Analytic structure of many-body Coulombic wave functions

Fournais, Søren; Hoffmann-Ostenhof, Maria; Hoffmann-Ostenhof, Thomas; Sørensen, Thomas Østergaard

Publication date:
2008

Document Version
Publisher's PDF, also known as Version of record

AALBORG UNIVERSITY

Analytic structure of many-body Coulombic wave functions

by

S. Fournais, M. Hoffmann-Ostenhof,T. Hoffmann-Ostenhof
and T. Østergaard Sørensen

R-2008-06 Juni 2008

Department of Mathematical Sciences
Aalborg University
Fredrik Bajers Vej 7 G ▪ DK - 9220 Aalborg Øst ▪ Denmark
Phone: +45 99 40 80 80 ▪ Telefax: +45 98 15 81 29
URL: http://www.math.aau.dk

ISSN 1399–2503 ▪ On-line version ISSN 1601–7811

ANALYTIC STRUCTURE OF MANY-BODY COULOMBIC WAVE FUNCTIONS

S. FOURNAIS, M. HOFFMANN-OSTENHOF, T. HOFFMANN-OSTENHOF, AND T. ØSTERGAARD SØRENSEN

Abstract. We investigate the analytic structure of solutions of non-relativistic Schrödinger equations describing Coulombic many-particle systems. We prove the following: Let $\psi(\mathbf{x})$ with $\mathbf{x} = (x_1, \dots, x_N) \in \mathbb{R}^{3N}$ denote an N-electron wavefunction of such a system with one nucleus fixed at the origin. Then in a neighbourhood of a coalescence point, for which $x_1 = 0$ and the other electron coordinates do not coincide, and differ from 0, ψ can be represented locally as $\psi(\mathbf{x}) = \psi^{(1)}(\mathbf{x}) + |x_1|\psi^{(2)}(\mathbf{x})$ with $\psi^{(1)}, \psi^{(2)}$ real analytic. A similar representation holds near two-electron coalescence points. The Kustaanheimo-Stiefel transform and analytic hypoellipticity play an essential role in the proof.

1. Introduction and results

1.1. Introduction. In quantum chemistry and atomic and molecular physics, the regularity properties of the Coulombic wavefunctions ψ, and of their corresponding one-electron densities ρ, are of great importance. These regularity properties determine the convergence properties of various (numerical) approximation schemes (see [26, 2, 3, 31, 32, 33] for some recent works). They are also of intrinsic mathematical interest.

The pioneering work is due to Kato [20], who proved that ψ is Lipschitz continuous, i.e., $\psi \in C^{0,1}$, near two-particle coalescence points.

In a series of recent papers the present authors have studied these properties in detail. In [7] we deduced an optimal representation of ψ of the form $\psi = \mathcal{F}\Phi$ with an explicit $\mathcal{F} \in C^{0,1}$, such that $\Phi \in C^{1,1}$, characterizing the singularities of ψ up to second derivatives; see [7, Theorem 1.1] for a precise statement. In particular, $\mathcal{F}$ contains logarithmic terms which stem from the singularities of the potential at three-particle coalescence points. This characterization has been applied in [8] and [9] in the study of the electron density ρ and (in the

Date: June 10, 2008.

atomic case) its spherical average $\widetilde{\rho}$ close to the nuclei. Real analyticity of ρ away from the nuclei was proved in [6]; see also [4], [5].

In this paper we derive a different representation of ψ which completely settles its analytic structure in the neighbourhood of two-particle coalescence points. The Kustaanheimo-Stiefel transform (KS-transform for short) and analytic hypoanalyticity of a certain degenerate elliptic operator are crucial for the proof.

We start with the one-particle case.

Theorem 1.1. *Let $\Omega \subset \mathbb{R}^3$ be a neighbourhood of the origin and assume that $W^{(1)}$, $W^{(2)}$, $F^{(1)}$, and $F^{(2)}$ are real analytic functions in Ω. Let*

$$H = -\Delta + \frac{W^{(1)}}{|x|} + W^{(2)}\,, \tag{1.1}$$

and assume that $\varphi \in W^{1,2}(\Omega)$ satisfies

$$H\varphi = \frac{F^{(1)}}{|x|} + F^{(2)} \tag{1.2}$$

in Ω in the distributional sense.

Then there exists a neighbourhood $\widetilde{\Omega} \subset \Omega$ of the origin, and real analytic functions $\varphi^{(1)}, \varphi^{(2)} : \widetilde{\Omega} \to \mathbb{C}$ such that

$$\varphi(x) = \varphi^{(1)}(x) + |x|\varphi^{(2)}(x)\,,\ x \in \widetilde{\Omega}\,. \tag{1.3}$$

Remark 1.2. Theorem 1.1 is a generalization of an almost 25 years old result by Hill [16]. The present investigations were partly motivated by this work. Hill considered solutions to

$$\big(-\Delta - \frac{Z}{|x|} + V^{(1)}(x) + |x|V^{(2)}(x)\big)\varphi = 0\,, \tag{1.4}$$

with $V^{(1)}$ and $V^{(2)}$ real analytic near the origin, and proved that φ satisfies (1.3). The statement (1.3) can easily be seen to hold for Hydrogenic eigenfunctions. These have the form $e^{-\beta|x|}P(x)$ for some $\beta > 0$, where $P(x)$ can be written as linear combinations of polynomials in $|x|$ times homogeneous harmonic polynomials. In particular, Hill's result implies that φ satisfies (1.3) near the origin for a one-electron molecule with fixed nuclei, one of them at the origin.

Remark 1.3. Hill's proof is rather involved. Our proof is quite different, also not easy, but has the advantage that it can be generalized to treat the Coulombic many-particle case; see Theorem 1.4 and its proof below, and also Remark 1.6.

The proof of Theorem 1.1 uses the KS-transform (see Section 2 for the definition). This transform was introduced in the 1960's [25] to regularize the Kepler problem in classical mechanics (see also [24, 30, 22]) and has found applications in problems related to the Coulomb potential in classical mechanics and quantum mechanics, see [1, 10, 13, 14, 15, 19]. The KS-transform is a homogeneous extension of the Hopf map (also called the Hopf fibration), the first example of a map from $\mathbb{S}^3$ to $\mathbb{S}^2$ which is not null-homotopic, discovered in the 1930's [17]. For more on the literature on the KS-transform, see [22, 14].

We move to the N-particle problem. For the sake of simplicity we consider the atomic case and mention extensions in the remarks. Let H be the non-relativistic Schrödinger operator of an N-electron atom with nuclear charge $Z > 0$ in the fixed nucleus approximation,

$$H = \sum_{j=1}^{N} \Big(-\Delta_j - \frac{Z}{|x_j|}\Big) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} =: -\Delta + V\,. \tag{1.5}$$

Here the $x_j = (x_{j,1}, x_{j,2}, x_{j,3}) \in \mathbb{R}^3$, $j = 1, \ldots, N$, denote the positions of the electrons, and the Δ_j are the associated Laplacians so that $\Delta = \sum_{j=1}^{N} \Delta_j$ is the $3N$-dimensional Laplacian. Let $\mathbf{x} = (x_1, x_2, \ldots, x_N) \in \mathbb{R}^{3N}$ and let $\nabla = (\nabla_1, \ldots, \nabla_N)$ denote the $3N$-dimensional gradient operator. The operator H is bounded from $W^{2,2}(\mathbb{R}^{3N})$ to $L^2(\mathbb{R}^{3N})$, and defines a bounded quadratic form on $W^{1,2}(\mathbb{R}^{3N})$ [21]. We investigate local solutions ψ of

$$H\psi = E\psi\ , \quad E \in \mathbb{R}\,, \tag{1.6}$$

in a neighbourhood of two-particle coalescence points.

More precisely, let Σ denote the set of coalescence points,

$$\Sigma := \Big\{ \mathbf{x} = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \,\Big|\, \prod_{j=1}^{N} |x_j| \prod_{1 \leq i < j \leq N} |x_i - x_j| = 0 \Big\}\,. \tag{1.7}$$

If, for some $\Omega \subset \mathbb{R}^{3N}$, ψ is a distributional solution to (1.6) in Ω, then [18, Section 7.5, pp. 177–180] ψ is real analytic away from Σ, that is, $\psi \in C^{\omega}(\Omega \setminus \Sigma)$.

Let, for $k, \ell \in \{1, \ldots, N\}, k \neq \ell$,

$$\Sigma_k' : = \Big\{ \mathbf{x} \in \mathbb{R}^{3N} \,\Big|\, \prod_{j=1, j\neq k}^{N} |x_j| \prod_{1 \leq i < j \leq N} |x_i - x_j| = 0 \Big\}\,, \tag{1.8}$$

$$\Sigma_{k,\ell}' : = \Big\{ \mathbf{x} \in \mathbb{R}^{3N} \,\Big|\, \prod_{j=1}^{N} |x_j| \prod_{1 \leq i < j \leq N, \{i,j\} \neq \{k,\ell\}} |x_i - x_j| = 0 \Big\}\,. \tag{1.9}$$

Then we denote

$$\Sigma_k := \Sigma \setminus \Sigma_k' \ , \quad \Sigma_{k,\ell} := \Sigma \setminus \Sigma_{k,\ell}' \tag{1.10}$$

the two kinds of 'two-particle coalescence points'.

