ELECTRON WAVEFUNCTIONS AND DENSITIES FOR ATOMS

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Abstract. With a special 'Ansatz' we analyse the regularity properties of atomic electron wavefunctions and electron densities. In particular we prove an a priori estimate, $\sup_{y\in B(x,R)}|\nabla\psi(y)| \le C(R)\sup_{y\in B(x,2R)}|\psi(y)|$ and obtain for the spherically averaged electron density, $\widetilde{\rho}(r)$, that $\widetilde{\rho}''(0)$ exists and is non-negative.

Avec un 'Ansatz' spécial nous analysons les proprietées de régularité des fonctions d'ondes atomiques et des densités d'electron. En particulier nous prouvons une éstimation a priori,

$$\sup_{y\in B(x,R)}|\nabla\psi(y)| \le C(R)\sup_{y\in B(x,2R)}|\psi(y)|$$

et obtient pour la densité d'electron moyennée sur la sphere $\widetilde{\rho}(r)$, que $\widetilde{\rho}''(0)$ existe et est non-négative.

1. Introduction and Results

Let V be the Coulomb potential for an atom consisting of a nucleus of charge Z (fixed at the origin) and N electrons:

$$V(\mathbf{x}) = V(x_1,\dots,x_N) = \sum_{j=1}^{N} -\frac{Z}{|x_j|} + \sum_{1\le j<k\le N}\frac{1}{|x_j-x_k|},$$
$$\mathbf{x} = (x_1,\dots,x_N)\in\mathbb{R}^{3N}, x_j = (x_{j,1},x_{j,2},x_{j,3})\in\mathbb{R}^3, j=1,\dots,N, \tag{1.1}$$

and let H be the corresponding N - electron Hamilton operator:

$$H \equiv H^N = -\Delta + V \tag{1.2}$$

with

$$-\Delta = \sum_{j=1}^{N} -\Delta_j \quad , \quad \Delta_j = \sum_{i=1}^{3}\frac{\partial^2}{\partial x_{j,i}^2}$$

being the kinetic energy operator of the N electrons. The quadratic form domain of H is $W^{1,2}(\mathbb{R}^{3N})$, see Reed and Simon [12]. Assume

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$\psi \in L^2(\mathbb{R}^{3N})$ is a real-valued normalised eigenfunction of the operator H:

$$(H-E)\psi = 0 \quad , \quad \|\psi\| \equiv \|\psi\|_{L^2(\mathbb{R}^{3N})} = 1. \tag{1.3}$$

It is known that then ψ is continuous with bounded derivatives, and $\psi \in W^{2,2}(\mathbb{R}^{3N})$ (Kato [8]) and that ψ is in fact analytic away from the singularities (in $\mathbb{R}^{3N}$) of V, since V is here real analytic (see Hopf [7]). In this paper we derive various qualitative and quantitative properties of the wave function ψ and of the corresponding one-electron density

$$\rho(x) = \int_{\mathbb{R}^{3(N-1)}} |\psi(x, x_2, \dots, x_N)|^2 \, dx_2 \dots dx_N \quad , \quad x \in \mathbb{R}^3, \tag{1.4}$$

as well as of its spherical average ($x = r\omega, r = |x|, \omega = x/|x| \in \mathbb{S}^2$)

$$\begin{aligned}\widetilde{\rho}(r) &= \int_{\mathbb{S}^2} \rho(r\omega)\, d\omega \\ &= \int_{\mathbb{S}^2}\int_{\mathbb{R}^{3(N-1)}} |\psi(r\omega, x_2, \dots, x_N)|^2 \, dx_2 \cdots dx_N \, d\omega \quad , \quad r \in [0,\infty).\end{aligned} \tag{1.5}$$

Remark 1.1. Aside from Kato's classical results (see Kato [8]), the local behaviour of electron wavefunctions has been investigated more recently by Hoffmann-Ostenhof et al. [4], [6]. The electron density itself has been studied extensively in the large-Z-limit, see Lieb [9]. Except for the spatial asymptotics, see Ahlrichs et al. [1], there are virtually no recent rigorous results on ρ despite the fact that the density is the central object in various popular numerical approximation schemes, as Density Functional Theory (DFT) and all the various descendants of Hartree-Fock theory.

We now present our results.

Theorem 1.2. *Let ψ be as in* (1.3). *For all $R \in (0,\infty)$, there exists a constant $C = C(R)$ such that*

$$\sup_{\mathbf{y} \in B(\mathbf{x},R)} |\nabla\psi(\mathbf{y})| \le C \sup_{\mathbf{y} \in B(\mathbf{x},2R)} |\psi(\mathbf{y})| \quad \textit{for all } \mathbf{x} \in \mathbb{R}^{3N}.$$

Remark 1.3. This result complements the result by Simon [14, Thm. C.2.5 (C14)] for the case of operators of the form (1.2), but with V in the Kato-class $K^{n,1}(\mathbb{R}^n)$: for $\delta \in [0,2)$ ($\delta = 0 : n \ge 3$),

$$V \in K^{n,\delta}(\mathbb{R}^n) \Leftrightarrow \lim_{\epsilon \to 0} \sup_{x \in \mathbb{R}^n} \int_{|x-y|<\epsilon} \frac{|V(y)|}{|x-y|^{n-2+\delta}}\, dy = 0.$$

The Coulomb potential (1.1) is in $K^{3N,\delta}(\mathbb{R}^{3N})$ for all $\delta \in [0,1)$, but is not in $K^{3N,1}(\mathbb{R}^{3N})$.

We recall the definition of Hölder continuity:

Definition 1.4. For $\Omega \subset \mathbb{R}^n$ an open set, $k \in \mathbb{N}$, and $\alpha \in (0,1]$, we say that the function u belongs to $C^{k,\alpha}_{\mathrm{loc}}(\Omega)$ whenever $u \in C^k(\Omega)$, and for all $\beta \in \mathbb{N}^n$ with $|\beta| = k$, and all open balls $B(x_0, r) \subset \Omega$, we have

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

As a consequence of the proof of Theorem 1.2 we get:

Proposition 1.5. *Let*

$$F(\mathbf{x}) = F(x_1, \dots, x_N) = \sum_{j=1}^N -\frac{Z}{2}|x_j| + \sum_{1 \leq j < k \leq N} \frac{1}{4}|x_j - x_k|. \tag{1.6}$$

Then the eigenfunction ψ given in (1.3) *can be represented as*

$$\psi = e^F \phi$$

with

$$\phi \in C^{1,\alpha}_{\mathrm{loc}}(\mathbb{R}^{3N}) \text{ for all } \alpha \in (0,1).$$

Remark 1.6. This result classifies the singularities of $\nabla\psi$ as those coming from ∇F: $\nabla\psi = \psi\nabla F + e^F \nabla\phi$. Kato [8] proved that $\nabla\psi$ is bounded, but as the ground state of Hydrogen-like systems ($N = 1, E = -Z^2/4$, $\psi(x) = c_0 e^{-Z|x|/2}, x \in \mathbb{R}^3$) shows, it is not in general continuous.

Remark 1.7. The results of Theorem 1.2 and Proposition 1.5 easily generalise to the case of molecules: L nuclei, of charge Z_l, fixed at $R_l \in \mathbb{R}^3$, $l = 1, \dots, L$, with corresponding N - electron Hamilton operator

$$H^{N,L} = \sum_{j=1}^N \Big(-\Delta_j - \sum_{l=1}^L \frac{Z_l}{|x_j - R_l|} \Big) + \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|}.$$

We assume throughout when studying ρ and $\widetilde{\rho}$ that E and ψ in (1.3) are such that there exist constants $C_0, \gamma > 0$ such that

$$|\psi(\mathbf{x})| \leq C_0\, e^{-\gamma|\mathbf{x}|} \text{ for all } \mathbf{x} \in \mathbb{R}^{3N}. \tag{1.7}$$

For references on the exponential decay of eigenfunctions, see e. g. Simon [14].

Remark 1.8. Inequality (1.7) holds when $E < \inf \sigma_{\mathrm{ess}}(H^N)$. In this case, we let $\varepsilon \equiv E_0^{N-1} - E$ with E_0^{N-1} the ground state energy of the $(N-1)$ - electron operator:

$$H^{N-1} = \sum_{j=2}^N \Big(-\Delta_j - \frac{Z}{|x_j|} \Big) + \sum_{2 \leq j < k \leq N} \frac{1}{|x_j - x_k|}. \tag{1.8}$$

By the HVZ-theorem (see Cycon et al. [2, Theorem 3.7], $\inf \sigma_{\text{ess}}(H^N) = E_0^{N-1}$, and so $\varepsilon > 0$ if $E < \inf \sigma_{\text{ess}}(H^N)$. When we study H in a symmetry sector, so that ψ transforms according to this symmetry, then E_0^{N-1} stands for the groundstate energy of the ionized particle system described by the Hamiltonian H^{N-1} in the appropriate symmetry subspace as determined by the symmetry behaviour of ψ. For this case a modified version of the HVZ-theorem holds (see e. g. Reed and Simon [13, Thm. XIII. 17'] and Zhislin and Sigalov [15]). This includes in particular the physically important case of real atoms (Pauli principle). So if E lies below the beginning of the essential spectrum of H considered in a symmetry sector, then analogously to the above the ionisation energy $\varepsilon > 0$ and ψ satisfies (1.7).

