota} \in \mathcal{J}_{\eta}^{\varpi,\infty}(\cup_{\mathfrak{c} \in \mathfrak{C}} B_D(\mathfrak{c}); A), \qquad \forall \, \iota = 1, \dots, N.$$

A.2. Local elliptic estimate. We report here, for the sake of self-containedness, a result on local weighted elliptic regularity. This has already been introduced in [MM19a], and has been proven, as an intermediate result, in [CDN12]. We denote the commutator by square brackets, i.e., we write

$$[A,B] = AB - BA$$

Proposition 7. Let 1 , <math>R > 0, and $\gamma \in \mathbb{R}$. Then, there exists $C_{\text{reg},p} \ge 1$ such that for all $k \in \mathbb{N}$ and $\rho \in (0, \frac{R}{2(k+1)}]$. and $j \in \mathbb{N}$ such that $1 \le j \le k$,

(40)
$$\sum_{|\alpha|=k+1} \|r^{k+1-\gamma}\partial^{\alpha}u\|_{L^{p}(B_{R-(j+1)\rho})} \leq C_{\operatorname{reg},p} \left(\sum_{|\beta|=k-1} \|r^{k+1-\gamma}\partial^{\beta}(\Delta u)\|_{L^{p}(B_{R-j\rho})} + \sum_{|\alpha|=k} \rho^{-1} \|r^{|\alpha|-\gamma}\partial^{\alpha}u\|_{L^{p}(B_{R-j\rho})} + \sum_{|\alpha|=k-1} \rho^{-2} \|r^{|\alpha|-\gamma}\partial^{\alpha}u\|_{L^{p}(B_{R-j\rho})} \right)$$

For the proof of Proposition 7, we introduce a smooth cutoff function $\eta \in C_0^{\infty}(B_{R-j\rho})$ such that for $\alpha \in \mathbb{N}^d$, $|\alpha| \leq 2$

(41)
$$0 \le \eta \le 1, \qquad \eta = 1 \text{ on } B_{R-(j+1)\rho}, \qquad |\partial^{\alpha}\eta| \le C_{\eta}\rho^{-|\alpha|}.$$

and we introduce an auxiliary estimate (see [MM19a] for the proof)

Lemma 8. [MM19a, Lemma 9] Let 1 , <math>R > 0, and $\gamma \in \mathbb{R}$. There exists C > 0 such that, for all $\beta \in \mathbb{N}_0^d$, $\rho \in (0, \frac{R}{2(|\beta|+2)}]$, and $j \in \mathbb{N}$ such that $1 \le j \le |\beta| + 1$,

(42)
$$\sum_{|\alpha|=2} \left\| \left[\partial^{\alpha}, r^{|\beta|+2-\gamma} \right] \eta \partial^{\beta} u \right\|_{L^{p}(B_{R-j\rho})} \leq C \sum_{|\alpha|\leq 1} \rho^{-2+|\alpha|} \|r^{|\beta|+|\alpha|-\gamma} \partial^{\alpha+\beta} u\|_{L^{p}(B_{R-j\rho})},$$

and C depends only on γ , R.

Proof of Proposition 7. Let us consider a multiindex β . First,

$$(43) \sum_{|\alpha|=2} \|r^{|\beta|+2-\gamma} \partial^{\alpha+\beta} u\|_{L^{p}(B_{R-(j+1)\rho})} \leq \sum_{|\alpha|=2} \left\{ \|\partial^{\alpha} \left(r^{|\beta|+2-\gamma} \partial^{\beta} u\right)\|_{L^{p}(B_{R-(j+1)\rho})} + \|\left[\partial^{\alpha}, r^{|\beta|+2-\gamma}\right] \partial^{\beta} u\|_{L^{p}(B_{R-(j+1)\rho})} \right\}$$

We consider the first term at the right hand side: using (41)

$$\sum_{|\alpha|=2} \|\partial^{\alpha} \left(r^{|\beta|+2-\gamma} \partial^{\beta} u \right)\|_{L^{p}(B_{R-(j+1)\rho})} \leq \sum_{|\alpha|=2} \|\partial^{\alpha} \left(r^{|\beta|+2-\gamma} \eta \partial^{\beta} u \right)\|_{L^{p}(B_{R-j\rho})}$$

and by elliptic regularity and using the triangular inequality, there exists C_Δ depending only on p and R such that

$$\begin{split} &\sum_{|\alpha|=2} \|\partial^{\alpha} \left(r^{|\beta|+2-\gamma} \eta \partial^{\beta} u \right) \|_{L^{p}(B_{R-j\rho})} \\ &\leq C_{\Delta} \|\Delta \left(r^{|\beta|+2-\gamma} \eta \partial^{\beta} u \right) \|_{L^{p}(B_{R-j\rho})} \\ &\leq C_{\Delta} \left(\|r^{|\beta|+2-\gamma} \eta \Delta \partial^{\beta} u\|_{L^{p}(B_{R-j\rho})} + \| \left[\Delta, r^{|\beta|+2-\gamma} \right] \eta \partial^{\beta} u\|_{L^{p}(B_{R-j\rho})} + \|r^{|\beta|+2-\gamma} \left[\Delta, \eta \right] \partial^{\beta} u\|_{L^{p}(B_{R-j\rho})} \right) \\ & \text{Combining the lact inequality with (43) we obtain} \end{split}$$