The main result of this paper is the following.

Theorem 1.4. *Let H be the non-relativistic Hamiltonian of an atom, given by* (1.5)*, let $\Omega \subset \mathbb{R}^{3N}$ be an open set, and assume that $\psi \in W^{1,2}(\Omega)$ satisfies, for some $E \in \mathbb{R}$,*

$$H\psi = E\psi \quad \text{in} \ \ \Omega \tag{1.11}$$

in the distributional sense. Let the sets Σ_k and $\Sigma_{k,\ell}$ be given by (1.10)*.*

Then, for all $k \in \{1, \ldots, N\}$, there exists a neighbourhood $\Omega_k \subset \Omega$ of $\Omega \cap \Sigma_k$, and real analytic functions $\psi_k^{(1)}, \psi_k^{(2)} : \Omega_k \to \mathbb{C}$ such that

$$\psi(\mathbf{x}) = \psi_k^{(1)}(\mathbf{x}) + |x_k|\psi_k^{(2)}(\mathbf{x}) \ , \ \ \mathbf{x} \in \Omega_k \ , \tag{1.12}$$

and for all $k, \ell \in \{1, \ldots, N\}$, $k \neq \ell$, there exists a neighbourhood $\Omega_{k,\ell} \subset \Omega$ of $\Omega \cap \Sigma_{k,\ell}$, and real analytic functions $\psi_{k,\ell}^{(1)}, \psi_{k,\ell}^{(2)} : \Omega_{k,\ell} \to \mathbb{C}$ such that

$$\psi(\mathbf{x}) = \psi_{k,\ell}^{(1)}(\mathbf{x}) + |x_k - x_\ell|\psi_{k,\ell}^{(2)}(\mathbf{x}) \ , \ \ \mathbf{x} \in \Omega_{k,\ell} \, . \tag{1.13}$$

Remark 1.5. The proof of Theorem 1.4 again uses the KS-transform. Due to the presence of the other electron coordinates we are confronted with additional problems. We have to deal with degenerate elliptic PDE's where the corresponding operators (of Grušin-type) are analytic hypoelliptic, see [12].

Remark 1.6. Theorem 1.4 extends in the obvious way to electronic eigenfunctions of Hamiltonians of N-electron molecules with K nuclei fixed at positions $(R_1, \ldots, R_K) \in \mathbb{R}^3$, given by

$$H = \sum_{j=1}^{N} \Big(-\Delta_j - \sum_{\ell=1}^{K} \frac{Z_\ell}{|x_j - R_\ell|} \Big) + \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} \, . \tag{1.14}$$

Furthermore we can replace in (1.14), as in Theorem 1.1, the potential terms by more general terms, and allow for inhomogeneities.

For instance, the result holds for general Coulombic many-particle systems described by

$$H = \sum_{j=1}^{n} -\frac{\Delta_j}{2m_j} + \sum_{1 \le i < j \le n} v_{ij}(x_i - x_j) \, , \tag{1.15}$$

where the $m_j > 0$ denote the masses of the particles, and $v_{ij} = v_{i,j}^{(1)}|x_i - x_j|^{-1} + v_{i,j}^{(2)}$ with $v_{ij}^{(k)}$, $k = 1, 2$, real analytic.

Remark 1.7. In separate work we will present additional regularity results (not primarily for Coulomb problems) obtained partly using the techniques developed in the present paper.

2. Proofs of the main theorems

As mentioned in the introduction our proofs are based on the Kustaanheimo-Stiefel (KS) transform. We will 'lift' the differential equations to new coordinates using that transform. The solutions to the new equations will be real analytic functions. By projecting to the original coordinates we get the structure results Theorem 1.1 and Theorem 1.4.

In the present section we will introduce the KS-transform and show how it allows to obtain Theorems 1.1 and 1.4. The more technical verifications of the properties of the KS-transform and its composition with real analytic functions needed for these proofs are left to Sections 3 and 4.

Define the KS-transform $K : \mathbb{R}^4 \to \mathbb{R}^3$ by

$$K(y) = \begin{pmatrix} y_1^2 - y_2^2 - y_3^2 + y_4^2 \\ 2(y_1y_2 - y_3y_4) \\ 2(y_1y_3 + y_2y_4) \end{pmatrix} . \tag{2.1}$$

It is a simple computation to verify that

$$|K(y)| := \|K(y)\|_{\mathbb{R}^3} = \|y\|_{\mathbb{R}^4}^2 =: |y|^2 \text{ for all } y \in \mathbb{R}^4 . \tag{2.2}$$

Let $f : \mathbb{R}^3 \to \mathbb{C}$ be any C^2-function, and define, with K as above,

$$f_K : \mathbb{R}^4 \to \mathbb{C} , \qquad f_K(y) := f(K(y)) . \tag{2.3}$$

Then for all $y \in \mathbb{R}^4 \setminus \{0\}$, (see Lemma 3.1),

$$(\Delta f)(K(y)) = \frac{1}{4|y|^2} \Delta f_K(y) . \tag{2.4}$$

2.1. **Proof of Theorem 1.1.** Assume $\varphi \in W^{1,2}(\Omega)$ satisfies (see (1.1)–(1.2))

$$\big(- \Delta + \frac{W^{(1)}}{|x|} + W^{(2)} \big)\varphi = \frac{F^{(1)}}{|x|} + F^{(2)} , \tag{2.5}$$

with $W^{(1)}, W^{(2)}, F^{(1)}, F^{(2)}$ real analytic in $\Omega \subset \mathbb{R}^3$.

Assume without loss that $\Omega = B_3(0, r)$ for some $r > 0$. (Here, and in the sequel, $B_n(x_0, r) = \{x \in \mathbb{R}^n \,|\, |x - x_0| < r\}$.) Since $\varphi \in L^2(\Omega)$, Remark 3.2 in Section 3 below implies that φ_K is well-defined, as an element of $L^2(K^{-1}(\Omega), \frac{4}{\pi}|y|^2 dy)$. We will show that φ_K satisfies (in the distributional sense)

$$\big(- \Delta_y + 4(W_K^{(1)} + |y|^2 W_K^{(2)})\big)\varphi_K = 4(F_K^{(1)} + |y|^2 F_K^{(2)}) \tag{2.6}$$

in $K^{-1}(\Omega) = B_4(0, \sqrt{r})$, with $W_K^{(i)}, F_K^{(i)}$, $i = 1, 2$, defined as in (2.3). Since $W^{(i)}, F^{(i)}$, $i = 1, 2$, are real analytic in $B_3(0, r)$ by assumption, and $K : \mathbb{R}^4 \to \mathbb{R}^3$ (see (2.1)) and $y \mapsto |y|^2$ are real analytic, the coefficients in the elliptic equation in (2.6) are real analytic in $B_4(0, \sqrt{r})$. It follows from elliptic regularity for equations with real analytic coefficients [18, Section 7.5, pp. 177–180] that $\varphi_K : B_4(0, \sqrt{r}) \to \mathbb{C}$ is real analytic. The statement of Theorem 1.1 then follows from Proposition 4.1 in Section 4 below.

It therefore remains to prove that φ_K satisfies (2.6).

By elliptic regularity, $\varphi \in W^{2,2}(\Omega')$ for all $\Omega' = B_3(0, r')$, $r' < r$. (To see this, use Hardy's inequality [28, Lemma p. 169] and that $\varphi \in W^{1,2}(\Omega)$ to conclude that $\Delta\varphi = G$ with $G \in L^2(\Omega')$. Then use [11, Theorem 8.8]).

It follows that both $(\Delta\varphi)_K$ and $(|\cdot|^{-1}\varphi)_K$ are well-defined, as elements of $L^2(K^{-1}(\Omega'), \frac{4}{\pi}|y|^2 dy)$ (see Remark 3.2 in Section 3 below; see also (3.5)). This and (2.5) imply that, as functions in $L^2(K^{-1}(\Omega')) = L^2(B_4(0, \sqrt{r'}))$,

$$|y|(\Delta\varphi)_K = |y|\big((W\varphi)_K - F_K\big)\,, \tag{2.7}$$

with

$$W(x) = \frac{W^{(1)}(x)}{|x|} + W^{(2)}(x)\,, \qquad F(x) = \frac{F^{(1)}(x)}{|x|} + F^{(2)}(x)\,. \tag{2.8}$$

Let $f \in C_0^\infty(K^{-1}(\Omega))$; then there exists $r' < r$ such that $\operatorname{supp}(f) \subset K^{-1}(\Omega')$, $\Omega' := B_3(0, r')$; choose $\{\varphi_n\}_{n\in\mathbb{N}} \subset C^\infty(\Omega')$ such that $\varphi_n \to \varphi$ and $\Delta\varphi_n \to \Delta\varphi$ in $L^2(\Omega')$-norm. This is possible since $\varphi \in W^{2,2}(\Omega')$. Note that both Δf and $4|y|^2 f$ belong to $C_0^\infty(K^{-1}(\Omega))$ when f does. Using (2.4) for $\varphi_n \in C^\infty(\Omega')$, Remark 3.2 in Section 3 below therefore implies that

$$\begin{aligned}
&\int_{K^{-1}(\Omega)} (\Delta f)(y)\, \varphi_K(y)\, dy = \lim_{n\to\infty} \int_{K^{-1}(\Omega)} (\Delta f)(y)\, (\varphi_n)_K(y)\, dy \\
&= \lim_{n\to\infty} \int_{K^{-1}(\Omega)} f(y)\, [\Delta_y(\varphi_n)_K](y)\, dy = \lim_{n\to\infty} \int_{K^{-1}(\Omega)} 4|y|^2 f(y)\, (\Delta_x\varphi_n)_K(y)\, dy \\
&= \int_{K^{-1}(\Omega)} 4|y|^2 f(y)\, (\Delta_x\varphi)_K(y)\, dy\,.
\end{aligned}$$