Remark 1.9. When assuming (1.7), Theorem 1.2 implies that $|\nabla\psi(\mathbf{x})|$ also decays exponentially for $|\mathbf{x}| \to \infty$.

Remark 1.10. From (1.7) and Lebesgue's Dominated Convergence Theorem follows that the density ρ is continuous in $\mathbb{R}^3$.

Theorem 1.11. *Let ψ be given according to* (1.3) *and assume that* (1.7) *holds. Then:*

(i) *The function ρ defined in* (1.4) *satisfies, in the distributional sense, the equation*

$$-\frac{1}{2}\Delta\rho - \frac{Z}{r}\rho + h = 0 \quad \textit{in} \quad \mathbb{R}^3, \tag{1.9}$$

where

$$h \in C^{\alpha}(\mathbb{R}^3 \setminus \{0\}) \cap L^{\infty}(\mathbb{R}^3) \ \ \textit{for all} \ \ \alpha \in (0,1)$$

and

$$\rho \in C^{2,\alpha}(\mathbb{R}^3 \setminus \{0\}) \cap C^{0,1}(\mathbb{R}^3) \ \ \textit{for all} \ \ \alpha \in (0,1).$$

(ii) *The function $\widetilde{\rho}$ defined in* (1.5) *satisfies*

$$-\frac{1}{2}\Delta\widetilde{\rho} - \frac{Z}{r}\widetilde{\rho} + \widetilde{h} = 0 \textit{ for } r > 0 \tag{1.10}$$

where $\widetilde{h}(r) = \int_{\mathbb{S}^2} h(r\omega)\,d\omega$. Thereby,

$$\widetilde{h} \in C^{\alpha}((0,\infty)) \cap C^0([0,\infty)) \textit{ for all } \alpha \in (0,1)$$

and

$$\widetilde{\rho} \in C^{2,\alpha}((0,\infty)) \cap C^2([0,\infty)) \textit{ for all } \alpha \in (0,1).$$

(iii)

$$h(x) \le C(R)\left(\int_{B(x,R)} \rho(y)\,dy + \rho(x)\right) \quad \textit{for all } x \in \mathbb{R}^3, \tag{1.11}$$

$$h(x) \ge \varepsilon\,\rho(x) \textit{ for all } x \in \mathbb{R}^3, \ \textit{if } \varepsilon = E_0^{N-1} - E > 0. \tag{1.12}$$

(iv)
$$\Big(\frac{d^2}{dr^2}\,\widetilde{\rho}\Big)(0) = \frac{2}{3}\big(\widetilde{h}(0) + Z^2\widetilde{\rho}(0)\big). \tag{1.13}$$

Remark 1.12. The results in (i) generalize to the case of molecules, where the continuity results for ρ and h hold in the complement of the set $\{R_1, \dots, R_L\} \subset \mathbb{R}^3$ (see Remark 1.7).

Remark 1.13. It is known that eigenfunctions obey (Kato's) Cusp Condition (see Kato [8]), and similar properties hold for particle densities. For more recent results see Hoffmann-Ostenhof et al. [4], [5], Hoffmann-Ostenhof and Seiler [6]. In the proof of Theorem 1.11, (iv) we make use of the Cusp Condition for $\widetilde{\rho}$, namely:
$$\widetilde{\rho}'(0) = \lim_{r\downarrow 0}\frac{\widetilde{\rho}(r) - \widetilde{\rho}(0)}{r} = -Z\widetilde{\rho}(0) \text{ and } \lim_{r\downarrow 0}\widetilde{\rho}'(r) = \widetilde{\rho}'(0) \tag{1.14}$$
and also present a proof for it.

Remark 1.14. Of course our results are only first steps in a thorough investigation of qualitative properties of the one-electron density. Here are some obvious open questions:

(i) Is $\rho(x) > 0$ for all $x \in \mathbb{R}^3$? We remark that this cannot be true in general, since it is false for some exited states of Hydrogen.

(ii) Is $\rho \in C^\infty(\mathbb{R}^3 \setminus \{0\})$ or even $C^\omega(\mathbb{R}^3 \setminus \{0\})$?

(iii) Is $\widetilde{\rho}$ smooth in $[0,\infty)$, in the sense that $\big(\frac{d^k}{dr^k}\widetilde{\rho}\big)(r)$ exists for $r \geq 0$ for all k?

(iv) Is $\frac{d}{dr}\widetilde{\rho}(r) \leq 0$ for $r \geq 0$? This is expected to be true for groundstate densities, but not known even for the bosonic case like Helium. Our results imply that $\frac{d}{dr}\widetilde{\rho}(r) \leq 0$ for $r \leq R_0$ for the bosonic case, where R_0 depends on the constant C in Theorem 1.2. Note that because of (1.9) and (1.12) we have $\Delta\rho \geq 0$ for $|x| \geq Z/\varepsilon$, and so the Maximum Principle gives that $\frac{d}{dr}\widetilde{\rho}(r) < 0$ for $r > Z/\varepsilon$.

Remark 1.15. In the proof of Theorem 1.11 we obtain (see Proposition 3.1): With $\nabla_1 = (\frac{\partial}{\partial x_{1,1}}, \frac{\partial}{\partial x_{1,2}}, \frac{\partial}{\partial x_{1,3}})$, the function
$$t_1(r) = \int_{\mathbb{S}^2}\int_{\mathbb{R}^{3(N-1)}} |\nabla_1\psi(r\omega, x_2, \dots, x_N)|^2\, dx_2 \dots dx_N\, d\omega$$
is continuous on $[0,\infty)$.

2. Proofs

Throughout the proofs, we will denote by C generic constants.

Crucial for our investigations is Corollary 8.36 in Gilbarg and Trudinger [3]. We shall make use of this result several times and for convenience we state it already here, adapted for our special case:

Proposition 2.1. *Let Ω be a bounded domain in $\mathbb{R}^n$ and suppose $u \in W^{1,2}(\Omega)$ is a weak solution of $\Delta u + \sum_{j=1}^n b_j D_j u + W u = g$ in Ω, where $b_j, W, g \in L^\infty(\Omega)$. Then $u \in C^{1,\alpha}(\Omega)$ for all $\alpha \in (0,1)$ and for any domain Ω', $\overline{\Omega'} \subset \Omega$ we have*

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

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

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

Thereby

$$|u|_{C^{1,\alpha}(\Omega')} = \|u\|_{L^\infty(\Omega')} + \|\nabla u\|_{L^\infty(\Omega')} + \sup_{x,y\in\Omega', x\neq y}\frac{|\nabla u(x) - \nabla u(y)|}{|x-y|^\alpha}.$$

Proof of Theorem 1.2 and Proposition 1.5.

Let the function F be as in (1.6) and define the function F_1 by

$$F_1(x_1,\dots,x_N) = \sum_{j=1}^N -\frac{Z}{2}\sqrt{|x_j|^2+1} + \sum_{1\leq j<k\leq N}\frac{1}{4}\sqrt{|x_j-x_k|^2+1}. \tag{2.1}$$

A computation shows that

$$\Delta F = V, \tag{2.2}$$

$$\|F - F_1\|_{L^\infty(\mathbb{R}^{3N})}\ ,\ \ \|\nabla(F-F_1)\|_{L^\infty(\mathbb{R}^{3N})}\ ,\ \ \|D^\beta F_1\|_{L^\infty(\mathbb{R}^{3N})} \leq C(\beta, N, Z)\ ,\ \ |\beta| \geq 1. \tag{2.3}$$

Make the 'Ansatz' $\psi = e^{F-F_1}\psi_1$. Using $(H-E)\psi = 0$ and (2.2) we get that ψ_1 satisfies the equation

$$\Delta\psi_1 + 2\nabla(F-F_1)\cdot\nabla\psi_1 + (|\nabla(F-F_1)|^2 - \Delta F_1 + E)\psi_1 = 0. \tag{2.4}$$

Due to (2.3) the coefficients in (2.4) are bounded in $\mathbb{R}^{3N}$. Then Proposition 2.1 implies that ψ_1 is $C^{1,\alpha}$ for all $\alpha \in (0,1)$, in any ball $B(\mathbf{x}, R) \subset \mathbb{R}^{3N}$, and

$$|\psi_1|_{C^{1,\alpha}(B(\mathbf{x},R))} \leq C \sup_{y\in B(\mathbf{x},2R)}|\psi_1(y)| \tag{2.5}$$

with C depending on R but not on $\mathbf{x}$. Since

$$|\nabla\psi(\mathbf{y})| \leq |\nabla(F-F_1)|\,|\psi(\mathbf{y})| + |e^{F-F_1}\nabla\psi_1(\mathbf{y})|$$

we obtain, via (2.3) and (2.5),

$$\begin{aligned}\sup_{\mathbf{y}\in B(\mathbf{x},R)}|\nabla\psi(\mathbf{y})| &\leq C\big(\sup_{\mathbf{y}\in B(\mathbf{x},R)}|\psi(\mathbf{y})| + \sup_{\mathbf{y}\in B(\mathbf{x},R)}|\nabla\psi_1(\mathbf{y})|\big)\\ &\leq C\big(\sup_{\mathbf{y}\in B(\mathbf{x},2R)}|\psi(\mathbf{y})| + \sup_{\mathbf{y}\in B(\mathbf{x},2R)}|\psi_1(\mathbf{y})|\big) \leq C\sup_{\mathbf{y}\in B(\mathbf{x},2R)}|\psi(\mathbf{y})|,\end{aligned}$$

with $C = C(R)$. This proves Theorem 1.2.

