A new proof of the analyticity of the electronic density of molecules.

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Abstract

We give a new, short proof of the regularity away from the nuclei of the electronic density of a molecule obtained in [FHHS1, FHHS2]. The new argument is based on the regularity properties of the Coulomb interactions underlined in [KMSW] and on well-known elliptic technics.

Keywords: Elliptic regularity, analytic elliptic regularity, molecular Hamiltonian, electronic density, Coulomb potential.

1 Introduction.

For the quantum description of molecules, it is very useful to study the so-called electronic density and, in particular, its regularity properties. This has be done for molecules with fixed nuclei: see [FHHS1, FHHS2, FHHS3] for details and references. The smoothness and the analyticity of the density away from the nuclei are proved in [FHHS1] and [FHHS2] respectively. In this paper, we propose an alternative proof.

Let us recall the framework and the precise results of [FHHS1, FHHS2]. We consider a molecule with N moving electrons ($N \geq 2$) and L fixed nuclei. While the distinct vectors $R_1, \cdots, R_L \in \mathbb{R}^3$ denote the positions of the nuclei, the positions of the electrons are given by $x_1, \cdots, x_N \in \mathbb{R}^3$. The charges of the nuclei are given by the positive $Z_1, \cdots, Z_L$ and the electronic charge is -1. In this picture, the Hamiltonian of the system is

$$H := \sum_{j=1}^{N}\Big(-\Delta_{x_j} - \sum_{k=1}^{L}\frac{Z_k}{|x_j - R_k|}\Big) + \sum_{1\leq j<j'\leq N}\frac{1}{|x_j - x_{j'}|} + E_0 \qquad (1.1)$$

$$\text{where } E_0 = \sum_{1\leq k<k'\leq L}\frac{Z_k Z_{k'}}{|R_k - R_{k'}|}$$

and $-\Delta_{x_j}$ stands for the Laplacian in the variable x_j. Setting $\Delta := \sum_{j=1}^{N}\Delta_{x_j}$, we define the potential V of the system as the multiplication operator satifying $H = -\Delta + V$. Thanks to Hardy's inequality

$$\exists c > 0\,;\ \forall f \in \mathrm{W}^{1,2}(\mathbb{R}^3)\,,\ \int_{\mathbb{R}^3}\Big(|t|^{-1}\,|f(t)|\Big)^2\,dt \ \leq\ c\int_{\mathbb{R}^3}|\nabla f(t)|^2\,dt\,, \qquad (1.2)$$

one can show that V is Δ-bounded with relative bound 0 and that H is self-adjoint on the domain of the Laplacian Δ, namely $\mathrm{W}^{2,2}(\mathbb{R}^{3N})$ (see Kato's theorem in [RS], p. 166-167). Let $\psi \in \mathrm{W}^{2,2}(\mathbb{R}^{3N}) \setminus \{0\}$ and $E \in \mathbb{R}$ such that $H\psi = E\psi$. Actually E is smaller than E_0 by [FH]. The electronic density associated to ψ is the following $\mathrm{L}^1(\mathbb{R}^3)$-function

$$\rho(x) := \sum_{j=1}^{N}\int_{\mathbb{R}^{3(N-1)}}\Big|\psi(x_1,\cdots,x_{j-1},x,x_j,\cdots,x_N)\Big|^2\,dx_1\cdots dx_{j-1}dx_j\cdots dx_N\,.$$

Here we used $N \geq 2$. The regularity result is the following

Theorem 1.1. [FHHS1, FHHS2]. *The density ρ is real analytic on $\mathbb{R}^3 \setminus \{R_1, \cdots, R_L\}$.*

Remark 1.2. *In [FHHS1], it is proved that ρ is smooth on $\mathbb{R}^3\setminus\{R_1, \cdots, R_L\}$. This result is then used in [FHHS2] to derive the analyticity.*