It follows from this and (2.7) that

$$\int_{K^{-1}(\Omega)} (\Delta f)(y)\, \varphi_K(y)\, dy = \int_{K^{-1}(\Omega)} 4|y|^2 f(y)\, \big((W\varphi)_K - F_K\big)(y)\, dy\,.$$

Since $(W\varphi)_K = W_K\varphi_K$, and, by (2.8) and (2.2),

$$\begin{aligned} W_K(y) &= |y|^{-2}\big(W_K^{(1)}(y) + |y|^2 W_K^{(2)}(y)\big)\,,\\ F_K(y) &= |y|^{-2}\big(F_K^{(1)}(y) + |y|^2 F_K^{(2)}(y)\big)\,, \end{aligned}$$

this implies that, for all $f \in C_0^\infty(K^{-1}(\Omega))$,

$$\begin{aligned} \int_{K^{-1}(\Omega)} &\varphi_K(y)\big[-\Delta_y f(y) + 4(W_K^{(1)}(y) + |y|^2 W_K^{(2)}(y))f(y)\big]\, dy\\ &= \int_{K^{-1}(\Omega)} 4(F_K^{(1)}(y) + |y|^2 F_K^{(2)}(y))f(y)\, dy\,, \end{aligned}$$

which means that φ_K satisfies (2.6) in the distributional sense, in $K^{-1}(\Omega) = B_4(0, \sqrt{r})$. □

2.2. **The N-particle problem.** In this section we prove Theorem 1.4. We only prove the statement (1.12), the proof of (1.13) is completely analogous, after an orthogonal transformation of coordinates. We assume $k = 1$, the proof for other k's is the same.

Let H be given by (1.5). Then, with $(x, x') \equiv (x_1, x') \in \mathbb{R}^3 \times \mathbb{R}^{3N-3}$, $x' = (x_2, \ldots, x_N)$,

$$H - E = -\Delta_x - \Delta_{x'} - \frac{Z}{|x|} + V_E(x, x')\,, \tag{2.9}$$

where

$$V_E(x_1, x') = \sum_{j=2}^{N} -\frac{Z}{|x_j|} + \sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|} - E \tag{2.10}$$

is real analytic on $\Omega \setminus \Sigma_1'$ (see (1.8) for Σ_1').

Assume $\psi \in W^{1,2}(\Omega)$ satisfies

$$(H - E)\psi = 0 \quad \text{on} \quad \Omega\,, \tag{2.11}$$

and let $(x_0, x_0') \in \Omega \cap \Sigma_1$; then (see (1.10)) $x_0 = 0$. We will first prove that there exists a neighbourhood $\Omega_1(P)$ of $P = (0, x_0')$ and real analytic functions $\psi_P^{(1)}, \psi_P^{(2)} : \Omega_1(P) \to \mathbb{C}$ such that

$$\psi(\mathbf{x}) = \psi_P^{(1)}(\mathbf{x}) + |x|\psi_P^{(2)}(\mathbf{x})\,,\ \mathbf{x} \in \Omega_1(P)\,. \tag{2.12}$$

By the above, V_E is real analytic on a neighbourhood of $(0, x_0')$, say, on

$$U(R) = \big\{(x, x') \in \mathbb{R}^3 \times \mathbb{R}^{3N-3}\,\big|\, |x| < R, |x' - x_0'| < R\big\} \subset \Omega$$

for some $R > 0$, R small. Let

$$U_K(R) := \left\{(y, x') \in \mathbb{R}^4 \times \mathbb{R}^{3N-3} \,\middle|\, |y| < \sqrt{R}, |x' - x_0'| < R\right\}. \tag{2.13}$$

Define now, with $K : \mathbb{R}^4 \to \mathbb{R}^3$ as in (2.1),

$$u : U_K(R) \to \mathbb{C}, \quad u(y, x') := \psi(K(y), x'), \tag{2.14}$$

$$W : U_K(R) \to \mathbb{R}, \quad W(y, x') := V_E(K(y), x'). \tag{2.15}$$

Since (by (2.2)) $(K(y), x') \in U(R)$ for $(y, x') \in U_K(R)$, it follows that u and W are well-defined, and W is real analytic on $U_K(R)$ since K is real analytic and V_E is real analytic on $U(R)$.

As in the proof of Theorem 1.1, we get that (2.11) implies that u satisfies

$$Q(y, x', D_y, D_{x'})u = 0 \quad \text{on} \quad U_K(R), \tag{2.16}$$

where

$$Q(y, x', D_y, D_{x'}) := -\Delta_y - 4|y|^2\Delta_{x'} + 4|y|^2 W(y, x') - 4Z \tag{2.17}$$

is a degenerate elliptic operator, a so-called 'Grušin-type operator'.

Since $|y|^2 W(y, x')$ is real analytic on $U_K(R)$, the operator Q is (real) analytic hypoelliptic due to [12, Theorem 5.1]. Therefore (2.16) implies that u is real analytic on some neighbourhood of $(0, x_0') \in \mathbb{R}^4 \times \mathbb{R}^{3N-3}$.

It follows from Proposition 4.4 in Section 4 below that there exist a neighbourhood $\Omega_1(P) \subset \mathbb{R}^{3N}$ of $P = (0, x_0') \in \mathbb{R}^3 \times \mathbb{R}^{3N-3}$ and real analytic functions $\psi_P^{(1)}, \psi_P^{(2)} : \Omega_1(P) \to \mathbb{C}$ such that (2.12) holds.

Let now

$$\Omega_1 := \bigcup_{P \in \Omega \cap \Sigma_1} \Omega_1(P) \subset \Omega \subset \mathbb{R}^{3N},$$

and define $\psi_1^{(1)}, \psi_1^{(2)} : \Omega_1 \to \mathbb{C}$ by

$$\psi_1^{(i)}(\mathbf{x}) = \psi_P^{(i)}(\mathbf{x}) \ \text{ when } \mathbf{x} \in \Omega_1(P) \ (i = 1, 2). \tag{2.18}$$

To see that this is well-defined, we need to verify that if $\mathbf{x} \in \Omega_1(P) \cap \Omega_1(Q)$, then $\psi_P^{(i)}(\mathbf{x}) = \psi_Q^{(i)}(\mathbf{x})$, $i = 1, 2$. Let therefore $\widetilde{\psi}^{(i)} = \psi_P^{(i)} - \psi_Q^{(i)}$, $i = 1, 2$, then

$$\widetilde{\psi}^{(1)}(\mathbf{x}) + |x|\widetilde{\psi}^{(2)}(\mathbf{x}) = 0, \ \mathbf{x} \in \Omega_1(P) \cap \Omega_1(Q), \tag{2.19}$$

with $\widetilde{\psi}^{(1)}, \widetilde{\psi}^{(2)}$ real analytic in $\Omega_1(P) \cap \Omega_1(Q)$. Let $\tilde{\mathbf{x}}_0 = (0, \tilde{x}_0') \in \Omega_1(P) \cap \Omega_1(Q)$. Then, since $\widetilde{\psi}^{(i)}, i = 1, 2$, are real analytic, there exist

$\delta > 0$ and $P_n^{(i)}, i = 1, 2$, homogeneous polynomials of degree n such that

$$\widetilde{\psi}^{(i)}(\mathbf{x}) = \sum_{n=0}^{\infty} P_n^{(i)}(x, x' - \tilde{x}'_0)\,, \quad i = 1, 2\,, \tag{2.20}$$

for $\mathbf{x} \in B_{3N}(\tilde{\mathbf{x}}_0, \delta)$. It follows from (2.19) (by homogeneity) that, for all $n \in \mathbb{N}$ and $\mathbf{x} = (x, x') \in B_{3N}(\tilde{\mathbf{x}}_0, \delta)$,

$$P_n^{(1)}(x, x' - \tilde{x}'_0) + |x| P_{n-1}^{(2)}(x, x' - \tilde{x}'_0) = 0\,.$$

But for n even, $P_n^{(1)}$ is an even function, while $P_{n-1}^{(2)}$, and therefore $|x|P_{n-1}^{(2)}$, is odd. Therefore, $P_n^{(1)} = P_{n-1}^{(2)} = 0$. Similarly for n odd. It follows that $\widetilde{\psi}^{(1)} = \widetilde{\psi}^{(2)} = 0$ on $B_{3N}(\tilde{\mathbf{x}}_0, \delta)$, and therefore also on $\Omega_1(P) \cap \Omega_1(Q)$, since $\widetilde{\psi}^{(1)}, \widetilde{\psi}^{(2)}$ are real analytic. This proves that $\psi_1^{(1)}$ and $\psi_1^{(2)}$ in (2.18) are well-defined. Since they are obviously real analytic, this finishes the proof of Thereom 1.4. □

3. The Kustaanheimo-Stiefel transform

The KS-transform turns out to be a very useful and natural tool for the investigation of Schrödinger equations with Coulombic interactions. In particular (2.2) and the following lemma are important for our proofs. Most of the facts stated here are well-known (see e. g. [13, Appendix A]).