Proposition 1.5 follows from $\psi = e^{F-F_1}\psi_1$, $\psi_1 \in C^{1,\alpha}_{\mathrm{loc}}(B(\mathbf{x}, R))$, since e^{-F_1} is smooth. $\square$

Proof of Theorem 1.11.

Multiplying the equation $(H - E)\psi = 0$ with ψ and integrating over $x_2, \dots, x_N$ gives the equation

$$\begin{aligned}
\int_{\mathbb{R}^{3(N-1)}} \psi\Delta_1\psi\, dx_2\cdots dx_N + \frac{Z}{|x_1|}\,\rho(x_1) = {}&\\
= \sum_{j=2}^{N}\int_{\mathbb{R}^{3(N-1)}} &\psi\big(-\Delta_j - \frac{Z}{|x_j|}\big)\psi\, dx_2\cdots dx_N\\
+ \sum_{1\le j<k\le N}\int_{\mathbb{R}^{3(N-1)}} &\frac{1}{|x_j - x_k|}\,\psi^2\, dx_2\cdots dx_N\\
= \int_{\mathbb{R}^{3(N-1)}} &\psi\big(H^{N-1} - E\big)\psi\, dx_2\cdots dx_N\\
+ \sum_{j=2}^{N}\int_{\mathbb{R}^{3(N-1)}} &\frac{1}{|x_1 - x_j|}\,\psi^2\, dx_2\cdots dx_N \qquad (2.6)
\end{aligned}$$

where H^{N-1} is the $(N-1)$ - electron operator defined in (1.8). Since $\Delta_1\big(\psi^2\big) = 2|\nabla_1\psi|^2 + 2\psi\Delta_1\psi$ and $\int \Delta_1(\psi^2)(x_1, x')\, dx' = \Delta_1\rho$ in the distributional sense, we get that

$$\begin{aligned}
\frac{1}{2}\Delta_1\rho(x_1) = \int_{\mathbb{R}^{3(N-1)}} &|\nabla_1\psi|^2\, dx_2\cdots dx_N\\
+ \int_{\mathbb{R}^{3(N-1)}} &\psi\Delta_1\psi\, dx_2\cdots dx_N \qquad (2.7)
\end{aligned}$$

which, together with (2.6), gives the equation $(r = |x|)$

$$\begin{aligned}
\frac{1}{2}\Delta\rho(x) + \frac{Z}{r}\rho(x) = \int_{\mathbb{R}^{3(N-1)}} &\psi\big(H^{N-1} - E\big)\psi\, dx_2\cdots dx_N\\
+ \sum_{j=2}^{N}\int_{\mathbb{R}^{3(N-1)}} &\frac{1}{|x_1 - x_j|}\,\psi^2\, dx_2\cdots dx_N\\
+ \int_{\mathbb{R}^{3(N-1)}} &|\nabla_1\psi|^2\, dx_2\cdots dx_N \equiv h(x), \qquad (2.8)
\end{aligned}$$

hence we obtain (1.9). Integration of (1.9) over $\mathbb{S}^2$ yields (1.10).

The proof of the regularity properties of the functions h and $\widetilde{h}$ are rather technical, and therefore postponed to the next section.

We now verify the regularity properties of the functions ρ and $\widetilde{\rho}$ under the assumption that the regularity properties of h and $\widetilde{h}$ stated in Theorem 1.11 have been shown. Define the function μ by the equation

$(r = |x|)$

$$\rho(x) = e^{-Zr}\big(\rho(0) + \mu(x)\big). \tag{2.9}$$

Then $\mu = e^{Zr}\rho - \rho(0)$, $\mu(0) = 0$, and (2.8) implies that

$$\Delta\mu - 2Z\,\frac{x}{r}\cdot\nabla\mu + Z^2\mu = 2he^{Zr} - Z^2\rho(0). \tag{2.10}$$

Since $h \in L^\infty_{\rm loc}$, all coefficients of (2.10) are $L^\infty_{\rm loc}$, and since $\rho \in W^{1,2}_{\rm loc}$, also $\mu \in W^{1,2}_{\rm loc}$. Therefore Proposition 2.1 leads to $\mu \in C^{1,\alpha}_{\rm loc}$, for all $\alpha \in (0,1)$. Due to (2.9), $\rho \in C^{0,1}(\mathbb{R}^3)$ follows.

Now consider

$$\Delta\rho = -\frac{2Z}{r}\rho + 2h \equiv g \quad \text{in} \quad \mathbb{R}^3 \setminus \{0\}. \tag{2.11}$$

Since $h \in C^\alpha(\mathbb{R}^3 \setminus \{0\})$, for all $\alpha \in (0,1)$ and due to the above, $\rho/r \in C^\alpha(\mathbb{R}^3 \setminus \{0\})$, for all $\alpha \in (0,1)$, we have

$$g \in C^\alpha(\mathbb{R}^3 \setminus \{0\}) \text{ for all } \alpha \in (0,1). \tag{2.12}$$

From (2.11) and (2.12) we obtain from regularity theory for the Poisson equation that $\rho \in C^{2,\alpha}(\mathbb{R}^3 \setminus \{0\})$ (see e. g. Gilbarg and Trudinger [3, Thm. 4.3 and 4.6] or Lieb and Loss [10, Thm. 10.3]).

We proceed analogously for $\widetilde{\rho}$: integrating (2.11) over $\mathbb{S}^2$, we get the equation

$$\Delta\widetilde{\rho} = -\frac{2Z}{r}\widetilde{\rho} + 2\widetilde{h} \equiv \widetilde{g} \quad \text{in} \quad \mathbb{R}^3 \setminus \{0\} \tag{2.13}$$

with

$$\widetilde{h}(r) = \int_{\mathbb{S}^2} h(r\omega)\,d\omega. \tag{2.14}$$

Since the R.H.S. of (2.13) is in $C^\alpha(\mathbb{R}^3 \setminus \{0\})$, we obtain that $\widetilde{\rho}$ as a (radially symmetric) function in $\mathbb{R}^3$ is $C^{2,\alpha}$ away from the origin, and therefore $\widetilde{\rho} : \mathbb{R}_+ \to \mathbb{R}$ satisfies $\widetilde{\rho} \in C^{2,\alpha}((0,\infty))$.

That $\widetilde{\rho} \in C^2([0,\infty))$ is shown in the proof of (iv).

Next we prove (iii). To prove the bound (1.12), let E_0^{N-1} be the groundstate energy for the operator H^{N-1}. From Remark 1.8 and the Variational Principle we get that for almost all $x_1 \in \mathbb{R}^3$,

$$\int_{\mathbb{R}^{3(N-1)}} \psi\big(H^{N-1} - E\big)\psi\,dx_2\cdots dx_N \geq (E_0^{N-1} - E)\rho(x_1),$$

and so $h(x) \geq \varepsilon\,\rho(x)$ with $\varepsilon = E_0^{N-1} - E > 0$.

As for the bound (1.11), note that due to the operator inequality $-\Delta - \beta/r \geq -\beta^2/4$ (true in dimension 3) and the translation invariance of $-\Delta$ we have, for almost all $x_k \in \mathbb{R}^3$ (fixed), $k \in \{1,\dots,N\}$, $k \neq j$,

$$\int_{\mathbb{R}^3} \frac{1}{|x_j - x_k|}\,|\psi|^2\,dx_j \leq \int_{\mathbb{R}^3} |\nabla_j\psi|^2\,dx_j + \frac{1}{4}\int_{\mathbb{R}^3} |\psi|^2\,dx_j.$$

In this way, using (2.7),

$$h(x) \leq C\Big(\int_{\mathbb{R}^{3(N-1)}} |\nabla\psi|^2\,dx_2\cdots dx_N + \int_{\mathbb{R}^{3(N-1)}} |\psi|^2\,dx_2\cdots dx_N\Big). \tag{2.15}$$

Due to Theorem 1.2 and a subsolution estimate (see Simon [14, Theorem C.1.2.]) we get, with $\mathbf{x} = (x_1, \cdots, x_N) = (x_1, x')$, $x' \in \mathbb{R}^{3(N-1)}$ and χ_Ω the characteristic function of the set Ω:

$$\begin{aligned}|\nabla\psi(\mathbf{x})|^2 \leq C \sup_{\mathbf{y}\in B(\mathbf{x},R)} |\psi(\mathbf{y})|^2 &\leq C\int_{\mathbf{y}\in B(\mathbf{x},2R)} |\psi(\mathbf{y})|^2\,d\mathbf{y}\\ &= C\int_{\mathbb{R}^{3N}} \chi_{B(\mathbf{x},2R)}(\mathbf{y})|\psi(\mathbf{y})|^2\,d\mathbf{y}.\end{aligned}$$