Combining the last inequality with (43) we obtain

$$(44) \sum_{|\alpha|=2} \|r^{|\beta|+2-\gamma}\partial^{\alpha+\beta}u\|_{L^{p}(B_{R-(j+1)\rho})}$$

$$\leq C_{\Delta}\left(\|r^{|\beta|+2-\gamma}\eta\partial^{\beta}(\Delta u)\|_{L^{p}(B_{R-j\rho})} + \sum_{i=1}^{d}\|r^{|\beta|+2-\gamma}(\partial_{ii}\eta)\partial^{\beta}u\|_{L^{p}(B_{R-j\rho})}\right)$$

$$+2\sum_{i=1}^{d}\|r^{|\beta|+2-\gamma}(\partial_{i}\eta)\partial^{\beta}\partial_{i}u\|_{L^{p}(B_{R-j\rho})}\right) + (1+C_{\Delta})\sum_{|\alpha|=2}\|\left[\partial^{\alpha},r^{|\beta|+2-\gamma}\right]\partial^{\beta}u\|_{L^{p}(B_{R-j\rho})}.$$

The bounds on the derivatives of η given in (41) and the estimate of Lemma 8 applied to (44) then imply the existence of a constant *C* dependent on *p*, γ , and *R* such that

$$\sum_{|\alpha|=2} \|r^{|\beta|+2-\gamma}\partial^{\alpha+\beta}u\|_{L^p(B_{R-(j+1)\rho})} \le C_\Delta \|r^{|\beta|+2-\gamma}\eta\partial^\beta (\Delta u)\|_{L^p(B_{R-j\rho})} + C\sum_{|\alpha|\le 1} \rho^{-2+|\alpha|} \|r^{|\beta|+|\alpha|-\gamma}\partial^{\alpha+\beta}u\|_{L^p(B_{R-j\rho})}$$

We can now sum over all multi indices β such that $|\beta| = k - 1$ to obtain the thesis (40).

A.3. Weighted interpolation estimate.

Lemma 9. Let R > 0 such that $B_R \subset B_1$, $\gamma - d/p \ge -2/3$, and $p \ge \frac{2}{3}d$. There exists a constant $C_{\text{interp}} > 0$ such that for all $\beta \in \mathbb{N}_0^d$ and $u \in \mathcal{K}_{\gamma}^{|\beta|+1,p}(B_R)$ the following "interpolation" estimate holds

$$(45) \quad \|r^{\frac{2-\gamma}{3}+|\beta|}\partial^{\beta}u\|_{L^{3p}(B_{R})} \leq C_{\text{interp}}\|r^{|\beta|-\gamma}\partial^{\beta}u\|_{L^{p}(B_{R})}^{1-\vartheta} \left\{ (|\beta|+1)^{\vartheta}\|r^{|\beta|-\gamma}\partial^{\beta}u\|_{L^{p}(B_{R})}^{\vartheta} + \sum_{i=1}^{d}\|r^{|\beta|+1-\gamma}\partial^{\beta}\partial_{i}u\|_{L^{p}(B_{R})}^{\vartheta} \right\},$$

with $\vartheta = \frac{2}{3} \frac{d}{p}$.

Proof. Consider a dyadic decomposition of B_1 given by the sets

$$V^{j} = \left\{ x \in B_{1} : 2^{-j} \le |x| \le 2^{-j+1} \right\}, \ j = 1, 2, \dots$$

and decompose the ball B_R into its intersections with the sets belonging to the decomposition, i.e., into $B^j = B_R \cap V^j$. Let us introduce the linear maps $\chi_j : V^1 \to V^j$ and write with a hat the pullback of functions by χ_j^{-1} , e.g., $\hat{r} = r \circ \chi_j^{-1}$ and $\hat{B}^j = \chi_j^{-1}(B^j)$. Then,

$$\|r^{\frac{2-\gamma}{3}+|\beta|}\partial^{\beta}u\|_{L^{3p}(B^{j})} \le 2^{\frac{j}{3}(\gamma-2-d/p)}\|\hat{r}^{\frac{2-\gamma}{3}+|\beta|}\hat{\partial}^{\beta}\hat{u}\|_{L^{3p}(\hat{B}^{j})}$$