Lemma 3.1. *Let $K : \mathbb{R}^4 \to \mathbb{R}^3$ be defined as in (2.1), let $f : \mathbb{R}^3 \to \mathbb{C}$ be any C^2-function, and define $f_K : \mathbb{R}^4 \to \mathbb{C}$ by (2.3). Finally, let*

$$L(y, D_y) := y_1 \frac{\partial}{\partial y_4} - y_4 \frac{\partial}{\partial y_1} + y_3 \frac{\partial}{\partial y_2} - y_2 \frac{\partial}{\partial y_3}\,. \tag{3.1}$$

(a) *Then, with $[A; B] = AB - BA$ the commutator of A and B,*

$$L(y, D_y) f_K = 0\ , \qquad \big[\Delta; L(y, D_y)\big] = 0\,, \tag{3.2}$$

and (2.4) holds.

(b) *Furthermore, for a function $g \in C^1(\mathbb{R}^4)$, the following two statements are equivalent:*

(i) *There exists a function $f : \mathbb{R}^3 \to \mathbb{C}$ such that $g = f_K$.*

(ii) *The function g satisfies*

$$Lg = 0\,. \tag{3.3}$$

(c) *Finally, let* $U = B_3(0,r) \subset \mathbb{R}^3$ *for* $r \in (0,\infty]$. *Then, for* $\phi \in C_0(\mathbb{R}^3)$ *(continuous with compact support),*

$$\int_{K^{-1}(U)} |\phi(K(y))|^2 \, dy = \frac{\pi}{4} \int_U \frac{|\phi(x)|^2}{|x|} \, dx \,. \tag{3.4}$$

In particular,

$$\big\| |y| \phi_K \big\|^2_{L^2(K^{-1}(U))} = \frac{\pi}{4} \|\phi\|^2_{L^2(U)} \,. \tag{3.5}$$

Remark 3.2. By a density argument, the isometry (3.5) allows to extend the composition by K given by (2.3) (the pull-back K^* by K) to a map

$$\begin{aligned} K^* : L^2(U, dx) &\to L^2(K^{-1}(U), \tfrac{4}{\pi}|y|^2 dy) \\ \phi &\mapsto \phi_K \end{aligned}$$

in the case when $U = B_3(0,r), r \in (0,\infty]$. This makes ϕ_K well-defined for any $\phi \in L^2(U)$. Furthermore, if $\phi_n \to \phi$ in $L^2(U)$, then, for all $g \in C^\infty(K^{-1}(U))$ ($g \in C_0^\infty(K^{-1}(U))$, if $r = \infty$)

$$\lim_{n\to\infty} \int_{K^{-1}(U)} g(y) (\phi_n)_K(y) \, dy = \int_{K^{-1}(U)} g(y) \phi_K(y) \, dy \,. \tag{3.6}$$

This follows from Schwarz' inequality and (3.5),

$$\begin{aligned} \Big| \int_{K^{-1}(U)} & g(y) \big((\phi_n)_K(y) - \phi_K(y) \big) \, dy \Big| \\ &\leq \Big(\int_{K^{-1}(U)} \frac{|g(y)|^2}{|y|^2} \, dy \Big)^{1/2} \big\| |y| \big((\phi_n)_K - \phi_K \big) \big\|_{L^2(K^{-1}(U))} \\ &= \frac{\sqrt{\pi}}{2} \Big(\int_{K^{-1}(U)} \frac{|g(y)|^2}{|y|^2} \, dy \Big)^{1/2} \|\phi_n - \phi\|_{L^2(U)} \to 0 \,, \ n \to \infty \,. \end{aligned}$$

Here the y-integral clearly converges since $g \in C^\infty(\mathbb{R}^4)$ ($g \in C_0^\infty(\mathbb{R}^4)$, if $r = \infty$).

Remark 3.3. As a consequence of (2.2) and (3.2) (choose $f(x) = |x|^j$), we have that

$$L(y, D_y) |y|^{2j} = 0 \ , \ j \in \mathbb{N} \,. \tag{3.7}$$

Proof of Lemma 3.1. The lemma is easier to prove in 'double polar coordinates' in $\mathbb{R}^4$. Let

$$(R, \Omega) := (r_1, r_2, \theta_1, \theta_2) \in (0,\infty)^2 \times [0, 2\pi)^2 \tag{3.8}$$

be defined by the relation

$$y \equiv y(R,\Omega) = \big(y_1(R,\Omega), y_2(R,\Omega), y_3(R,\Omega), y_4(R,\Omega)\big)\,, \tag{3.9}$$

$$(y_1, y_4) = r_1(\cos\theta_1, \sin\theta_1)\ , \quad (y_3, y_2) = r_2(\cos\theta_2, \sin\theta_2)\,. \tag{3.10}$$

Then it follows directly from (2.1) that

$$K(y(R,\Omega)) = \begin{pmatrix} r_1^2 - r_2^2 \\ -2r_1r_2\sin(\theta_1-\theta_2) \\ 2r_1r_2\cos(\theta_1-\theta_2) \end{pmatrix}\,. \tag{3.11}$$

We note in passing that the relation (2.2) is immediate from (3.11). In the double polar coordinates,

$$L = \frac{\partial}{\partial\theta_1} + \frac{\partial}{\partial\theta_2}\,, \tag{3.12}$$

and

$$\Delta = \Big(\frac{\partial^2}{\partial r_1^2} + \frac{1}{r_1}\frac{\partial}{\partial r_1} + \frac{1}{r_1^2}\frac{\partial^2}{\partial\theta_1^2}\Big) + \Big(\frac{\partial^2}{\partial r_2^2} + \frac{1}{r_2}\frac{\partial}{\partial r_2} + \frac{1}{r_2^2}\frac{\partial^2}{\partial\theta_2^2}\Big)\,.$$

Therefore, it is obvious that L and Δ commute. Furthermore, from (3.11) we see that f_K only depends on the angles through the expression $\theta_1 - \theta_2$ and therefore,

$$Lf_K = \big(\frac{\partial}{\partial\theta_1} + \frac{\partial}{\partial\theta_2}\big)f_K = 0\,.$$

The proof of (2.4) is merely an elementary computation, which we leave to the reader. This finishes the proof of point (a) of the lemma.

From (3.2) we infer that in order to prove point (b) we have to show that (ii) implies (i).

To do so, we need to define a function $f : \mathbb{R}^3 \to \mathbb{C}$ such that $g = f_K$. If $x = 0$, let $f(x) := g(0)$, then $g(0) = f(0) = f(K(0)) = f_K(0)$ by (2.2). Assume now that $x \in \mathbb{R}^3 \setminus \{0\}$. We claim that the pre-image of x under K, $K^{-1}(\{x\})$, is a circle in $\mathbb{R}^4$ (in the literature called the 'Hopf circle') and that g is constant on this circle. Then, taking any $y \in K^{-1}(\{x\})$ and letting $f(x) := g(y)$, we have that f is well-defined, and satisfies $f_K(y) = f(K(y)) = f(x) = g(y)$. This will finish the proof of point (b) of the lemma.

To prove the claim, assume first that $x \in \mathbb{R}^3 \setminus \{0\}$, $x = (x_1, x_2, x_3)$ with $(x_2, x_3) \neq (0,0)$. Then the equations (see (3.11) and (2.2))

$$\begin{aligned} r_1^2 - r_2^2 &= x_1, \\ -2r_1r_2\sin\vartheta &= x_2, \\ 2r_1r_2\cos\vartheta &= x_3, \\ (r_1^2 + r_2^2)^2 &= x_1^2 + x_2^2 + x_3^2 \end{aligned} \tag{3.13}$$

uniquely determine $r_1, r_2 \in (0,\infty)$, and determine ϑ modulo 2π; choose the solution $\vartheta \in [0,2\pi)$. That is, the pre-image of x under K is the set of points in $\mathbb{R}^4$ with double polar coordinates $(r_1, r_2, \theta_1, \theta_2)$, where (r_1, r_2) is the unique solution to (3.13), and $\theta_1 - \theta_2 = \vartheta$ modulo 2π, with $\vartheta \in [0,2\pi)$. Defining new angles $\theta = \theta_1 + \theta_2, \vartheta = \theta_1 - \theta_2$, this set is the circle in $\mathbb{R}^4$ with centre at the origin and radius $(x_1^2 + x_2^2 + x_3^2)^{1/4} = \sqrt{r_1^2 + r_2^2}$, parametrized by $\theta \in [0,2\pi)$. Since, by (3.12), the function g (strictly speaking, g composed with the map in (3.9)) is independent of $\theta = \theta_1 + \theta_2$, g is, as claimed, constant on this circle.