Using this, and that for fixed $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{3N}$:

$$\chi_{B(\mathbf{x},2R)}(\mathbf{y}) = \chi_{B(\mathbf{y},2R)}(\mathbf{x}) = \begin{cases} 1 & \text{if } |\mathbf{x}-\mathbf{y}| < 2R,\\ 0 & \text{otherwise}\end{cases}$$

we get, by Fubini,

$$\begin{aligned}&\int_{\mathbb{R}^{3(N-1)}} |\nabla\psi(x_1,x')|^2\,dx'\\ &\leq C\int_{\mathbb{R}^{3(N-1)}} \Big(\int_{\mathbb{R}^{3N}} \chi_{B(\mathbf{x},2R)}(\mathbf{y})|\psi(\mathbf{y})|^2\,d\mathbf{y}\Big)\,dx'\\ &= C\int_{\mathbb{R}^{3N}} |\psi(\mathbf{y})|^2\Big(\int_{\mathbb{R}^{3(N-1)}} \chi_{B(\mathbf{y},2R)}(\mathbf{x})\,dx'\Big)\,d\mathbf{y}.\end{aligned} \tag{2.16}$$

Note that with $\mathbf{z} = \mathbf{x} - \mathbf{y}$ we have

$$\chi_{B(\mathbf{y},2R)}(\mathbf{x}) = \chi_{B(\mathbf{y},2R)}(\mathbf{z}+\mathbf{y}) = \chi_{B(\mathbf{0},2R)}(\mathbf{z})$$

and so (with $r' = |z'|$ and $\omega' = z'/r'$)

$$\begin{aligned}&\int_{\mathbb{R}^{3(N-1)}} \chi_{B(\mathbf{y},2R)}((x_1,x'))\,dx' = \int_{\mathbb{R}^{3(N-1)}} \chi_{B(\mathbf{0},2R)}((z_1,z'))\,dz'\\ &= \int_{|(z_1,z')|\leq 2R} dz' = \chi_{B(0,2R)}(z_1)\int_{\mathbb{S}^{3(N-1)-1}}\int_0^{\sqrt{4R^2-|z_1|^2}} r'^{3(N-1)-1}\,dr'\,d\omega'\\ &= C(N)\big(4R^2-|z_1|^2\big)^{3(N-1)/2}\chi_{B(0,2R)}(z_1)\\ &\leq \widetilde{C}(N)R^{3(N-1)}\chi_{B(x_1,2R)}(y_1).\end{aligned} \tag{2.17}$$

From (2.16) and (2.17) we get

$$\begin{aligned}&\int_{\mathbb{R}^{3(N-1)}} |\nabla\psi(x_1,x')|^2\,dx'\\ &\leq C(R)\int_{|x_1-y_1|<2R}\int_{\mathbb{R}^{3(N-1)}} |\psi(y_1,y')|^2\,dy'\,dy_1 = C(R)\int_{B(x_1,2R)} \rho(y_1)\,dy_1.\end{aligned} \tag{2.18}$$

Combining (2.15) and (2.18) proves (1.11).

We now prove (iv). We first prove Kato's Cusp Condition (1.14) for the function $\widetilde{\rho}$:

$$\widetilde{\rho}'(0) = \lim_{r\downarrow 0}\frac{\widetilde{\rho}(r)-\widetilde{\rho}(0)}{r} = -Z\widetilde{\rho}(0) \text{ and } \lim_{r\downarrow 0}\widetilde{\rho}'(r) = \widetilde{\rho}'(0).$$

First, define the function $\widetilde{\mu}$ by the equation (see also (2.9))

$$\widetilde{\rho}(r) = e^{-Zr}\big(\widetilde{\rho}(0) + \widetilde{\mu}(r)\big). \tag{2.19}$$

Note that $\widetilde{\mu}(0) = 0$. Then, using (1.10), $\widetilde{\mu}$ satisfies the equation

$$\Delta\widetilde{\mu} - 2Z\,\frac{x}{r}\cdot\nabla\widetilde{\mu} + Z^2\widetilde{\mu} = 2\widetilde{h}e^{Zr} - Z^2\widetilde{\rho}(0),$$

and, since $\widetilde{h}$ is continuous, Proposition 2.1 gives that $\widetilde{\mu}$, as a (radially symmetric) function in $\mathbb{R}^3$, is $C^{1,\alpha}$ in a neighbourhood of the origin. In particular, $\lim_{r\downarrow 0}\widetilde{\mu}'(r) = \widetilde{\mu}'(0)$. Since (see (2.19))

$$\widetilde{\rho}'(r) = -Z\widetilde{\rho}(0) + e^{-Zr}\widetilde{\mu}'(r) \tag{2.20}$$

this means that

$$\lim_{r\downarrow 0}\widetilde{\rho}'(r) = -Z\widetilde{\rho}(0) + \lim_{r\downarrow 0}\widetilde{\mu}'(r) = \widetilde{\mu}'(0) - Z\widetilde{\rho}(0). \tag{2.21}$$

From (2.19) we also get that

$$\frac{\widetilde{\mu}(r)}{r} = e^{Zr}\,\frac{\widetilde{\rho}(r)-\widetilde{\rho}(0)}{r} + \frac{e^{Zr}-1}{r}\,\widetilde{\rho}(0).$$

This, together with (2.21) and $\widetilde{\mu}(0) = 0$, implies that

$$\begin{aligned}\lim_{r\downarrow 0}\widetilde{\rho}'(r) &= \widetilde{\mu}'(0) - Z\widetilde{\rho}(0) = \lim_{r\downarrow 0}\frac{\widetilde{\mu}(r)}{r} - \widetilde{\rho}(0)\lim_{r\downarrow 0}\frac{e^{Zr}-1}{r}\\ &= \lim_{r\downarrow 0} e^{Zr}\frac{\widetilde{\rho}(r)-\widetilde{\rho}(0)}{r} = \widetilde{\rho}'(0),\end{aligned} \tag{2.22}$$

and by (2.20) and (2.22), $\widetilde{\rho}'(0) = -Z\widetilde{\rho}(0)$. This proves (1.14).

Next, define the function $\widetilde{\eta}$ by the equations

$$\widetilde{\rho}(r) = e^{-Zr}\big(\widetilde{\rho}(0) + \beta r^2 + \widetilde{\eta}(r)\big), \tag{2.23}$$
$$\beta = \frac{1}{3}\big(\widetilde{h}(0) - \frac{Z^2}{2}\widetilde{\rho}(0)\big).$$

Then $\widetilde{\eta}(0) = 0$, and due to (1.14), $\widetilde{\eta}'(0) = 0$. Together with (1.9) this gives

$$\begin{aligned}\Delta\widetilde{\eta}(r) &= \Big(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\Big)\widetilde{\eta}\\ &= 2\big[e^{Zr}\widetilde{h}(r) - \frac{Z^2}{2}\widetilde{\rho}(r)e^{Zr} - 3\beta + 2Z\beta r + Z\widetilde{\eta}'(r)\big]\\ &\equiv 2G(r).\end{aligned} \tag{2.24}$$

From the foregoing regularity properties of $\widetilde{\rho}$, in particular (1.14) and (2.23), we obtain that $\widetilde{\eta}' \in C^0([0,\infty))$. From this, together with the regularity properties of $\widetilde{h}$ shown in Section 3, we conclude that $G \in C^0([0,\infty))$ and

$$G(r) \to \widetilde{h}(0) - \frac{Z^2}{2}\widetilde{\rho}(0) - 3\beta = 0 \quad \text{as} \quad r \downarrow 0. \tag{2.25}$$

From (2.25) and (2.24) we get that

$$\widetilde{\eta}(r) = 2\int_0^r \frac{1}{t^2}\int_0^t G(s)s^2\,ds\,dt,$$

and

$$\frac{\widetilde{\eta}'(r) - \widetilde{\eta}'(0)}{r} = \frac{2}{r^3}\int_0^r G(s)s^2\,ds = \frac{2}{3}\frac{1}{\mathrm{Vol}_{\mathbb{R}^3}(B(0,r))}\int_{B(0,r)} G(|x|)\,d^3x,$$

so that

$$\eta''(0) = \lim_{r\downarrow 0}\frac{\eta'(r) - \eta'(0)}{r} = \frac{2}{3}\,G(0) = 0. \tag{2.26}$$

Then by (2.23) $\widetilde{\rho}''(0)$ exists, and

$$\widetilde{\rho}''(0) = Z^2\widetilde{\rho}(0) + 2\beta = \frac{2}{3}\big(\widetilde{h}(0) + Z^2\widetilde{\rho}(0)\big).$$

This verifies (1.13).