We can now use the interpolation inequality

$$\|v\|_{L^{3p}(B)} \le C \|v\|_{L^{p}(B)}^{1-\vartheta} \|v\|_{W^{1,p}(B)}^{\vartheta},$$

for $B \subset \mathbb{R}^d$, $v \in W^{1,p}(B)$ and with ϑ defined as above, see [DFØS12]. Therefore,

$$(46) \quad \|r^{\frac{2-\gamma}{3}+|\beta|}\partial^{\beta}u\|_{L^{3p}(B^{j})} \leq C2^{\frac{j}{3}(\gamma-2-d/p)}\|\hat{r}^{\frac{2-\gamma}{3}+|\beta|}\hat{\partial}^{\beta}\hat{u}\|_{L^{p}(\widehat{B}^{j})}^{1-\vartheta} \sum_{|\alpha|=1} \|\hat{\partial}^{\alpha}\hat{r}^{\frac{2-\gamma}{3}+|\beta|}\hat{\partial}^{\beta}\hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta}.$$

Let us now consider the first norm in the product above. Since $\hat{r} \in (1/2, 1)$, we can inject in the norm a term $\hat{r}^{\frac{2}{3}\gamma} \leq \max(1, 2^{\frac{2}{3}|\gamma|}) = C(\gamma)$, i.e.,

$$\|\hat{r}^{\frac{2-\gamma}{3}+|\beta|}\hat{\partial}^{\beta}\hat{u}\|_{L^{p}(\widehat{B}^{j})}^{1-\vartheta} \leq C\|\hat{r}^{|\beta|-\gamma}\hat{\partial}^{\beta}\hat{u}\|_{L^{p}(\widehat{B}^{j})}^{1-\vartheta}.$$

We now compute more explicitly the second norm in the product in (46):

$$\sum_{|\alpha|=1} \|\hat{\partial}^{\alpha} \hat{r}^{\frac{2-\gamma}{3}+|\beta|} \hat{\partial}^{\beta} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} \leq \left(|\beta|+\frac{2-\gamma}{3}\right)^{\vartheta} \|\hat{r}^{\frac{2-\gamma}{3}+|\beta|-1} \hat{\partial}^{\beta} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} + \sum_{i=1}^{d} \|\hat{r}^{\frac{2-\gamma}{3}+|\beta|} \hat{\partial}^{\beta} \partial_{i} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} + \sum_{i=1}^{d} \|\hat{r}^{\frac{2-\gamma}{3}+|\beta|} \hat{\partial}^{\beta} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} + \sum_{i=1}^{d} \|\hat{r}^{\frac{2-\gamma}{3}+|\beta|} \hat{\partial}^{\beta} \partial_{i} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} + \sum_{i=1}^{d} \|\hat{r}^{\frac{2-\gamma}{3}+|\beta|} \hat{\partial}^{\beta} \partial_{i} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} + \sum_{i=1}^{d} \|\hat{r}^{\frac{2-\gamma}{3}+|\beta|} \hat{\partial}^{\beta} \partial_{i} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} + \sum_{i=1}^{d} \|\hat{r}^{\frac{2-\gamma}{3}+|\beta|} \hat{\partial}^{\beta} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} + \sum_{i=1}^{d} \|\hat{r}^{\frac{2-\gamma}{3}+|\beta|} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} + \sum_{i=1}^{d} \|\hat{r}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} + \sum_$$

and we may adjust the exponents of \hat{r} and the term in $\frac{2-\gamma}{3}$ introducing a constant that depends on γ , d and p, obtaining

$$\sum_{|\alpha|=1} \|\hat{\partial}^{\alpha} \hat{r}^{\frac{2-\gamma}{3}+|\beta|} \hat{\partial}^{\beta} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} \leq C \left(|\beta|+1\right)^{\vartheta} \|\hat{r}^{|\beta|-\gamma} \hat{\partial}^{\beta} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta} + \sum_{i=1}^{a} \|\hat{r}^{|\beta|-\gamma+1} \hat{\partial}^{\beta} \partial_{i} \hat{u}\|_{L^{p}(\widehat{B}^{j})}^{\vartheta}.$$

Scaling everything back to B^j and adjusting the exponents,

$$\begin{aligned} \|r^{\frac{2-\gamma}{3}+|\beta|}\partial^{\beta}u\|_{L^{3p}(B^{j})} &\leq C2^{j(\gamma-d/p-2/3)}\|r^{|\beta|-\gamma}\partial^{\beta}u\|_{L^{p}(B^{j})}^{1-\vartheta} \left\{ \left(|\beta|+1\right)^{\vartheta}\|r^{|\beta|-\gamma}\partial^{\beta}u\|_{L^{p}(B^{j})}^{\vartheta} + \sum_{i=1}^{d}\|r^{|\beta|-\gamma+1}\partial^{\beta}\partial_{i}u\|_{L^{p}(B^{j})}^{\vartheta} \right\}.\end{aligned}$$

If $\gamma - d/p \ge -2/3$ then we can sum over all j = 1, 2, ... thus obtaining the estimate (40) on the whole ball B_R .