Now let us sketch the new proof of Theorem 1.1, the complete proof and the notation used are given in Section 2. We consider the almost everywhere defined L^2-function

$$\tilde{\psi}\ :\ \mathbb{R}^3 \ni x \mapsto \psi(x,\cdot,\cdots,\cdot) \in \mathrm{W}^{2,2}(\mathbb{R}^{3(N-1)}) \qquad (1.3)$$

and denote by $\|\cdot\|$ the $\mathrm{L}^2(\mathbb{R}^{3(N-1)})$-norm. By permutation of the variables, it suffices to show that the map $\mathbb{R}^3 \ni x \mapsto \|\tilde{\psi}(x)\|^2$ belongs to $C^\omega(\mathbb{R}^3 \setminus \{R_1, \cdots, R_L\}; \mathbb{R})$, the space of real analytic functions on $\mathbb{R}^3 \setminus \{R_1, \cdots, R_L\}$. We define the potentials V_0, V_1 by

$$V \;=\; V_0 + V_1 \quad \text{with} \quad V_0(x) \;=\; E_0 - \sum_{k=1}^{L} \frac{Z_k}{|x - R_k|} \;\in\; C^\omega(\mathbb{R}^3 \setminus \{R_1, \cdots, R_L\}; \mathbb{R})\,. \quad (1.4)$$

We view the function $\tilde{\psi}$ as a distributional solution in $\mathcal{D}'(\mathbb{R}^3; \mathrm{W}^{2,2}(\mathbb{R}^{3(N-1)}))$ of

$$-\Delta_x \tilde{\psi} \,+\, Q(x)\tilde{\psi} = 0\,, \quad (1.5)$$

where the x-dependent operator $Q(x) \in \mathcal{B} := \mathcal{L}(\mathrm{W}^{2,2}(\mathbb{R}^{3(N-1)}); \mathrm{L}^2(\mathbb{R}^{3(N-1)}))$ is given by

$$Q(x) \;=\; -\Delta_{x'} \,+\, V_0 \,-\, E \,+\, V_1 \quad \text{with} \quad \Delta_{x'} \;=\; \sum_{j=2}^{N} \Delta_{x_j}\,. \quad (1.6)$$

Considering (1.5) in a small enough neighbourhood Ω of some $x_0 \in \mathbb{R}^3 \setminus \{R_1, \cdots, R_L\}$, we pick from [KMSW] a x-dependent unitary operator $U_{x_0}(x)$ on $\mathrm{L}^2(\mathbb{R}^{3(N-1)})$ such that

$$W:\; \Omega \ni x \mapsto U_{x_0}(x) V_1(x) U_{x_0}(x)^{-1} \in \mathcal{B} \quad (1.7)$$

belongs to $C^\omega(\Omega; \mathcal{B})$. It turns out that $P_0 = U_{x_0}(-\Delta_x - \Delta_{x'})U_{x_0}^{-1}$ is an elliptic differential operator in x with analytic, differential coefficients in $\mathcal{B}$. Applying U_{x_0} to (1.5) and setting $\varphi = U_{x_0}\tilde{\psi}$, we obtain

$$\Big(P_0 \,+\, W(x) \,+\, V_0(x) \,-\, E\Big)\varphi \;=\; 0\,. \quad (1.8)$$

Since $U_{x_0}(x)$ is unitary on $\mathrm{L}^2(\mathbb{R}^{3(N-1)})$, $\|\tilde{\psi}(x)\| = \|\varphi(x)\|$. Thus, it suffices to show that $\varphi \in C^\omega(\Omega; \mathrm{L}^2(\mathbb{R}^{3(N-1)}))$. Using (1.8), a parametrix of the operator $P_0 + W + V_0$, we show by induction that, for all k, $\varphi \in \mathrm{W}^{k,2}(\Omega; \mathrm{W}^{2,2}(\mathbb{R}^{3(N-1)}))$. Thus $\varphi \in C^\infty(\Omega; \mathrm{W}^{2,2}(\mathbb{R}^{3(N-1)}))$. Finally we can adapt the arguments in [H1] p. 178-180 to get $\varphi \in C^\omega(\Omega; \mathrm{W}^{2,2}(\mathbb{R}^{3(N-1)}))$, yielding $\varphi \in C^\omega(\Omega; \mathrm{L}^2(\mathbb{R}^{3(N-1)}))$.