Furthermore, by (2.24),

$$\Delta\widetilde{\eta}(r) = \widetilde{\eta}''(r) + \frac{2}{r}\widetilde{\eta}'(r) = 2G(r)$$

and so

$$\widetilde{\eta}''(r) = 2G(r) - \frac{2}{r}\widetilde{\eta}'(r) = 2G(r) - 2\left(\frac{\widetilde{\eta}'(r) - \widetilde{\eta}'(0)}{r}\right)$$

since $\widetilde{\eta}'(0) = 0$. This implies, by (2.26),

$$\lim_{r\downarrow 0}\widetilde{\eta}''(r) = 2\big(\lim_{r\downarrow 0} G(r) - \lim_{r\downarrow 0}\left(\frac{\widetilde{\eta}'(r) - \widetilde{\eta}'(0)}{r}\right)\big) = \widetilde{\eta}''(0) = 0,$$

so that due to (2.23) $\widetilde{\rho}''(r)$ is continuous at $r = 0$. Hence formula (1.13) follows from (2.23) and $\widetilde{\eta}''(0) = 0$. This finishes the proof of Theorem 1.11. ☐

3. Regularity of h and $\widetilde{h}$

In this section we prove the statements in Theorem 1.11 on the regularity of the functions h and $\widetilde{h}$. More precisely, we prove the following:

Proposition 3.1. *Let ψ satisfy* (1.3) *and let h be as in* (2.8)*:*

$$\begin{aligned} h(x) = &\int_{\mathbb{R}^{3(N-1)}} |\nabla\psi|^2 \, dx_2 \cdots dx_N \\ &- \sum_{j=2}^{N} \int_{\mathbb{R}^{3(N-1)}} \frac{Z}{|x_j|} \psi^2 \, dx_2 \cdots dx_N \\ &+ \sum_{1 \le j < k \le N} \int_{\mathbb{R}^{3(N-1)}} \frac{1}{|x_j - x_k|} \psi^2 \, dx_2 \cdots dx_N, \end{aligned} \tag{3.1}$$

and $\widetilde{h}$ as in (2.14)*:*

$$\widetilde{h}(r) = \int_{\mathbb{S}^2} h(r\omega) \, d\omega.$$

Then $h \in C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \{0\})$ and $\widetilde{h} \in C^0([0,\infty)) \cap C^{\alpha}_{\mathrm{loc}}((0,\infty))$ for all $\alpha \in (0,1)$.

Remark 3.2. From the proof of Proposition 3.1 follows the continuity of the function t_1 in Remark 1.15.

Proof. For convenience, we shall often write $\int \equiv \int_{\mathbb{R}^{3(N-1)}}$. Let

$$\begin{aligned} J_1(x) &= \int |\nabla\psi|^2 \, dx_2 \cdots dx_N, \\ J_2(x) &= \sum_{j=2}^{N} \int \frac{Z}{|x_j|} \psi^2 \, dx_2 \cdots dx_N, \\ J_3(x) &= \sum_{1 \le j < k \le N} \int \frac{1}{|x_j - x_k|} \psi^2 \, dx_2 \cdots dx_N. \end{aligned} \tag{3.2}$$

For the proof of the regularity of the functions J_1, J_2, J_3 we shall make use of the following lemmas. The proof of the first lemma is trivial, using $|(x_1, x_2, \ldots, x_N)| \ge |(x_2, \ldots, x_N)|$.

Lemma 3.3. *Let $\alpha \in (0,1)$ and $x_0 \in \mathbb{R}^3$. Assume that the real function $G = G(x_1, \ldots, x_N)$ satisfies: For all $R > 0$ there exists constants C, γ such that*

$$\begin{aligned} &\sup_{x,y \in B(x_0,R)} \frac{|G(x, x_2, \ldots, x_N) - G(y, x_2, \ldots, x_N)|}{|x-y|^{\alpha}} \le \\ &C \exp\big(-\gamma |(x_0, x_2, \ldots, x_N)|\big) \quad \text{for all} \quad (x_0, x_2, \ldots, x_N) \in \mathbb{R}^{3N}. \end{aligned} \tag{3.3}$$

Then the function

$$\eta(x) \equiv \int_{\mathbb{R}^{3(N-1)}} G(x, x_2, \ldots, x_N) \, dx_2 \cdots dx_N$$

is in $C^{\alpha}_{loc}(\mathbb{R}^3)$.

We next prove the following lemma.

Lemma 3.4. *Let $\alpha \in (0,1)$. Assume that the real valued function $K = K(x_1, \dots, x_N)$ satisfies (3.3) and that there exists constants C, γ such that*

$$|K(x_1, \dots, x_N)| \\ \leq C \exp\big(-\gamma|(x_1, \dots, x_N)|\big) \text{ for all } (x_1, \dots, x_N) \in \mathbb{R}^{3N}. \tag{3.4}$$

Then:

(a)

For all $j, k \in \{1, \dots, N\}, j \neq k$, the function

$$\zeta(x_1) \equiv \int_{\mathbb{R}^{3(N-1)}} \frac{1}{|x_j - x_k|} K(x_1, \dots, x_N)\, dx_2 \cdots dx_N$$

is in $C^\alpha_{\mathrm{loc}}(\mathbb{R}^3)$.

(b)

For $j \geq 2$ the function

$$\mu(x_1) \equiv \int_{\mathbb{R}^{3(N-1)}} \frac{1}{|x_j|} K(x_1, \dots, x_N)\, dx_2 \cdots dx_N$$

is in $C^\alpha_{\mathrm{loc}}(\mathbb{R}^3)$.

Proof. Assume first that $j \neq 1 \neq k$. Let $x, y \in B(x_0, R)$, then by (3.3),

$$\frac{|\zeta(x) - \zeta(y)|}{|x-y|^\alpha} \leq \\ \int \frac{1}{|x_j - x_k|} \frac{|K(x, x_2, \dots, x_N) - K(y, x_2, \dots, x_N)|}{|x-y|^\alpha}\, dx_2 \cdots dx_N \\ \leq C \int \frac{1}{|x_j - x_k|} \exp\big(-\gamma|(x_0, x_2, \dots, x_N)|\big)\, dx_2 \cdots dx_N.$$

By equivalence of norms in $\mathbb{R}^{3N}$ there is a constant c_0 such that

$$\frac{|\zeta(x) - \zeta(y)|}{|x-y|^\alpha} \leq C\Big(\prod_{l=2, l\neq j,k}^{N} \int_{\mathbb{R}^3} \exp(-\gamma c_0 |x_l|)\, dx_l\Big) \times \\ \times \int_{\mathbb{R}^6} \frac{1}{|x_j - x_k|} \exp(-\gamma c_0(|x_j| + |x_k|))\, dx_j\, dx_k \leq C,\ x, y \in B(x_0, R).$$

The last inequality is an application of the following inequality (with $n = 3, \lambda = 1, p = r = 6/5$): (see Lieb and Loss [10, Theorem 4.3])

Hardy-Littlewood-Sobolev Inequality: *Let $p, r > 1$ and $0 < \lambda < n$ with $1/p + \lambda/n + 1/r = 2$. Let $f \in L^p(\mathbb{R}^n)$ and $h \in L^r(\mathbb{R}^n)$. Then there exists a sharp constant $C(n, \lambda, p)$, independent of f and h, such that*

$$\left| \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f(x) |x-y|^{-\lambda} h(y)\, dx\, dy \right| \leq C(n, \lambda, p) \|f\|_p \|h\|_r.$$

This proves Lemma 3.4 (a) when $j \neq 1 \neq k$.

Assume now that $j=1$. We assume without loss that $k=2$. Then, with $x_1, \bar{x}_1 \in B(x_0, R)$,

$$
\begin{aligned}
&\frac{|\zeta(x_1)-\zeta(\bar{x}_1)|}{|x_1-\bar{x}_1|^\alpha} \leq \\
&\int \frac{1}{|x_1-x_2|} \frac{|K(x_1,x_2,\dots,x_N)-K(\bar{x}_1,x_2,\dots,x_N)|}{|x_1-\bar{x}_1|^\alpha}\,dx_2\cdots dx_N \\
&+\int \left|\frac{1}{|x_1-x_2|}-\frac{1}{|\bar{x}_1-x_2|}\right| |x_1-\bar{x}_1|^{-\alpha}|K(\bar{x}_1,x_2,\dots,x_N)|\,dx_2\cdots dx_N \\
&\equiv (\mathrm{A})+(\mathrm{B}).
\end{aligned}
$$

For (A), using (3.3) and equivalence of norms in $\mathbb{R}^{3N}$, we get

$$
\begin{aligned}
(\mathrm{A}) &\leq C\int \frac{1}{|x_1-x_2|}\exp\big(-\gamma c_0(|x_0|+|x_2|+\cdots+|x_N|)\big)\,dx_2\cdots dx_N \\
&\leq C\int_{\mathbb{R}^3} \frac{1}{|x_1-x_2|}\exp(-\gamma c_0|x_2|)\,dx_2 \leq C(x_0,R).
\end{aligned}
$$

As for (B), we apply the following inequality; for the convenience of the reader, we give the proof (borrowed from Lieb and Loss [10, (3) p. 225]).