A.4. An imbedding result.

Lemma 10. Let $p \ge 2$, R > 0, and $\gamma \in \mathbb{R}$ such that $\gamma - d/p > 0$. Then, there exists C such that for all $\ell \in \mathbb{N}_0$ and all $v \in \mathcal{K}^{\infty,p}_{\gamma}(B_R)$.

$$||v||_{\mathcal{K}^{\ell,\infty}_{\gamma-d/p}(B_R)} \le C(\ell+1)^2 ||v||_{\mathcal{K}^{\ell+2,p}_{\gamma}(B_R)}.$$

Proof. We prove the lemma for R = 1; the general case with R > 0 follows by homothety (with constants depending on R). Consider the annuli

$$\Gamma_j = \left\{ x \in B_1 : 2^{-j-1} < |x| < 2^{-j} \right\}, \ j \in \mathbb{N}_0$$

and let $\widehat{\Gamma} = \Gamma_0$. For all $j \in \mathbb{N}$, let χ_j be the homothety from $\widehat{\Gamma}$ to Γ_j and denote with a hat the quantities rescaled on $\widehat{\Gamma}$, e.g., $\hat{v} = v \circ \chi$. Then, by a scaling argument and since $1/2 < \hat{r}_{|_{\widehat{\Gamma}}} < 1$, we have

$$\max_{|\alpha| \le \ell} \|r^{|\alpha| - \gamma + d/p} \partial^{\alpha} v\|_{L^{\infty}(\Gamma_j)} \le 2^{j(\gamma - d/p)} \max_{|\alpha| \le \ell} \|\hat{r}^{|\alpha|} \widehat{\partial}^{\alpha} \hat{v}\|_{L^{\infty}(\widehat{\Gamma})}.$$

By the embedding of $W^{2,p}(\widehat{\Gamma})$ in $L^{\infty}(\widehat{\Gamma})$, then, there exists C > 0 independent of ℓ and j such that

$$\max_{|\alpha| \le \ell} \|r^{|\alpha| - \gamma + d/p} \partial^{\alpha} v\|_{L^{\infty}(\Gamma_j)} \le C 2^{j(\gamma - d/p)} \max_{|\alpha| \le \ell} \|\hat{r}^{|\alpha|} \widehat{\partial}^{\alpha} \hat{v}\|_{W^{2,p}(\widehat{\Gamma})}$$

Hence, by a simple differentiation, injecting the necessary weight, using again that $1/2 < \hat{r}_{|_{\hat{\Gamma}}} < 1$, and bounding the maximum over $|\alpha| \le \ell$ with the respective sum, we arrive at

$$\max_{|\alpha| \le \ell} \|r^{|\alpha| - \gamma + d/p} \partial^{\alpha} v\|_{L^{\infty}(\Gamma_j)} \le C 2^{j(\gamma - d/p)} (\ell + 1)^2 \left(\sum_{|\alpha| \le \ell + 2} \|\hat{r}^{|\alpha| - \gamma} \widehat{\partial}^{\alpha} \hat{v}\|_{L^p(\widehat{\Gamma})}^p \right)^{1/p}.$$

Scaling back to the original domain, we obtain the existence of C>0 independent of ℓ and j such that

$$\max_{|\alpha| \le \ell} \|r^{|\alpha| - \gamma + d/p} \partial^{\alpha} v\|_{L^{\infty}(\Gamma_j)} \le C(\ell + 1)^2 \|v\|_{\mathcal{K}^{\ell+2,p}_{\gamma}(\Gamma_j)},$$

hence there exists C > 0 such that for all $\ell \in \mathbb{N}$ holds

$$\|v\|_{\mathcal{K}^{\ell,\infty}_{\gamma-d/p}(B_1)} = \sup_{j\in\mathbb{N}_0} \|v\|_{\mathcal{K}^{\ell,\infty}_{\gamma-1}(\Gamma_j)} \le C(\ell+1)^2 \|u\|_{\mathcal{K}^{\ell+2,p}_{\gamma}(B_1)}.$$

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