On the other hand, assume $x = (t,0,0), t \in \mathbb{R} \setminus \{0\}$. Then the equations

$$\begin{aligned} r_1^2 - r_2^2 &= t, \\ (r_1^2 + r_2^2)^2 &= t^2 \end{aligned} \tag{3.14}$$

have a unique solution (r_1, r_2); in fact, $(r_1, r_2) = (\sqrt{t}, 0)$ if $t > 0$ and $(r_1, r_2) = (0, \sqrt{-t})$ if $t < 0$. In both cases, the pre-image of x under K is a circle, namely (see also (3.8))

$$\begin{aligned} C_+ &= \{(\sqrt{t}\cos\theta_1, 0, 0, \sqrt{t}\sin\theta_1)\} \in \mathbb{R}^4 \,|\, \theta_1 \in [0,2\pi)\} \qquad (t > 0)\,, \\ C_- &= \{(0, \sqrt{-t}\sin\theta_2, \sqrt{-t}\cos\theta_2, 0)\} \in \mathbb{R}^4 \,|\, \theta_2 \in [0,2\pi)\} \quad (t > 0)\,. \end{aligned}$$

Since $y_2 = y_3 = 0$ for any $y = (y_1, y_2, y_3, y_4) \in C_+$, (3.1) and (3.3) imply that $\partial g/\partial\theta_1 = 0$, with θ_1 the angle parametrizing C_+, and so g is, as claimed, constant on C_+; similarly for C_-. This finishes the proof of point (b) of the lemma.

We finish by proving point (c); this is merely a calculation which we for simplicity also do in 'double polar coordinates': Recall that $|y|^2 = r_1^2 + r_2^2 = |x|$ (see (2.2)). By (3.10) and (3.11), and since $U = B_3(0,r)$ and $K^{-1}(U) = B_4(0,\sqrt{r})$,

$$\begin{aligned} \int_{K^{-1}(U)} |\phi(K(y))|^2\,dy = \int_0^{2\pi} \Big\{ \int_0^{\sqrt{r}} r_1\,dr_1 \int_0^{\sqrt{r - r_1^2}} r_2\,dr_2 \int_0^{2\pi} d\theta_1 \\ \big|\phi\big(r_1^2 - r_2^2, -2r_1r_2\sin(\theta_1 - \theta_2), 2r_1r_2\cos(\theta_1 - \theta_2)\big)\big|^2 \Big\}\,d\theta_2\,. \end{aligned}$$

In the triple integral inside $\{\cdot\}$ we make (for fixed θ_2) the change of variables

$$x = K_{\theta_2}(r_1, r_2, \theta_1) = \big(r_1^2 - r_2^2, -2r_1r_2\sin(\theta_1 - \theta_2), 2r_1r_2\cos(\theta_1 - \theta_2)\big)\,.$$

From the foregoing (see after (3.14)) it follows that the image of K_{θ_2} is U. The determinant of the Jacobian is

$$
\begin{aligned}
&\det(DK_{\theta_2}) \\
&= \left| \begin{bmatrix} 2r_1 & -2r_2 & 0 \\ -2r_2\sin(\theta_1-\theta_2) & -2r_1\sin(\theta_1-\theta_2) & -2r_1r_2\cos(\theta_1-\theta_2) \\ 2r_2\cos(\theta_1-\theta_2) & 2r_1\cos(\theta_1-\theta_2) & -2r_1r_2\sin(\theta_1-\theta_2) \end{bmatrix} \right| \\
&= 8r_1r_2(r_1^2+r_2^2)\,.
\end{aligned}
$$

Recall that $|y|^2 = r_1^2 + r_2^2 = |x|$. Therefore the integral is

$$
\int_{K^{-1}(U)} |\phi(K(y)|^2\,dy = \int_0^{2\pi} \Big\{ \int_U |\phi(x)|^2 \frac{dx}{8|x|} \Big\}\, d\theta_2 = \frac{\pi}{4}\int_U \frac{|\phi(x)|^2}{|x|}\,dx\,.
$$

This proves (3.4); applying it to $\sqrt{|x|}\phi$ gives (3.5). This finishes the proof of point (c), and therefore, of Lemma 3.1. $\square$

Lemma 3.4. *Let the differential operator $L = L(y,D)$ be given by* (3.1)*, and let P_{2k} be a harmonic, homogeneous polynomial of degree $2k$ in $\mathbb{R}^4$ such that $LP_{2k} = 0$.*

Then there exists a harmonic polynomial in $\mathbb{R}^3$, Y_k, homogeneous of degree k, such that

$$
P_{2k}(y) = Y_k(K(y)) \quad \textit{for all } y \in \mathbb{R}^4\,, \tag{3.15}
$$

with $K : \mathbb{R}^4 \to \mathbb{R}^3$ from (2.1).

Proof. Using that $LP_{2k} = 0$ we get from Lemma 3.1 the existence of a function Y_k such that $P_{2k}(y) = Y_k(K(y))$. Since the KS-transform is homogeneous of degree 2, Y_k is necessarily homogeneous of degree k. Furthermore, by (2.4), Y_k is harmonic. So we only have left to prove that Y_k is a polynomial.

Let $\mathcal{L}_n$ be the (positive) Laplace-Beltrami operator on the sphere $\mathbb{S}^{n-1}$. Then one can express the Laplace operator in $\mathbb{R}^n$ as

$$
\Delta = \frac{\partial^2}{\partial r^2} + \frac{n-1}{r}\frac{\partial}{\partial r} - \frac{\mathcal{L}_n}{r^2}\,. \tag{3.16}
$$

Furthermore, $\sigma(\mathcal{L}_n) = \{\ell(\ell+n-1)\}_{\ell=0}^{\infty}$ and the eigenspace corresponding to the eigenvalue $\ell(\ell+n-1)$ is exactly spanned by the restrictions to $\mathbb{S}^{n-1}$ of the harmonic, homogeneous polymials in $\mathbb{R}^n$ of degree ℓ.

Using the fact that $\Delta Y_k = 0$ and that Y_k is homogeneous of degree k in $\mathbb{R}^3$ we find that $Y_k\big|_{\mathbb{S}^2}$ is an eigenfunction of $\mathcal{L}_3$ with eigenvalue $k(k+2)$. Thus there exists a homogeneous, harmonic polynomial $\widetilde{Y}_k$ of degree k such that

$$
\widetilde{Y}_k\big|_{\mathbb{S}^2} = Y_k\big|_{\mathbb{S}^2}\,.
$$

Since the functions have the same homogeneity, they are identical everywhere. This finishes the proof of the lemma. □

4. Analyticity and the KS-transform

In this section we study the regularity of functions given as a composition with the Kustaanheimo-Stiefel transform. We start with the one-particle case.

Proposition 4.1. *Let $U \subset \mathbb{R}^3$ be open with $0 \in U$, and let $\varphi : U \to \mathbb{C}$ be a function. Let $\mathcal{U} = K^{-1}(U) \subset \mathbb{R}^4$, with $K : \mathbb{R}^4 \to \mathbb{R}^3$ from* (2.1)*, and suppose that*

$$\varphi_K = \varphi \circ K : \mathcal{U} \to \mathbb{C} \tag{4.1}$$

is real analytic.

Then there exist functions $\varphi^{(1)}, \varphi^{(2)}$, real analytic in a neighbourhood of $0 \in \mathbb{R}^3$, such that

$$\varphi(x) = \varphi^{(1)}(x) + |x|\varphi^{(2)}(x)\,. \tag{4.2}$$

Proof. Note that $K(-y) = K(y)$ for all $y \in \mathbb{R}^4$, so that $\varphi_K(-y) = \varphi_K(y)$ for all $y \in \mathbb{R}^4$. It follows that φ_K can be written as an absolutely convergent power series containing only terms of even order. Furthermore, since the sum is absolutely convergent, the order of summation is unimportant, and so, for some $R > 0$, $c_\beta \in \mathbb{C}$,

$$\varphi_K(y) = \sum_{\beta \in \mathbb{N}^4, |\beta|/2 \in \mathbb{N}} c_\beta y^\beta = \sum_{n=0}^{\infty} \sum_{|\beta|=2n} c_\beta y^\beta \quad \text{for} \quad |y| < R\,. \tag{4.3}$$

This implies (see e. g. [23, sections 2.1–2.2]) that there exists constants $C_1, M_1 > 0$ such that

$$|c_\beta| \le C_1 M_1^{|\beta|} \quad \text{for all } \beta \in \mathbb{N}^4\,. \tag{4.4}$$

Note that for fixed $n \in \mathbb{N}$,

$$Q^{(2n)}(y) := \sum_{\beta \in \mathbb{N}^4, |\beta| = 2n} c_\beta\, y^\beta \tag{4.5}$$

is a homogeneous polynomial of degree $2n$. By [29, Theorem 2.1],

$$Q^{(2n)}(y) = \sum_{j=0}^{n} |y|^{2j} H^{(2n)}_{2n-2j}(y)\,, \tag{4.6}$$

where $H^{(2n)}_{2n-2j}$ is a homogeneous *harmonic* polynomial of degree $2n-2j$, $j = 0, 1, \ldots, n$. It follows that

$$\varphi_K(y) = \sum_{n=0}^{\infty} Q^{(2n)}(y) = \sum_{n=0}^{\infty}\sum_{j=0}^{n} |y|^{2j} H^{(2n)}_{2n-2j}(y)\,. \tag{4.7}$$

We need the following lemma.