For $\alpha \in (0,1)$:

$$
\begin{aligned}
&\left|\frac{1}{|x-z|}-\frac{1}{|y-z|}\right| |x-y|^{-\alpha} \leq \\
&|x-z|^{-1-\alpha}+|y-z|^{-1-\alpha} \quad \text{for all} \quad x,y,z\in\mathbb{R}^3.
\end{aligned} \tag{3.5}
$$

Proof of (3.5). By Hölder's inequality we have, for $b>1$, $\alpha\in(0,1)$,

$$
1-b^{-1}=\int_1^b t^{-2}\,dt \leq \left(\int_1^b dt\right)^\alpha \left(\int_1^\infty t^{-2/(1-\alpha)}\,dt\right)^{1-\alpha} \leq (b-1)^\alpha.
$$

Substituting b/a for b, with $a>0$, this gives

$$
\left|b^{-1}-a^{-1}\right| \leq |b-a|^\alpha \max\{a^{-1-\alpha}, b^{-1-\alpha}\}.
$$

So, for $x,y,z\in\mathbb{R}^3$, using $\max\{s,t\}\leq s+t$ and the triangle inequality in $\mathbb{R}^3$, we have

$$
\left||x-z|^{-1}-|y-z|^{-1}\right| \leq |x-y|^\alpha\left\{|x-z|^{-1-\alpha}+|y-z|^{-1-\alpha}\right\}.
$$

$\square$

In this way, by (3.4) and equivalence of norms in $\mathbb{R}^{3N}$,

$$
\begin{aligned}
\text{(B)} &\leq \int \left(\frac{|K(\bar{x}_1, x_2, \dots, x_N)|}{|x_1 - x_2|^{1+\alpha}} + \frac{|K(\bar{x}_1, x_2, \dots, x_N)|}{|\bar{x}_1 - x_2|^{1+\alpha}} \right) dx_2 \cdots dx_N \\
&\leq C \prod_{j=3}^{N} \int_{\mathbb{R}^3} \exp(-\gamma c_0 |x_j|)\, dx_j \\
&\quad \times \int_{\mathbb{R}^3} \left(\frac{1}{|\bar{x}_1 - x_2|^{1+\alpha}} + \frac{1}{|x_1 - x_2|^{1+\alpha}} \right) \exp(-\gamma c_0 |x_2|)\, dx_2 \\
&\leq C(x_0, R),
\end{aligned}
$$

since $x_1, \bar{x}_1 \in B(x_0, R)$. This finishes the proof of Lemma 3.4 (a).

The proof of (b) is similar to that of (a) so we omit the details. □

The proof of the following fact is straightforward:

There exist constants $C = C(\gamma, R)$ and $\widetilde{\gamma} = \widetilde{\gamma}(\gamma)$ such that

$$\exp(-\gamma|(x, \dots, x_N)|) \leq C \exp(-\widetilde{\gamma}|(x_0, \dots, x_N)|) \tag{3.6}$$

for all $x \in B(x_0, R)$.

Using this and Lemma 3.3, 3.4, we shall prove the following lemma on the regularity of the functions J_1, J_2 and J_3 from (3.2).

Lemma 3.5. *Let J_1, J_2 and J_3 be as in* (3.2). *Then*

(i) $J_2, J_3 \in C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$ *for all* $\alpha \in (0,1)$.
(ii) $J_1 \in C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \{0\})$ *for all* $\alpha \in (0,1)$.

Herefrom follow the regularity properties of the function h stated in Proposition 3.1.

Proof of Lemma 3.5 (i).

Firstly, by Theorem 1.2 and Remark 1.8,

$$|\psi(\mathbf{x})|\ ,\ \ |\nabla\psi(\mathbf{x})| \leq C \exp(-\gamma|\mathbf{x}|)\ ,\ \ \mathbf{x} \in \mathbb{R}^{3N}, \tag{3.7}$$

which gives (3.4) for $K = \psi^2$.

Next we verify that for $G = \psi^2$, (3.3) is fulfilled. Then Lemma 3.4 can be applied with $K = \psi^2$, and the Hölder-continuity of J_2 and J_3 follows.

Given $x_0 \in \mathbb{R}^3, R > 0, \alpha \in (0,1)$, and $x, y \in B(x_0, R)$. Using that (see e. g. Malý and Ziemer [11, Theorem 1.41]) (here, $(x, x_2, \dots, x_N) = (x, x')$, $x' \in \mathbb{R}^{3(N-1)}$)

$$
\begin{aligned}
\psi^2(x, x') - \psi^2(y, x') &= \int_0^1 \frac{\partial}{\partial s} \left[\psi^2(sx + (1-s)y, x') \right] ds \\
&= \int_0^1 \left[\nabla_1(\psi^2)(sx + (1-s)y, x') \right] \cdot (x - y)\, ds \qquad (3.8)
\end{aligned}
$$

and that $sx + (1-s)y \in B(x_0, R)$ for all $s \in [0,1]$ we get, with (3.7) and (3.6),

$$\begin{aligned}
&\frac{|\psi^2(x,x') - \psi^2(y,x')|}{|x-y|^\alpha} \\
&\leq 2|x-y|^{1-\alpha} \int_0^1 |\nabla_1 \psi(sx + (1-s)y, x')| \cdot |\psi(sx + (1-s)y, x')| \, ds \\
&\leq 2(2R)^{1-\alpha} \int_0^1 C \, \exp(-2\gamma |(sx + (1-s)y, x')|) \, ds \\
&\leq C \, \exp(-\widetilde{\gamma} |(x_0, \ldots, x_N)|), \qquad (3.9)
\end{aligned}$$

so (3.3) follows for $\alpha \in (0,1)$.

This proves (i) of Lemma 3.5.

To prove (ii), we write ψ as in the proof of Theorem 1.2: $\psi = e^{F-F_1}\psi_1$, with F and F_1 as in (1.6) and (2.1). Then

$$\begin{aligned}
J_1(x) = \int |\nabla \psi|^2 \, dx' &= \int |\nabla F|^2 \psi^2 \, dx' + \int |\nabla F_1|^2 \psi^2 \, dx' \\
&- 2 \int \big(\nabla F \cdot \nabla F_1\big) \psi^2 \, dx' + \int e^{2(F-F_1)} |\nabla \psi_1|^2 \, dx' \\
&+ 2 \int \big(\nabla F \cdot \nabla \psi_1\big) e^{2(F-F_1)} \psi_1 \, dx' - 2 \int \big(\nabla F_1 \cdot \nabla \psi_1\big) e^{2(F-F_1)} \psi_1 \, dx' \\
&\equiv I_1(x) + I_2(x) + I_3(x) + I_4(x) + I_5(x) + I_6(x). \qquad (3.10)
\end{aligned}$$

Using the idea from (3.8) twice (on $|\nabla F_1|^2$ and ψ^2, respectively), the estimates (2.3), (3.7), (3.9), and (3.6), we have, with $x_0 \in \mathbb{R}^3, R > 0, \alpha \in (0,1)$, and $x, y \in B(x_0, R)$:

$$\begin{aligned}
&\frac{\big||\nabla F_1|^2 \psi^2(x,x') - |\nabla F_1|^2 \psi^2(y,x')\big|}{|x-y|^\alpha} \leq \\
&\qquad \frac{\big||\nabla F_1(x,x')|^2 - |\nabla F_1(y,x')|^2\big|}{|x-y|^\alpha} |\psi(x,x')|^2 \\
&\qquad + |\nabla F_1(y,x')|^2 \frac{\big|\psi^2(x,x') - \psi^2(y,x'x)\big|}{|x-y|^\alpha} \\
&\qquad \leq C\,|x-y|^{1-\alpha} \big\|\nabla\big(|\nabla F_1|^2\big)\big\|_\infty \exp(-2\gamma|(x, x_2, \ldots, x_N)|) \\
&\qquad\qquad + 2\widetilde{C}|x-y|^{1-\alpha} \big\||\nabla F_1|^2\big\|_\infty \exp(-\widetilde{\gamma}|(x_0, \ldots, x_N)|) \\
&\qquad \leq \bar{C} \, \exp(-\bar{\gamma}(x_0, \ldots, x_N)|).
\end{aligned}$$

By Lemma 3.3, with $G = |\nabla F_1|^2 \psi^2(x_1, \cdots, x_N)$, this implies that $I_2 \in C^\alpha_{\mathrm{loc}}(\mathbb{R}^3)$.

Using the same ingredients, writing $\nabla \psi_1 = \nabla(e^{F_1 - F}\psi)$, gives (3.3) and (3.4) with

$$G = K = e^{2(F-F_1)} |\nabla \psi_1|^2$$

and

$$G = K = \big(\nabla F_1 \cdot \nabla \psi_1\big) e^{2(F-F_1)} \psi_1,$$

and so by Lemma 3.3, $I_4, I_6 \in C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$.

The remaining terms are those involving the function F, namely I_1, I_3 and I_5.