The main idea in the construction of the unitary operator U_{x_0} is to change, locally in x, the variables $x_2, \cdots, x_N$ in a x-dependent way such that the x-dependent singularities $1/|x - x_j|$ becomes locally x-independent (see Section 2). In [KMSW], where this clever method was introduced, the nuclei positions play the role of the x variable and the $x_2, \cdots, x_N$ are the electronic degrees of freedom. The validity of the Born-Oppenheimer approximation is proved there for the computation of the eigenvalues and eigenvectors of the molecule. We point out that this method is the core of a recently introduced, semiclassical pseudodifferential calculus adapted to the treatment of Coulomb singularities in molecular systems, namely the twisted h-pseudodifferential calculus (h being the semiclassical parameter). This calculus is due to A. Martinez and V. Sordoni in [MS].

As one can see in [KMSW, MS], the above method works in a larger framework. So do Theorem 1.1 and our proof. For instance, we do not need the positivity of the charges Z_k, the fact that $E < E_0$, and the precise form of the Coulomb interaction. We do not use the self-adjointness (or the symmetry) of the operator H. We could replace in (1.1) each $-\Delta_{x_j}$ by $|i\nabla_{x_j} + A(x)|^2$, where A is a suitable, analytic, magnetic vector potential. We could also add a suitable, analytic exterior potential.

Let us now compare our proof with the one in [FHHS1, FHHS2]. Here we only use (almost) classical arguments of elliptic regularity. In [FHHS1, FHHS2], the elliptic regularity is essentially replaced by some Hölder continuity regularity result on ψ. The authors introduced an adapted, smartly chosen variable w.r.t. which they can derivate ψ. Here the x-dependent change of variables produces regularity with respect to x. As external tools, we only exploit basic notions of pseudodifferential calculus, the rest being elementary. In [FHHS1, FHHS2], a general, involved regularity result from the literature on "PDE" is an important ingredient of the arguments. We believe that, in spirit, the two proofs are similar. The shortness and the relative simplicity of the new proof is due to the clever method borrowed from [KMSW], which transforms the singular potential V_1 in an analytic function with values in $\mathcal{B}$.

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2 Details of the proof.

Here we complete the proof of Theorem 1.1, sketched in Section 1.

Notation and basic facts. For a function $f : \mathbb{R}^d \times \mathbb{R}^n \ni (x,y) \mapsto f(x,y) \in \mathbb{R}^p$, let $d_x f$ be the total derivative of f w.r.t. x, by $\partial_x^\alpha f$ with $\alpha \in \mathbb{N}^d$ the corresponding partial derivatives. For $\alpha \in \mathbb{N}^d$ and $x \in \mathbb{R}^d$, $D_x^\alpha := (-i\partial_x)^\alpha := (-i\partial_{x_1})^{\alpha_1} \cdots (-i\partial_{x_d})^{\alpha_d}$, $D_x = -i\nabla_x$, $x^\alpha := x_1^{\alpha_1} \cdots x_d^{\alpha_d}$, $|\alpha| := \alpha_1 + \cdots + \alpha_d$, $\alpha! := (\alpha_1!) \cdots (\alpha_d!)$, $|x|^2 = x_1^2 + \cdots + x_d^2$, and $\langle x \rangle := (1 + |x|^2)^{1/2}$. If $\mathcal{A}$ is a Banach space and O an open subset of $\mathbb{R}^d$, we denote by $C_c^\infty(O; \mathcal{A})$ (resp. $C_b^\infty(O; \mathcal{A})$, resp. $C^\omega(O; \mathcal{A})$) the space of functions from O to $\mathcal{A}$ which are smooth with compact support (resp. smooth with bounded derivatives, resp. analytic). Let $\mathcal{D}'(O; \mathcal{A})$ denotes the topological dual of $C_c^\infty(O; \mathcal{A})$. We use the traditional notation $W^{k,2}(O; \mathcal{A})$ for the Sobolev spaces of $\mathrm{L}^2(O; \mathcal{A})$-functions with k derivatives in $\mathrm{L}^2(O; \mathcal{A})$ when $k \in \mathbb{N}$ and for the dual of $W^{-k,2}(O; \mathcal{A})$ when $-k \in \mathbb{N}$. If $\mathcal{A}'$ is another Banach space, we denote by $\mathcal{L}(\mathcal{A}; \mathcal{A}')$ the space of the continuous linear maps from $\mathcal{A}$ to $\mathcal{A}'$ and set $\mathcal{L}(\mathcal{A}) = \mathcal{L}(\mathcal{A}; \mathcal{A})$. For $A \in \mathcal{L}(\mathcal{A})$ with finite dimensional $\mathcal{A}$, A^{T} denotes the transpose of A and $\mathrm{Det}A$ its determinant. By the Sobolev injections,

$$\bigcap_{k \in \mathbb{N}} W^{k,2}(O; \mathcal{A}) \ \subset \ C^\infty(O; \mathcal{A}) \, . \tag{2.1}$$