Lemma 4.2. *There exist harmonic polynomials $Y^{(2n)}_{n-j} : \mathbb{R}^3 \to \mathbb{C}$, homogeneous of degree $n-j$, such that*

$$H^{(2n)}_{2n-2j}(y) = Y^{(2n)}_{n-j}(K(y)) \quad \textit{for all } y \in \mathbb{R}^4\,, \tag{4.8}$$

with $K : \mathbb{R}^4 \to \mathbb{R}^3$ from (2.1). In particular, the function

$$q^{(2n)}(x) := \sum_{j=0}^{n} |x|^j Y^{(2n)}_{n-j}(x) \tag{4.9}$$

satisfies

$$q^{(2n)}(K(y)) = Q^{(2n)}(y) \quad \textit{for all } y \in \mathbb{R}^4\,. \tag{4.10}$$

Proof of Lemma 4.2: Recall (see (3.2)) that, with $L \equiv L(y, D_y)$ as in (3.1), $L\varphi_K = 0$, and therefore, since power series can be differentiated termwise (see (4.7)),

$$0 = L\varphi_K = \sum_{n=0}^{\infty} LQ^{(2n)}\,. \tag{4.11}$$

Since $LQ^{(2n)}$ is again a homogeneous polynomial of degree $2n$, it follows that

$$LQ^{(2n)} = 0\,,\ n = 0, 1, \ldots\,. \tag{4.12}$$

Since L is a first order differential operator, (3.7) implies that

$$L[|y|^{2j} H^{(2n)}_{2n-2j}] = |y|^{2j}[LH^{(2n)}_{2n-2j}]\,, \tag{4.13}$$

where $LH^{(2n)}_{2n-2j}$ is again a homogeneous polynomial of order $2(n-j)$. Then (4.6), (4.12), and (4.13) imply that

$$\sum_{j=0}^{n} |y|^{2j}[LH^{(2n)}_{2n-2j}](y) = 0 \quad \text{for all } y \in \mathbb{R}^4\,. \tag{4.14}$$

Since $H^{(2n)}_{2n-2j}$ is harmonic, and (see (3.2)) $[\Delta; L] = 0$, we get that $LH^{(2n)}_{2n-2j}$ is a homogeneous *harmonic* polynomial of degree $2(n-j)$. Note that for $|y| = 1$, the left side of (4.14) is a linear combination of spherical harmonics of different degrees. From the linear independence of such spherical harmonics it follows that

$$LH^{(2n)}_{2n-2j} = 0 \text{ for all } j = 0, \dots, n, \text{ and } n \in \mathbb{N}\,. \tag{4.15}$$

From Lemma 3.4 it follows that there exist harmonic polynomials in $\mathbb{R}^3$, $Y^{(2n)}_{n-j}$, homogeneous of degree $n-j$, such that (4.8) holds.

Now (4.10) follows from this and (2.2). This finishes the proof of the lemma. □

Lemma 4.2, (4.7), and $|K(y)| = |y|^2$, imply that

$$\varphi_K(y) = \varphi(K(y)) = \sum_{n=0}^{\infty}\sum_{j=0}^{n} |K(y)|^j\, Y^{(2n)}_{n-j}(K(y))\,. \tag{4.16}$$

Formally, we can now finish the proof of Proposition 4.1 by defining

$$\varphi^{(1)}(x) := \sum_{n=0}^{\infty}\sum_{j=0, j \text{ even}}^{n} |x|^j\, Y^{(2n)}_{n-j}(x)\,, \tag{4.17}$$

$$\varphi^{(2)}(x) := \sum_{n=0}^{\infty}\sum_{j=1, j \text{ odd}}^{n} |x|^{j-1}\, Y^{(2n)}_{n-j}(x)\,. \tag{4.18}$$

However, it is not *a priori* clear that these sums converge and thus define real analytic functions. The remainder of the proof will establish the necessary convergence.

Lemma 4.3. *There exists $r > 0$ such that the two series in* (4.17) *and* (4.18) *converge for $|x| < r$.*

More precisely, there exists a universal constant $R > 0$ such that with $\widetilde{C}_1 := RC_1$, $\widetilde{M}_1 = 2M_1^2$ (with C_1, M_1 from (4.4)*),*

$$|Y^{(2n)}_{n-j}(x)| \le \widetilde{C}_1 \widetilde{M}_1^n |x|^{n-j}. \tag{4.19}$$

Proof. Clearly, the convergence of the series in (4.17) and (4.18) is a consequence of (4.19): take $r < 1/(2\widetilde{M}_1)$. Thus we only have to prove the estimate (4.19).

We return to (4.3). For fixed β, with $|\beta| = 2n > 0$ we have (again using [29, Theorem 2.1]) that, for some $d_j^{(\beta)} \in \mathbb{C}$,

$$y^\beta = \sum_{j=0}^{n} |y|^{2j} d_j^{(\beta)} P^{(\beta)}_{2n-2j}(y)\,, \tag{4.20}$$

where $P^{(\beta)}_{2n-2j}$ is a harmonic homogeneous polynomial of degree $2n-2j$, which depends on β, and satisfies $\|P^{(\beta)}_{2n-2j}\|_{L^2(\mathbb{S}^3)} = 1$. It follows from

(4.5) and (4.20) that

$$Q^{(2n)}(y) = \sum_{j=0}^{n} |y|^{2j} \sum_{|\beta|=2n} c_\beta d_j^{(\beta)} P_{2n-2j}^{(\beta)}(y)\,. \tag{4.21}$$

Comparing (4.6) with (4.21) we see that

$$\sum_{j=0}^{n} |y|^{2j} \big[H_{2n-2j}^{(2n)}(y) - \sum_{|\beta|=2n} c_\beta d_j^{(\beta)} P_{2n-2j}^{(\beta)}(y)\big] = 0\,. \tag{4.22}$$

Restricting to $|y| = 1$, (4.22) becomes a sum of spherical harmonics with different degrees, which are linearly independent, implying that (see (4.8))

$$Y_{n-j}^{(2n)}(K(y)) = H_{2n-2j}^{(2n)}(y) = \sum_{|\beta|=2n} c_\beta d_j^{(\beta)} P_{2n-2j}^{(\beta)}(y)\,. \tag{4.23}$$

We are now going to bound the $Y_{n-j}^{(2n)}$'s in L^∞. Since the (restriction to $\mathbb{S}^3$ of the) $P_{2n-2j}^{(\beta)}$'s in (4.20) are orthogonal in $L^2(\mathbb{S}^3)$ (they are homogeneous of different degrees), we get (by Parseval's identity), from setting $|y| = 1$ in (4.20), that

$$\sum_{j=0}^{n} |d_j^{(\beta)}|^2 = \int_{\mathbb{S}^3} |y^\beta|^2\, d\omega \le \int_{\mathbb{S}^3} |y|^{2|\beta|}\, d\omega = \int_{\mathbb{S}^3} 1\, d\omega = \mathrm{Vol}(\mathbb{S}^3)\,, \tag{4.24}$$

and so the $d_j^{(\beta)}$'s are bounded, uniformly in j and β, by $\mathrm{Vol}(\mathbb{S}^3)^{1/2}$.

Due to homogeneity, and using [27, Lemma 8], we get, for any $y \in \mathbb{R}^3 \setminus \{0\}$ and $j \le n$, that

$$\begin{aligned} \big|P_{2n-2j}^{(\beta)}(y)\big| &= |y|^{2n-2j}\big|P_{2n-2j}^{(\beta)}(y/|y|)\big| \le |y|^{2n-2j}\big\|P_{2n-2j}^{(\beta)}\big\|_{L^\infty(\mathbb{S}^3)} \\ &\le |y|^{2n-2j}\frac{2n-2j+1}{\mathrm{Vol}(\mathbb{S}^3)^{1/2}} \le |y|^{2n-2j}\frac{3n}{\mathrm{Vol}(\mathbb{S}^3)^{1/2}}\,. \end{aligned} \tag{4.25}$$

Note that (see [29, pp. 138–139])

$$\#\big\{\sigma \in \mathbb{N}^k \,\big|\, |\sigma| = \ell\big\} = \binom{k+\ell-1}{k-1}\,, \tag{4.26}$$

and so

$$\begin{aligned} \#\big\{\beta \in \mathbb{N}^4 \,\big|\, |\beta| = 2n\big\} &= \frac{(4+2n-1)!}{(4-1)!(2n)!} \\ &= \frac{1}{6}(2n+3)(2n+2)(2n+1) \le 10n^3\,. \end{aligned} \tag{4.27}$$

It follows from (4.23), (4.4), (4.24) (4.25), and (4.27) that (with C_1 and M_1 the constants in (4.4))

$$\begin{aligned}\big|Y^{(2n)}_{n-j}(K(y))\big| &\leq \sum_{|\beta|=2n} |c_\beta|\, |d^{(\beta)}_j|\, \big|P^{(\beta)}_{2n-2j}(y)\big| \\ &\leq 10C_1 n^4 |y|^{2n-2j} M_1^{2n} = 10C_1 n^4 |K(y)|^{n-j} M_1^{2n}\,.\end{aligned} \tag{4.28}$$

The desired estimate (4.19) clearly follows, using the surjectivity of K, with $R := 10 \max_n n^4 2^{-n}$. ☐

Recall that each term $|x|^j Y^{(2n)}_{n-j}(x)$ in the definition (4.17) of $\varphi^{(1)}$ is a homogeneous *polynomial* (of degree n) in x, and similarly for $\varphi^{(2)}$. Therefore, the series (4.17) and (4.18) are convergent power series. This implies that $\varphi^{(1)}, \varphi^{(2)}$ define real analytic functions on $\{|x| < r\}$ (see [23, sections 2.1–2.2]).