Note that

$$\begin{aligned}\nabla F(x_1, \dots, x_N) = & -\frac{Z}{2}\Big(\frac{x_1}{|x_1|}, \dots, \frac{x_N}{|x_N|}\Big) \\ & + \frac{1}{4}\left(\sum_{k=2}^{N} \frac{x_1 - x_k}{|x_1 - x_k|}, \dots, \sum_{k=1, k\neq j}^{N} \frac{x_j - x_k}{|x_j - x_k|}, \dots, \sum_{k=1}^{N-1} \frac{x_N - x_k}{|x_N - x_k|}\right)\end{aligned} \tag{3.11}$$

and so

$$\begin{aligned}|\nabla F(x_1, \dots, x_N)|^2 = & \frac{NZ^2}{4} - \frac{Z}{8}\sum_{j,k=1,k\neq j}^{N} \frac{x_j}{|x_j|} \cdot \frac{x_j - x_k}{|x_j - x_k|} \\ & + \frac{1}{16}\sum_{j,k,l=1,k\neq j,l\neq j}^{N} \frac{x_j - x_k}{|x_j - x_k|} \cdot \frac{x_j - x_l}{|x_j - x_l|}.\end{aligned}$$

In this way,

$$\begin{aligned}I_1(x_1) = & \frac{NZ^2}{4}\int \psi^2 \, dx_2 \cdots dx_N \\ & - \frac{Z}{8}\sum_{j,k=1,k\neq j}^{N} \int \frac{x_j}{|x_j|} \cdot \frac{x_j - x_k}{|x_j - x_k|} \, \psi^2 \, dx_2 \cdots dx_N \\ & + \frac{1}{16}\sum_{j,k,l=1,k\neq j,l\neq j}^{N} \frac{x_j - x_k}{|x_j - x_k|} \cdot \frac{x_j - x_l}{|x_j - x_l|} \, \psi^2 \, dx_2 \cdots dx_N \\ = & \frac{NZ^2}{4}\rho(x_1) - \frac{Z}{8}\sum_{j,k=1,k\neq j}^{N} \kappa_{j,k}(x_1) + \frac{1}{16}\sum_{j,k,l=1,k\neq j,l\neq j}^{N} \nu_{j,k,l}(x_1).\end{aligned} \tag{3.12}$$

Note that $\nu_{j,k,l} = \nu_{j,l,k}$.

Using the ideas above, Lemma 3.3 implies that the following functions from (3.12) (with the mentioned choices of G satisfying (3.3)) are all in $C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$:

$$\begin{aligned}
\rho:\quad & G=\psi^2,\\
\kappa_{j,k},\quad j,k\neq 1, j\neq k:\quad & G=\frac{x_j}{|x_j|}\cdot\frac{x_j-x_k}{|x_j-x_k|}\,\psi^2,\\
\nu_{j,k,k}, j\neq k:\quad & G=\frac{x_j-x_k}{|x_j-x_k|}\cdot\frac{x_j-x_k}{|x_j-x_k|}\,\psi^2=\psi^2,\\
\nu_{j,k,l},\quad j,k,l\neq 1, l\neq j\neq k:\quad & G=\frac{x_j-x_k}{|x_j-x_k|}\cdot\frac{x_j-x_l}{|x_j-x_l|}\,\psi^2.
\end{aligned}$$

Likewise, Lemma 3.4 implies (with the mentioned choices of $G=K$ satisfying (3.3) and (3.4)) that the following functions from (3.12) are all in $C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$:

$$\begin{aligned}
\kappa_{j,1},\quad j\neq 1:\quad & G=K=\frac{x_j\cdot(x_j-x_1)}{|x_j|}\,\psi^2,\\
\nu_{j,1,l},\quad j,l\neq 1, j\neq l:\quad & G=K=\frac{(x_j-x_1)\cdot(x_j-x_l)}{|x_j-x_l|}\,\psi^2,
\end{aligned}$$

From the decomposition of I_1 in (3.12) we are left with

$$\kappa_{1,k}(x_1)=\int\frac{x_1}{|x_1|}\cdot\frac{x_1-x_k}{|x_1-x_k|}\,\psi^2\,dx' \quad,\quad k=2,\dots,N, \tag{3.13}$$

and

$$\nu_{1,k,l}(x_1)=\int\frac{x_1-x_k}{|x_1-x_k|}\cdot\frac{x_1-x_l}{|x_1-x_l|}\,\psi^2\,dx' \quad,\quad k,l\in\{2,\dots,N\}, k\neq l. \tag{3.14}$$

Note that

$$\begin{aligned}
&\int\frac{x_1}{|x_1|}\cdot\frac{x_1-x_k}{|x_1-x_k|}\,\psi^2\,dx_2\cdots dx_N\\
&\qquad=\frac{1}{|x_1|}\int\frac{1}{|x_1-x_k|}\big(x_1\cdot(x_1-x_k)\,\psi^2\big)\,dx_2\cdots dx_N.
\end{aligned}$$

The function $1/|x_1|$ is smooth for $x_1\neq 0$ and therefore in $C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3\setminus\{0\})$. The function $x_1\cdot(x_1-x_k)\,\psi^2$ satisfies (3.3) and (3.4) (by the same ideas as above), so Lemma 3.4 (a) implies that the function

$$\int\frac{1}{|x_1-x_k|}\big(x_1\cdot(x_1-x_k)\,\psi^2\big)\,dx_2\cdots dx_N$$

is in $C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$. The functions in (3.13) are therefore in $C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3\setminus\{0\})$.

As for the functions in (3.14), these are all in $C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$, which can be seen by applying the previous ideas, in particular Lemma 3.5, (3.6), (3.7) and (3.9).

This proves that $I_1\in C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3\setminus\{0\})$.

As for I_3 (see (3.10) and (3.11)), with $\nabla = (\nabla_1, \dots, \nabla_N)$,

$$I_3(x) = Z\sum_{j=1}^{N}\int\Big(\frac{x_j}{|x_j|}\cdot\nabla_j F_1\Big)\psi^2\,dx_2\cdots dx_N - \frac{1}{2}\sum_{j,k=1,j\neq k}^{N}\int\Big(\frac{x_j-x_k}{|x_j-x_k|}\cdot\nabla_j F_1\Big)\psi^2\,dx_2\cdots dx_N. \tag{3.15}$$

The terms in the first sum with $j \neq 1$ are in $C^{\alpha}_{\text{loc}}(\mathbb{R}^3)$, due to Lemma 3.4 (b), with $G = K = (x_j\cdot\nabla_j F_1)\,\psi^2$ satisfying (3.3) and (3.4). (To see this, use the previous ideas; to apply the idea from (3.8) to $\nabla_j F_1$ we use that F_1 is smooth). The terms in the second sum in (3.15) are all in $C^{\alpha}_{\text{loc}}(\mathbb{R}^3)$, due to Lemma 3.4 (a), applied with $G = K = \big((x_j - x_k)\cdot\nabla_j F_1\big)\,\psi^2$. The term with $j = 1$ is in $C^{\alpha}_{\text{loc}}(\mathbb{R}^3\setminus\{0\})$. This can be seen by following the ideas in the proof of the regularity properties of the function in (3.13), now using Lemma 3.3 with $G = (x_1\cdot\nabla_1 F_1)\psi^2$.

The statements and proofs are similar for

$$I_5(x) = -Z\sum_{j=1}^{N}\int\Big(\frac{x_j}{|x_j|}\cdot\nabla_j\psi_1\Big)e^{2(F-F_1)}\psi_1\,dx_2\cdots dx_N + \frac{1}{2}\sum_{j,k=1,j\neq k}^{N}\int\Big(\frac{x_j-x_k}{|x_j-x_k|}\cdot\nabla_j\psi_1\Big)e^{2(F-F_1)}\psi_1\,dx_2\cdots dx_N. \tag{3.16}$$

That is, the functions in the first sum in (3.16) with $j \geq 2$ and those in the second sum are all in $C^{\alpha}_{\text{loc}}(\mathbb{R}^3)$, whereas the function in the first sum with $j = 1$ is only in $C^{\alpha}_{\text{loc}}(\mathbb{R}^3\setminus\{0\})$. To prove this we use the inequality (with $\mathbf{x} = (x_1, \dots, x_N)$):

$$|\psi_1|_{C^{1,\alpha}(B(\mathbf{x},R/2))} \leq C\sup_{y\in(B(\mathbf{x},R))}|\psi_1(y)| \leq C\,\exp(-\gamma|(x_1,\dots,x_N)|).$$

This inequality follows from (2.3), (2.5) and (3.7) (remember that $\psi_1 = e^{F_1-F}\psi$).