Denoting by $\| \cdot \|_{\mathcal{A}}$ the norm of $\mathcal{A}$, it is well-known (cf. [H3]) that a function $u \in C^\infty(O; \mathcal{A})$ is analytic if and only if, for any compact $K \subset O$, there exists some $C > 0$ such that

$$\forall \alpha \in \mathbb{N}^d \, , \quad \sup_{x \in K} \left\| (D_x^\alpha u)(x) \right\|_{\mathcal{A}} \ \leq \ C^{|\alpha|+1} \cdot (\alpha!) \, . \tag{2.2}$$

For convenience, we set $\mathcal{W}_k = \mathrm{W}^{k,2}(\mathbb{R}^{3(N-1)})$, for $k \in \mathbb{N}$. Recall that $\mathcal{B} = \mathcal{L}(\mathcal{W}_2; \mathcal{W}_0)$. Let $\mathcal{B}' = \mathcal{L}(\mathcal{W}_0; \mathcal{W}_2)$, $\mathcal{B}_0 = \mathcal{L}(\mathcal{W}_0)$, and $\mathcal{B}_2 = \mathcal{L}(\mathcal{W}_2)$.

Construction of U_{x_0} (see [KMSW, MS]). Let $\tau \in C_c^\infty(\mathbb{R}^3; \mathbb{R})$ such that $\tau(x_0) = 1$ and $\tau = 0$ near R_k, for all $k \in \{1; \cdots ; L\}$. For $x, s \in \mathbb{R}^3$, we set $f(x,s) = s + \tau(s)(x - x_0)$.

Notice that

$$\forall (x;s)\in(\mathbb{R}^3)^2\,,\ f(x,x_0)=x \text{ and } f(x,s)=s \text{ if } s\notin \operatorname{supp}\tau\,. \tag{2.3}$$

Since $(d_sf)(x,s).s' = s' + \langle\nabla\tau(s), s'\rangle(x-x_0)$, we can choose a small enough, relatively compact neighborhood Ω of x_0 such that

$$\forall x\in\Omega\,,\quad \sup_s \|(d_sf)(x,s) - \mathrm{I}_3\|_{\mathcal{L}(\mathbb{R}^3)} \le 1/2\,, \tag{2.4}$$

I_3 being the identity matrix of $\mathcal{L}(\mathbb{R}^3)$. Thus, for $x\in\Omega$, $f(x,\cdot)$ is a C^∞-diffeomorphism on $\mathbb{R}^3$ and we denote by $g(x,\cdot)$ its inverse. By (2.4) and a Neumann expansion in $\mathcal{L}(\mathbb{R}^3)$,

$$\Big((d_sf)(x,s)\Big)^{-1} = \mathrm{I}_3 + \Big(\sum_{n=1}^{\infty}\Big(-\langle\nabla\tau(s),(x-x_0)\rangle\Big)^{n-1}\Big)\langle\nabla\tau(s),\cdot\rangle(x-x_0)\,,$$

for $(x,s)\in\Omega\times\mathbb{R}^3$. Notice that the power series converges uniformly w.r.t. s. This is still true for the series of the derivatives ∂_s^β, for $\beta\in\mathbb{N}^3$. Since

$$(d_sg)(x,f(x,s)) = \Big((d_sf)(x,s)\Big)^{-1} \text{ and } (d_xg)(x,f(x,s)) = -(d_sg)(x,f(x,s))\cdot(d_xf)(x,s),$$