Finally, using (4.16), (4.17) and (4.18),

$$\begin{aligned}&\varphi^{(1)}(K(y)) + |K(y)|\varphi^{(2)}(K(y)) \\ &\qquad = \sum_{n=0}^{\infty}\sum_{j=0}^{n} |K(y)|^j\, Y^{(2n)}_{n-j}(K(y)) = \varphi(K(y))\,.\end{aligned} \tag{4.29}$$

This, and the surjectivity of K, imply (4.2) and therefore finishes the proof of Proposition 4.1. ☐

For the N-particle case, we have the following analogous result.

Proposition 4.4. *Let $U \subset \mathbb{R}^3$, $U' \subset \mathbb{R}^{3N-3}$ be open, with $0 \in U$, $x_0' \in U'$ and let $\psi : U \times U' \to \mathbb{C}$ be a function. Let $\mathcal{U} = K^{-1}(U) \subset \mathbb{R}^4$, with $K : \mathbb{R}^4 \to \mathbb{R}^3$ from* (2.1)*, and suppose that*

$$\begin{aligned}u : \mathcal{U} \times U' &\to \mathbb{C} \\ (y, x') &\mapsto \psi(K(y), x')\end{aligned} \tag{4.30}$$

is real analytic.

Then there exist functions $\psi^{(1)}, \psi^{(2)}$, real analytic in a neighbourhood $\mathcal{W}$ of $(0, x_0') \in \mathbb{R}^{3N}$, such that

$$\psi(x, x') = \psi^{(1)}(x, x') + |x|\psi^{(2)}(x, x')\ , \quad (x, x') \in \mathcal{W}\,. \tag{4.31}$$

Proof. Define

$$\varphi_\gamma(x) := \frac{1}{\gamma!}\partial^\gamma_{x'}\psi(x, x')\big|_{x'=x_0'}\,, \quad \varphi_{\gamma,K}(y) := \varphi_\gamma(K(y))\,. \tag{4.32}$$

This is well defined by the assumption on u.

Since, as in the proof of Proposition 4.1, u is even with respect to $y \in \mathbb{R}^4$, and the series converges absolutely, we have, for $|y| < \sqrt{R}$, $|x' - x_0'| < R$ for some $R > 0$, $c_{\beta\gamma} \in \mathbb{C}$,

$$u(y, x') = \sum_{\beta \in \mathbb{N}^4, |\beta|/2 \in \mathbb{N}, \gamma \in \mathbb{N}^{3N-3}} c_{\beta\gamma}\, y^\beta (x' - x_0')^\gamma\,,$$

with

$$|c_{\beta\gamma}| \le C_2 M_2^{|\beta+\gamma|} = C_2 M_2^{|\beta|} M_2^{|\gamma|} \quad \text{for all } \beta \in \mathbb{N}^4, \gamma \in \mathbb{N}^{3N-3}\,, \tag{4.33}$$

for some constants $C_2, M_2 > 0$. Clearly it follows that

$$\varphi_{\gamma,K}(y) = \sum_{\beta \in \mathbb{N}^4, |\beta|/2 \in \mathbb{N}} c_{\beta\gamma}\, y^\beta\,, \tag{4.34}$$

so that

$$\begin{aligned} u(y, x') &= \sum_{\gamma \in \mathbb{N}^{3N-3}} \Big(\sum_{\beta \in \mathbb{N}^4, |\beta|/2 \in \mathbb{N}} c_{\beta\gamma}\, y^\beta \Big) (x' - x_0')^\gamma \\ &= \sum_{\gamma \in \mathbb{N}^{3N-3}} \varphi_{\gamma,K}(y)\, (x' - x_0')^\gamma\,. \end{aligned} \tag{4.35}$$

Moreover, from (4.33) we have that, for all $\gamma \in \mathbb{N}^{3N-3}$,

$$|c_{\beta\gamma}| \le C_1(\gamma) M_2^{|\beta|} \quad \text{where} \quad C_1(\gamma) := C_2 M_2^{|\gamma|}\,. \tag{4.36}$$

In particular, (4.34) and (4.36) show that $\varphi_{\gamma,K}$ is real analytic near $y = 0$. Repeating the arguments in the proof of Proposition 4.1 for $\varphi_{\gamma,K}$ for fixed $\gamma \in \mathbb{N}^{3N-3}$, we get that

$$\begin{aligned} \varphi_\gamma(x) &= \sum_{n=0}^{\infty} \sum_{\ell=0}^{[n/2]} |x|^{2\ell}\, Y_{n-2\ell}^{(2n),\gamma}(x) \\ &\quad + |x| \sum_{n=0}^{\infty} \sum_{\ell=0}^{[(n-1)/2]} |x|^{2\ell}\, Y_{n-(2\ell+1)}^{(2n),\gamma}(x)\,, \end{aligned} \tag{4.37}$$

where $Y_{n-k}^{(2n),\gamma} : \mathbb{R}^3 \to \mathbb{C}$ are harmonic polynomials, homogeneous of degree $n-k$, depending on $\gamma \in \mathbb{N}^{3N-3}$. Therefore, for some $a_\alpha(\gamma), b_\alpha(\gamma) \in \mathbb{C}$, $\alpha \in \mathbb{N}^3$,

$$\sum_{\ell=0}^{[n/2]} |x|^{2\ell}\, Y_{n-2\ell}^{(2n),\gamma}(x) = \sum_{|\alpha|=n} a_\alpha(\gamma) x^\alpha\,, \tag{4.38}$$

$$\sum_{\ell=0}^{[(n-1)/2]} |x|^{2\ell}\, Y_{n-(2\ell+1)}^{(2n),\gamma}(x) = \sum_{|\alpha|=n-1} b_\alpha(\gamma) x^\alpha\,, \tag{4.39}$$

with (see (4.19)),

$$\Big|\sum_{|\alpha|=n} a_\alpha(\gamma)x^\alpha\Big| \leq RC_1(\gamma)n(2M_2^2)^n|x|^n, \tag{4.40}$$

$$\Big|\sum_{|\alpha|=n-1} b_\alpha(\gamma)x^\alpha\Big| \leq RC_1(\gamma)n(2M_2^2)^n|x|^n. \tag{4.41}$$

Recall that (see (4.26))

$$\#\{\gamma \in \mathbb{N}^{3N-3}\,|\,|\gamma| = k\} = \binom{3N+k-4}{3N-4}. \tag{4.42}$$

By definition, discarding part of the denominator,

$$\binom{3N+k-4}{3N-4} \leq \frac{(3N+k-4)!}{k!} = (3N+k-4)\cdot\ldots\cdot(k+1)\,.$$

This last product contains $(3N-4)$ terms each of which are smaller than $(3N+k)$. Thus

$$\binom{3N+k-4}{3N-4} \leq (3N+k)^{3N-4} \leq C_3 k^{3N}\,,$$

for some C_3 (depending on N) and all $k \geq 1$.

It follows that, for $|x| < 1/(4M_2^2)$, $|x'-x_0'| < 1/(2M_2)$,

$$\begin{aligned}
&\Big|\sum_{\gamma\in\mathbb{N}^{3N-3}}\sum_{n=0}^{\infty}\sum_{|\alpha|=n} a_\alpha(\gamma)x^\alpha(x'-x_0')^\gamma\Big| \\
&\qquad\leq RC_2\sum_{k=0}^{\infty}\sum_{\gamma\in\mathbb{N}^{3N-3},|\gamma|=k}\sum_{n=0}^{\infty}(2M_2^2)^n|x|^n M_2^{|\gamma|}|x'-x_0'|^{|\gamma|} \\
&\qquad\leq RC_2C_3\Big(\sum_{k=0}^{\infty}\frac{k^{3N}}{2^k}\Big)\Big(\sum_{n=0}^{\infty}\frac{n}{2^n}\Big) < \infty\,,
\end{aligned}$$

and so, with $a_{\alpha\gamma} := a_\alpha(\gamma)$,

$$\psi^{(1)}(x,x') := \sum_{\gamma\in\mathbb{N}^{3N-3}}\sum_{\alpha\in\mathbb{N}^3} a_{\alpha\gamma}x^\alpha(x'-x_0')^\gamma \tag{4.43}$$

defines a real analytic function in a neighborhood of $(0,x_0')$. Similarly, with $b_{\alpha\gamma} := b_\alpha(\gamma)$,

$$\psi^{(2)}(x,x') := \sum_{\gamma\in\mathbb{N}^{3N-3}}\sum_{\alpha\in\mathbb{N}^3} b_{\alpha\gamma}x^\alpha(x'-x_0')^\gamma \tag{4.44}$$

defines a real analytic function in a neighborhood of $(0, x'_0)$. From the above observations and from (4.35), (4.32), (4.37), (4.38) and (4.39) it follows that

$$\begin{aligned}
&\psi^{(1)}(K(y), x') + |K(y)|\,\psi^{(2)}(K(y), x') \\
&\quad = \sum_{\gamma\in\mathbb{N}^{3N-3}} \sum_{n=0}^{\infty} \sum_{\ell=0}^{[n/2]} |K(y)|^{2\ell}\, Y^{(2n),\gamma}_{n-2\ell}(K(y))(x'-x'_0)^\gamma \\
&\qquad + \sum_{\gamma\in\mathbb{N}^{3N-3}} |K(y)| \sum_{n=0}^{\infty} \sum_{\ell=0}^{[(n-1)/2]} |K(y)|^{2\ell}\, Y^{(2n),\gamma}_{n-(2\ell+1)}(K(y))(x'-x'_0)^\gamma \\
&\quad = \sum_{\gamma\in\mathbb{N}^{3N-3}} \varphi_{\gamma,K}(y)(x'-x'_0)^\gamma = u(y,x') = \psi(K(y), x')\,, \qquad (4.45)
\end{aligned}$$

and so, by the surjectivity of K,

$$\psi(x, x') = \psi^{(1)}(x, x') + |x|\,\psi^{(2)}(x, x')\,, \qquad (4.46)$$

with $\psi^{(i)}, i = 1, 2$, real analytic on

$$\big\{(x, x') \in \mathbb{R}^{3N} \,\big|\, |x| < 1/(4M_2^2)\,,\ |x' - x'_0| < 1/(2M_2)\big\}\,.$$