This proves that $I_5 \in C^{\alpha}_{\text{loc}}(\mathbb{R}^3\setminus\{0\})$, and so finishes the proof that $J_1 \in C^{\alpha}_{\text{loc}}(\mathbb{R}^3\setminus\{0\})$. (See (3.10)). This proves (ii) and therefore Lemma 3.5. $\square$

That $\widetilde{h} \in C^{\alpha}_{\text{loc}}((0,\infty))$ is a consequence of the foregoing and of the following proposition:

Proposition 3.6. *Assume $f \in C^{\alpha}_{\text{loc}}(\mathbb{R}^3\setminus\{0\})$, $\alpha \in (0,1)$. Then $\widetilde{f} \in C^{\alpha}_{\text{loc}}((0,\infty))$, where*

$$\widetilde{f}(r) = \int_{\mathbb{S}^2} f(r\omega)\,d\omega.$$

Proof. Let $r \in (0,\infty)$. For all $x_0 \in A = \{x \in \mathbb{R}^3 \,|\, |x| = r\}$, choose $R = R(x_0)$ and $C = C(x_0)$ such that

$$\sup_{x,y\in B(x_0,R(x_0))} \frac{|f(x)-f(y)|}{|x-y|^\alpha} \le C(x_0). \tag{3.17}$$

This is possible, since $f \in C^\alpha_{\mathrm{loc}}(\mathbb{R}^3 \setminus \{0\})$. Then

$$A \subset \bigcup_{x_0\in A} B(x_0, R(x_0)).$$

Using compactness of A, choose $x_1, \dots, x_m \in A$ such that

$$A \subset \bigcup_{j=1}^m B(x_j, R(x_j)).$$

Choose $\epsilon \in (0,r)$ such that

$$\{y \in \mathbb{R}^3 \,|\, r-\epsilon < |y| < r+\epsilon\} \subset \bigcup_{j=1}^m B(x_j, R(x_j)).$$

Then, for all $s,t \in (r-\epsilon, r+\epsilon)$ and all $\omega \in \mathbb{S}^2$ there exists $j \in \{1,\dots,m\}$ such that $s\omega, t\omega \in B(x_j, R(x_j))$ and therefore by (3.17),

$$\frac{|f(s\omega)-f(t\omega)|}{|s-t|^\alpha} = \frac{|f(s\omega)-f(t\omega)|}{|s\omega-t\omega|^\alpha} \le C(x_j).$$

So with $C = \max\{C(x_1),\dots,C(x_m)\}$,

$$\frac{|f(s\omega)-f(t\omega)|}{|s-t|^\alpha} \le C, \text{ for all } s,t \in (r-\epsilon,r+\epsilon) \text{ and all } \omega \in \mathbb{S}^2.$$

This implies that

$$\begin{aligned}\frac{|\widetilde{f}(s)-\widetilde{f}(t)|}{|s-t|^\alpha} &= \frac{|\int_{\mathbb{S}^2}(f(s\omega)-f(t\omega))\,d\omega|}{|s-t|^\alpha} \\ &\le \int_{\mathbb{S}^2} \frac{|f(s\omega)-f(t\omega)|}{|s\omega-t\omega|^\alpha}\,d\omega \le C, \quad \text{for all } s,t \in (r-\epsilon,r+\epsilon).\end{aligned}$$

This proves that $\widetilde{f} \in C^\alpha_{\mathrm{loc}}((0,\infty))$. □

To prove that $\widetilde{h} \in C^0([0,\infty))$, we apply the following:

Proposition 3.7. *Assume $f \in C^\alpha_{\mathrm{loc}}(\mathbb{R}^3)$. Then $\widetilde{f} \in C^0([0,\infty))$, where*

$$\widetilde{f}(r) = \int_{\mathbb{S}^2} f(r\omega)\,d\omega.$$

Proof. The function f is continuous in $\mathbb{R}^3$, since it is in $C^\alpha_{\mathrm{loc}}(\mathbb{R}^3)$. Let $r \in [0,\infty)$. Then

$$\lim_{s\to r} f(s\omega) = f(r\omega) \quad \text{for all } \omega \in \mathbb{S}^2.$$

Using the supremum of f on a sufficiently large compact set in $\mathbb{R}^3$ as a dominant, Lebesque's Dominated Convergence Theorem gives us that

$$\lim_{s\to r}\int_{\mathbb{S}^2} f(s\omega)\,d\omega = \int_{\mathbb{S}^2} f(r\omega)\,d\omega.$$

Therefore $f \in C^0([0,\infty))$. □

Recall the proof of the fact that $h \in C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3\setminus\{0\})$. In fact, the only terms in the decomposition of h (see (3.1), (3.2), (3.10), and (3.11)) that are only in $C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3\setminus\{0\})$ and not in $C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$ are the functions

$$\begin{aligned}
&\int \frac{x_1}{|x_1|}\cdot\frac{x_1-x_k}{|x_1-x_k|}\,\psi^2\,dx_2\cdots dx_N \quad , \quad k=2,\dots,N,\\
&\int \Big(\frac{x_1}{|x_1|}\cdot\nabla_1 F_1\Big)\psi^2\,dx_2\cdots dx_N,\\
&\int \Big(\frac{x_1}{|x_1|}\cdot\nabla_1 \psi_1\Big)e^{2(F-F_1)}\psi_1\,dx_2\cdots dx_N.
\end{aligned}\tag{3.18}$$

Comparing (3.10), (3.13), (3.15) and (3.16), it can be seen that all the terms in (3.18) stem from the function J_1, namely from I_1, I_3, and I_5.

All other terms in the decomposition of h are in $C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$. When integrating them over $\mathbb{S}^2$, we get something continuous in $[0,\infty)$, according to Proposition 3.7 above.

For the terms in (3.18) we note that they are all of the form

$$\int \frac{x_1}{|x_1|}\cdot\mathbf{K}(x_1,x')\,dx' = \frac{x_1}{|x_1|}\cdot\int \mathbf{K}(x_1,x')\,dx'. \tag{3.19}$$

In each case, we have

$$\mathbf{L}(x_1) = \big(L_1(x_1),L_2(x_1),L_3(x_1)\big) = \int \mathbf{K}(x_1,x')\,dx',\, L_j \in C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3). \tag{3.20}$$

To see this, apply Lemma 3.3 to each of the coordinate functions L_j, $j=1,2,3$. The integrands are easily seen to satisfy (3.3) in each case, by the previous ideas. To get continuity in $[0,\infty)$ of the functions in (3.18) we use (3.19) and (3.20), and the following lemma:

Proposition 3.8. *Assume* $\mathbf{f} = (f_1,f_2,f_3)$, $f_j \in C^{\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$. *Then* $\bar f \in C^0([0,\infty))$, *where*

$$\bar f(r) = \int_{\mathbb{S}^2}\big(\omega\cdot\mathbf{f}(r\omega)\big)\,d\omega.$$

Proof. The same as for Proposition 3.7, noting that for all $r\in[0,\infty)$ and fixed $\omega\in\mathbb{S}^2$:

$$\lim_{s\to r}\omega\cdot\mathbf{f}(s\omega) = \omega\cdot\mathbf{f}(r\omega).$$

□

This holds even in the case $r = 0$, for which

$$\lim_{s\downarrow 0} \int_{\mathbb{S}^2} \omega \cdot \mathbf{f}(s\omega)\, d\omega = \int_{\mathbb{S}^2} \omega \cdot \mathbf{f}(0)\, d\omega = 0.$$

This proves that the functions in (3.18) are in $C^0([0,\infty))$. Therefore $\widetilde{h} \in C^0([0,\infty))$, which finishes the proof of Proposition 3.1. $\square$

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References

[1] R. Ahlrichs, M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, and J.D. Morgan, III, *Bounds on the decay of electron densities with screening*, Phys. Rev. A (3) **23** (1981), 2106–2117.

[2] H.L. Cycon, R.G. Froese, W. Kirsch, and B. Simon, *Schrödinger Operators with Application to Quantum Mechanics and Global Geometry*, Texts and Monographs in Physics, Springer-Verlag, Berlin, 1987.

[3] D. Gilbarg and N.S. Trudinger, *Elliptic Partial Differential Equations of Second Order*, second ed., Springer-Verlag, Berlin, 1983.

[4] M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, and H. Stremnitzer, *Local properties of Coulombic wave functions*, Comm. Math. Phys. **163** (1994), 185–215.

[5] M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, and W. Thirring, *Simple bounds to the atomic one-electron density at the nucleus and to expectation values of one-electron operators*, J. Phys. B **11** (1978), L571–L575.

[6] M. Hoffmann-Ostenhof and R. Seiler, *Cusp conditions for eigenfunctions of n-electron systems*, Phys. Rev. A **23** (1981), 21–23.

[7] E. Hopf, *Über den funktionalen, insbesondere den analytischen Charakter der Lösungen elliptischer Differentialgleichungen zweiter Ordnung*, Math. Z. **34** (1931), 194–233.

[8] T. Kato, *On the eigenfunctions of many-particle systems in quantum mechanics*, Comm. Pure Appl. Math. **10** (1957), 151–177.

[9] E.H. Lieb, *The Stability of Matter: From Atoms to Stars. Selecta of Elliot H. Lieb*, second ed., Springer - Verlag, Berlin/Heidelberg, 1997.

[10] E.H. Lieb and M. Loss, *Analysis*, American Mathematical Society, Providence, RI, 1997.

[11] Jan Malý and William P. Ziemer, *Fine regularity of solutions of elliptic partial differential equations*, American Mathematical Society, Providence, RI, 1997.

[12] M. Reed and B. Simon, *Methods of modern mathematical physics. II. Fourier analysis, self-adjointness*, Academic Press, New York, 1975.

[13] ______, *Methods of modern mathematical physics. IV. Analysis of operators*, Academic Press, New York, 1978.

[14] B. Simon, *Schrödinger semigroups*, Bull. Amer. Math. Soc. (N.S.) **7** (1982), 447–526.

[15] G.M. Zhislin and A.G. Sigalov, *On the spectrum of the energy operator for atoms with fixed nuclei on subspaces corresponding to irreducible representations of a group of permutations*, Am. Math. Soc., Transl., II. Ser. **91** (1970), 263–295.

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