we see by induction that, for $\alpha,\beta\in\mathbb{N}^3$,

$$\Big(\partial_x^\alpha\partial_s^\beta g\Big)(x,f(x,s)) = \sum_{\gamma\in\mathbb{N}^3}(x-x_0)^\gamma a_{\alpha\beta\gamma}(s) \tag{2.5}$$

on $\Omega\times\mathbb{R}^3$, with coefficients $a_{\alpha\beta\gamma}\in C^\infty(\mathbb{R}^3;\mathcal{L}(\mathbb{R}^3))$. For $\alpha=\beta=0$, this follows from $g(x,f(x,s))=s$. Notice that, except for $(\alpha,\beta,\gamma)=(0,0,0)$ and for $|\beta|=1$ with $(\alpha,\gamma)=(0,0)$, the coefficients $a_{\alpha\beta\gamma}$ are supported in the compact support of τ.
For $x\in\mathbb{R}^3$ and $y=(y_2,\cdots,y_N)\in\mathbb{R}^{3(N-1)}$, let $F(x,y)=(f(x,y_2),\cdots,f(x,y_N))$. For $x\in\Omega$, $F(x,\cdot)$ is a C^∞-diffeomorphism on $\mathbb{R}^{3(N-1)}$ satisfying the following properties: There exists $C_0>0$ such that, for all $\alpha\in\mathbb{N}^3$, for all $x\in\Omega$, for all $y,y'\in\mathbb{R}^{3(N-1)}$,

$$C_0^{-1}|y-y'| \le |F(x,y)-F(x,y')| \le C_0|y-y'|\,, \tag{2.6}$$

$$|\partial_x^\alpha F(x,y)-\partial_x^\alpha F(x,y')| \le C_0|y-y'|\,, \tag{2.7}$$

$$\text{and, for } |\alpha|\ge 1\,,\ |\partial_x^\alpha F(x,y)| \le C_0\,. \tag{2.8}$$

For $x\in\Omega$, denote by $G(x,\cdot)$ the inverse diffeomorphism of $F(x,\cdot)$. By (2.5), the functions

$$\Omega\times\mathbb{R}^{3(N-1)}\ni(x,y) \mapsto \Big(\partial_x^\alpha\partial_y^\beta G\Big)(x,F(x,y))\,,$$

for $(\alpha,\beta)\in\mathbb{N}^3\times\mathbb{N}^{3(N-1)}$, are also given by a power series in x with smooth coefficients in y. Given $x\in\Omega$, let $U_{x_0}(x)$ be the unitary operator on $\mathrm{L}^2(\mathbb{R}^{3(N-1)})$ defined by

$$(U_{x_0}(x)\theta)(y) = |\mathrm{Det}(d_yF)(x,y)|^{1/2}\theta(F(x,y))\,.$$

Computation of the terms in (1.8) **(cf. [KMSW, MS]).** Consider the functions

$$
\begin{aligned}
\Omega \ni x \mapsto J_1(x,\cdot) &\in C_c^\infty\Big(\mathbb{R}^{3(N-1)}; \mathcal{L}(\mathbb{R}^{3(N-1)}; \mathbb{R}^3)\Big)\,,\\
\Omega \ni x \mapsto J_2(x,\cdot) &\in C_c^\infty(\mathbb{R}^{3(N-1)}; \mathbb{R}^3)\,,\\
\Omega \ni x \mapsto J_3(x,\cdot) &\in C_b^\infty\Big(\mathbb{R}^{3(N-1)}; \mathcal{L}(\mathbb{R}^{3(N-1)})\Big)\,,\\
\Omega \ni x \mapsto J_4(x,\cdot) &\in C_c^\infty(\mathbb{R}^{3(N-1)}; \mathbb{R}^{3(N-1)})\,,\\
\text{defined by }\ J_1(x,y) &= (d_xG(x,y'))^{\mathrm{T}}\Big(x, y' = F(x,y)\Big)\,,\\
J_2(x,y) &= \Big|\mathrm{Det}\, d_yF(x,y)\Big|^{1/2} D_x\Big(\Big|\mathrm{Det}\, d_{y'}G(x,y')\Big|^{1/2}\Big)\Big|_{y'=F(x,y)}\,,\\
J_3(x,y) &= (d_{y'}G(x,y'))^{\mathrm{T}}\Big(x, y' = F(x,y)\Big)\,,\\
J_4(x,y) &= \Big|\mathrm{Det}\, d_yF(x,y)\Big|^{1/2} D_{y'}\Big(\Big|\mathrm{Det}\, d_{y'}G(x,y')\Big|^{1/2}\Big)\Big|_{y'=F(x,y)}\,.
\end{aligned}
$$