This finishes the proof of Proposition 4.4. □

Acknowledgement. Financial support from the Danish Natural Science Research Council, under the grant Mathematical Physics and Partial Differential Equations (TØS), and from the European Science Foundation Programme *Spectral Theory and Partial Differential Equations* (SPECT), is gratefully acknowledged. SF is supported by a Skou Grant and a Young Elite Researcher Award from the Danish Research Council. The authors wish to thank Bernard Helffer (SF, TØS), Günther Hörmann (MHO), Gerd Grubb (TØS), Andreas Knauf (TØS), and Heinz Siedentop (TØS) for helpful discussions.

References

[1] François Castella, Thierry Jecko, and Andreas Knauf, *Semiclassical Resolvent Estimates for Schrödinger Operators with Coulomb Singularities*, Ann. Henri Poincaré (*Online First*) (2008).

[2] Heinz-Jürgen Flad, Wolfgang Hackbusch, and Reinhold Schneider, *Best N-term approximation in electronic structure calculations. I. One-electron reduced density matrix*, M2AN Math. Model. Numer. Anal. **40** (2006), no. 1, 49–61.

[3] ———, *Best N-term approximation in electronic structure calculations. II. Jastrow factors*, M2AN Math. Model. Numer. Anal. **41** (2007), no. 2, 261–279.

[4] Søren Fournais, Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and Thomas Østergaard Sørensen, *The Electron Density is Smooth Away from the Nuclei*, Comm. Math. Phys. **228** (2002), no. 3, 401–415.

[5] ______, *On the regularity of the density of electronic wavefunctions*, **307** (2002), 143–148.
[6] ______, *Analyticity of the density of electronic wavefunctions*, Ark. Mat. **42** (2004), no. 1, 87–106.
[7] ______, *Sharp Regularity Results for Coulombic Many-Electron Wave Functions*, Comm. Math. Phys. **255** (2005), no. 1, 183–227.
[8] ______, *Non-Isotropic Cusp Conditions and Regularity of the Electron Density of Molecules at the Nuclei*, Ann. Henri Poincaré **8** (2007), no. 4, 731–748.
[9] Søren Fournais, Maria Hoffmann-Ostenhof, and Thomas Østergaard Sørensen, *Third derivative of the one-electron density at the nucleus*, `arXiv:math-ph/0607004v1` (2006).
[10] Christian Gérard and Andreas Knauf, *Collisions for the Quantum Coulomb Hamiltonian*, Comm. Math. Phys. **143** (1991), no. 1, 17–26.
[11] David Gilbarg and Neil S. Trudinger, *Elliptic partial differential equations of second order*, Classics in Mathematics, Springer-Verlag, Berlin, 2001, Reprint of the 1998 edition.
[12] V. V. Grušin, *A certain class of elliptic pseudodifferential operators that are degenerate on a submanifold*, Mat. Sb. (N.S.) **84 (126)** (1971), 163–195, (English translation: Math. USSR-Sb. 13 (1971), 155–185).
[13] Bernard Helffer, Andreas Knauf, Heinz Siedentop, and Rudi Weikard, *On the absence of a first order correction for the number of bound states of a Schrödinger operator with Coulomb singularity*, Comm. Partial Differential Equations **17** (1992), no. 3-4, 615–639.
[14] Bernard Helffer and Heinz Siedentop, *Regularization of atomic Schrödinger operators with magnetic field*, Math. Z. **218** (1995), no. 3, 427–437.
[15] ______, *A generalization of the Kustaanheimo-Stiefel transform for two-centre systems*, Bull. London Math. Soc. **28** (1996), no. 1, 33–42.
[16] Robert Nyden Hill, *On the analytic structure of the wave function for a hydrogen atom in an analytic potential*, J. Math. Phys. **25** (1984), no. 5, 1577–1583.
[17] Heinz Hopf, *Über die Abbildungen der dreidimensionalen Sphäre auf die Kugelfläche*, Math. Ann. **104** (1931), no. 1, 637–665.
[18] Lars Hörmander, *Linear partial differential operators*, Third revised printing. Die Grundlehren der mathematischen Wissenschaften, Band 116, Springer-Verlag, Berlin, 1976.
[19] Res Jost, *Das H-Atom nach Kustaanheimo-Stiefel-Scheifele*, Lecture notes by Hanruedi Tschudi of a course by Res Jost on theoretical physics for mathematicians, Winter Semester 1974/75, ETH-Zürich, 1975.
[20] Tosio Kato, *On the eigenfunctions of many-particle systems in quantum mechanics*, Comm. Pure Appl. Math. **10** (1957), 151–177.
[21] ______, *Perturbation theory for linear operators*, Classics in Mathematics, Springer-Verlag, Berlin, 1995, Reprint of the 1980 edition.
[22] Andreas Knauf, *The n-centre problem of celestial mechanics for large energies*, J. Eur. Math. Soc. (JEMS) **4** (2002), no. 1, 1–114.
[23] Steven G. Krantz and Harold R. Parks, *A primer of real analytic functions*, second ed., Birkhäuser Advanced Texts: Basler Lehrbücher. [Birkhäuser Advanced Texts: Basel Textbooks], Birkhäuser Boston Inc., Boston, MA, 2002.
[24] Paul E. Kustaanheimo, *Spinor regularization of the Kepler motion*, Ann. Univ. Turku. Ser. A I No. **73** (1964), 7.

[25] Paul E. Kustaanheimo and Eduard L. Stiefel, *Perturbation theory of Kepler motion based on spinor regularization*, J. Reine Angew. Math. **218** (1965), 204–219.

[26] Claude Le Bris and Pierre-Louis Lions, *From atoms to crystals: a mathematical journey*, Bull. Amer. Math. Soc. (N.S.) **42** (2005), no. 3, 291–363 (electronic).

[27] Claus Müller, *Spherical harmonics*, Lecture Notes in Mathematics, vol. 17, Springer-Verlag, Berlin, 1966.

[28] Michael Reed and Barry Simon, *Methods of modern mathematical physics. II. Fourier Analysis, Self-Adjointness*, Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1975.

[29] Elias M. Stein and Guido Weiss, *Introduction to Fourier analysis on Euclidean spaces*, Princeton University Press, Princeton, N.J., 1971, Princeton Mathematical Series, No. 32.

[30] Eduard L. Stiefel and Gerhard Scheifele, *Linear and regular celestial mechanics. Perturbed two-body motion, numerical methods, canonical theory*, Springer-Verlag, New York, 1971, Die Grundlehren der mathematischen Wissenschaften, Band 174.

[31] Harry Yserentant, *On the regularity of the electronic Schrödinger equation in Hilbert spaces of mixed derivatives*, Numer. Math. **98** (2004), no. 4, 731–759.

[32] ———, *Sparse grid spaces for the numerical solution of the electronic Schrödinger equation*, Numer. Math. **101** (2005), no. 2, 381–389.

[33] ———, *The hyperbolic cross space approximation of electronic wavefunctions*, Numer. Math. **105** (2007), no. 4, 659–690.

(S. Fournais) Department of Mathematical Sciences, University of Aarhus, Ny Munkegade, Building 1530, DK-8000 Århus C, Denmark.
E-mail address: fournais@imf.au.dk

(S. Fournais on leave from) CNRS and Laboratoire de Mathématiques d'Orsay, Univ Paris-Sud, Orsay CEDEX, F-91405, France.

(M. Hoffmann-Ostenhof) Fakultät für Mathematik, Universität Wien, Nordbergstrasse 15, A-1090 Vienna, Austria.
E-mail address: maria.hoffmann-ostenhof@univie.ac.at

(T. Hoffmann-Ostenhof) Institut für Theoretische Chemie, Währingerstrasse 17, Universität Wien, A-1090 Vienna, Austria.

(T. Hoffmann-Ostenhof, 2nd address) The Erwin Schrödinger International Institute for Mathematical Physics, Boltzmanngasse 9, A-1090 Vienna, Austria.
E-mail address: thoffman@esi.ac.at

(T. Østergaard Sørensen) Department of Mathematical Sciences, Aalborg University, Fredrik Bajers Vej 7G, DK-9220 Aalborg East, Denmark.
E-mail address: sorensen@math.aau.dk