Actually, the support of $J_k(x,\cdot)$, for $k \neq 3$, is contained in the x-independent, compact support of the function τ (cf. (2.3)). So do also the supports of the derivatives $\partial_x^\alpha \partial_y^\beta J_3$ of J_3, for $|\alpha| + |\beta| > 0$. Thanks to (2.5), the $J_k(\cdot,y)$'s can also be written as a power series in x with smooth coefficients depending on y. Now

$$U_{x_0}\nabla_x U_{x_0}^{-1} \;=\; \nabla_x \,+\, J_1\nabla_y \,+\, J_2 \quad\text{and}\quad U_{x_0}\nabla_{x'} U_{x_0}^{-1} \;=\; J_3\nabla_y \,+\, J_4\,. \tag{2.9}$$

In particular, $U_{x_0}(x)$ preserves $\mathrm{W}^{2,2}(\mathbb{R}^{3(N-1)})$, for all $x \in \Omega$. Furthermore,

$$P_0 \;=\; U_{x_0}\Big(-\Delta_x \,-\, \Delta_{x'}\Big)U_{x_0}^{-1} \;=\; -\Delta_x \,+\, \mathcal{J}_1(x;y;D_y)\cdot D_x \,+\, \mathcal{J}_2(x;y;D_y)\,, \tag{2.10}$$

where $\mathcal{J}_2(x;y;D_y)$ is a scalar differential operator of order 2 and $\mathcal{J}_1(x;y;D_y)$ is a column vector of 3 scalar differential operators of order 1. More precisely, the coefficients of $\mathcal{J}_1(x;y;D_y)$ and of $\mathcal{J}_2(x;y;D_y) + \Delta_y$ are compactly supported, uniformly w.r.t. x. In particular, these scalar differential operators belong to $\mathcal{B}$. By (2.5), they are given on Ω by a power series of x with coefficients in $\mathcal{B}$ and therefore are analytic functions on Ω with values in $\mathcal{B}$ (cf. [H3]). Next, we look at W defined in (1.7). By (2.3), for $j \neq j'$ in $\{2; \cdots; N\}$, for $k \in \{1; \cdots; L\}$, and for $x \in \Omega$,

$$
\begin{aligned}
U_{x_0}(x)\Big(|x - x_j|^{-1}\Big)U_{x_0}^{-1}(x) &= |f(x;x_0) - f(x;y_j)|^{-1}\,, &(2.11)\\
U_{x_0}(x)\Big(|x_j - R_k|^{-1}\Big)U_{x_0}^{-1}(x) &= |f(x;y_j) - f(x;R_k)|^{-1}\,, &(2.12)\\
U_{x_0}(x)\Big(|x_j - x_{j'}|^{-1}\Big)U_{x_0}^{-1}(x) &= |f(x;y_j) - f(x;y_{j'})|^{-1}\,. &(2.13)
\end{aligned}
$$

Lemma 2.1. *The potential W in* (1.7) *is an analytic function from Ω to $\mathcal{B}$.*

Proof: We prove the stronger result: W is analytic from Ω to $\tilde{\mathcal{B}} := \mathcal{L}(\mathcal{W}_1; \mathcal{W}_0)$. Notice that W is a sum of terms of the form (2.11), (2.12), and (2.13). We show the regularity of (2.11). Similar arguments apply for the other terms. We first recall the arguments in [KMSW], which proves the C^∞ regularity.
Using the fact that $d_x(f(x,x_0) - f(x,y_j))$ does not depend on x,

$$D_x^\alpha\Big(|f(x,x_0) - f(x,y_j)|^{-1}\Big) \;=\; (\tau(x_0) - \tau(y_j))^{|\alpha|}\,\Big(D^\alpha \frac{1}{|\cdot|}\Big)(f(x,x_0) - f(x,y_j))$$

for $x_0 \neq y_j$. By (2.6) and (2.7), we see that, for all $\alpha \in \mathbb{N}^3$ and for $x_0 \neq y_j$,

$$\begin{aligned}\Big|D_x^\alpha\Big(|f(x,x_0)-f(x,y_j)|^{-1}\Big)\Big| &\leq C_0^{2|\alpha|}|f(x,x_0)-f(x,y_j)|^{|\alpha|}\Big|D^\alpha\frac{1}{|\cdot|}\Big|(f(x,x_0)-f(x,y_j))\\ &\leq C_0^{2|\alpha|}C(\alpha!)\cdot|f(x,x_0)-f(x,y_j)|^{-1}\,,\end{aligned}$$

thanks to

$$\forall\alpha\in\mathbb{N}^3\,,\ \exists C>0\,,\ \forall y\in\mathbb{R}^3\setminus\{0\}\,,\quad \Big|D^\alpha\frac{1}{|\cdot|}\Big|(y)\ \leq\ \frac{C(\alpha!)}{|y|^{|\alpha|+1}}\,. \tag{2.14}$$

Since $|x'|^{-1}$ is $\nabla_{x'}$-bounded by (1.2) and since $U(x_0)(x)$ is unitary, $|f(x,x_0)-f(x,y_j)|^{-1}$ is $U(x_0)(x)\nabla_{x'}(U(x_0)(x))^{-1}$-bounded with the same bounds. But, by (2.9),

$$U(x_0)(x)\nabla_{x'}U(x_0)(x)^{-1}\Big(-\Delta_y\,+\,1\Big)^{-1/2}$$

is uniformly bounded w.r.t. x. Thus

$$\Big\|D_x^\alpha\Big(|f(x,x_0)-f(x,y_j)|^{-1}\Big)\Big\|_{\tilde{\mathcal{B}}}\ \leq\ C_1C_0^{2|\alpha|}C(\alpha!)\,, \tag{2.15}$$

uniformly w.r.t. $\alpha\in\mathbb{N}^3$ and $x\in\Omega$. Therefore W is a distribution on Ω the derivatives of which belong to $\mathrm{L}^\infty(\Omega)$, thus to $\mathrm{L}^2(\Omega)$. By (2.1), W is smooth.
To show the analyticity of W, we just add the following improvement of (2.14), that we prove in appendix below. There exists $K>0$ such that

$$\forall\alpha\in\mathbb{N}^3\,,\ \forall y\in\mathbb{R}^3\setminus\{0\}\,,\quad \Big|D^\alpha\frac{1}{|\cdot|}\Big|(y)\ \leq\ \frac{K^{|\alpha|+1}(\alpha!)}{|y|^{|\alpha|+1}}\,. \tag{2.16}$$

Now the l.h.s. of (2.15) is, for $\alpha\in\mathbb{N}^3$ and $x\in\Omega$, bounded above by $C_1C_0^{2|\alpha|}K^{|\alpha|+1}(\alpha!)\leq K_1^{|\alpha|+1}(\alpha!)$, for some $K_1>0$. This yields the result by (2.2). □

Smoothness. Now we view (1.8) as an "elliptic" differential equation w.r.t. x with coefficients in $\mathcal{B}$ and want to follow usual arguments of elliptic regularity to prove the smoothness of φ. In fact, we shall use the basic pseudodifferential calculus in [H2] (p. 65-75). Since the symbol of P_0+W+V_0 takes its values in $\mathcal{B}$, which is not an algebra of operators, we verify the validity of the basic calculus in our situation.
By (2.10), P_0+W+V_0 is a differential operator in the x variable the symbol of which

$$p(x;\xi)\ =\ |\xi|^2\,+\,\mathcal{J}_1(x;y;D_y)\cdot\xi\,+\,\mathcal{J}_2(x;y;D_y)\,+\,W(x)\,+\,V_0(x) \tag{2.17}$$

and belongs to the Hörmander class $S(m^2,g;\mathcal{B})$ on $\Omega\times\mathbb{R}^3$ with values in $\mathcal{B}$, where

$$m(x;\xi)\ =\ \Big(|\xi|^2\,+\,1\Big)^{1/2}\quad\text{and}\quad g\ =\ dx^2\,+\,d\xi^2/\langle\xi\rangle^2\,.$$

We can check that the basic calculus of [H2] actually works with the symbols classes $S(m',g;\mathcal{B})$, $S(m',g;\mathcal{B}')$, $S(m',g;\mathcal{B}_0)$, and $S(m',g;\mathcal{B}_2)$, for any (scalar) order function m' on $\Omega\times\mathbb{R}^3$. In particular, we have the following properties: We can give a sense to asymptotic sums of symbols in $S(m',g;\mathcal{A})$, for $\mathcal{A}\in\{\mathcal{B},\mathcal{B}',\mathcal{B}_0,\mathcal{B}_2\}$. The composition of operators $a_1(x, D_x)a_2(x, D_x) = b(x, D_x)$ with $b \in S(m', g; \mathcal{B}_0)$ if $a_1, a_2 \in S(m', g; \mathcal{B}_0)$ and if $a_1 \in S(m', g; \mathcal{B})$ and $a_2 \in S(m', g; \mathcal{B}')$, also with $b \in S(m', g; \mathcal{B}_2)$ if $a_1, a_2 \in S(m', g; \mathcal{B}_2)$ and if $a_1 \in S(m', g; \mathcal{B}')$ and $a_2 \in S(m', g; \mathcal{B})$. The adjoint of an operator $b(x, D_x)$ is $b^*(x, D_x)$ with $b^* \in S(m', g; \mathcal{B}_j)$ if $b \in S(m', g; \mathcal{B}_j)$, $b^* \in S(m', g; \mathcal{B}')$ if $b \in S(m', g; \mathcal{B})$, and $b^* \in S(m', g; \mathcal{B})$ if $b \in S(m', g; \mathcal{B}')$. For $\mathcal{A} \in \{\mathcal{B}, \mathcal{B}', \mathcal{B}_0, \mathcal{B}_2\}$, $k \in \mathbb{Z}$, and $a \in S(m^k, g; \mathcal{A})$,

$$\forall \ell \in \mathbb{Z}\,,\ a(x, D_x) \in \mathcal{L}\Big(\mathrm{W}^{\ell,2}(\Omega; \mathcal{A}); \mathrm{W}^{\ell-k,2}(\Omega; \mathcal{A})\Big)\,. \tag{2.18}$$

By the proof of Lemma 2.1, $W(x)(-\Delta_y + 1)^{-1/2}$ is uniformly bounded on Ω. By the properties of $\mathcal{J}_1$ and $\mathcal{J}_2$, so are $\xi \cdot \mathcal{J}_1(x; y; D_y)(|\xi|^2 - \Delta_y + 1)^{-1/2}$ and $(\mathcal{J}_2(x; y; D_y) + \Delta_y)(-\Delta_y + 1)^{-1/2}$ on $\Omega \times \mathbb{R}^3$. Thus, we can find $a \in (0; 1)$ and $b \in \mathbb{R}$ such that, for all $(x, \xi) \in \Omega \times \mathbb{R}^3$, for all $u \in \mathcal{W}_2$,

$$\begin{aligned} \|Tu\|_{\mathcal{W}_0} &\leq a\|(|\xi|^2 - \Delta_y + 1)u\|_{\mathcal{W}_0} + b\|u\|_{\mathcal{W}_0} \\ \text{with } T &= \xi \cdot \mathcal{J}_1(x; y; D_y) + (\mathcal{J}_2(x; y; D_y) + \Delta_y) + W(x) + V_0(x)\,. \end{aligned}$$

By Theorem 4.11, p. 291 in [K], there exists $C > 0$ such that, for all $(x, \xi) \in \Omega \times \mathbb{R}^3$, $p(x, \xi)$ is bounded below by $-C + 1$. In particular, $(C + p)^{-1}$ is a well-defined symbol in $S(m^{-2}, g; \mathcal{B}')$ on $\Omega \times \mathbb{R}^3$ (this is the "ellipticity" we use).
By composition, $(C + p)^{-1}(x, D_x) \cdot (p + C)(x, D_x) = 1 - q(x, D_x)$ with $q \in S(m^{-1}, g; \mathcal{B}_2)$. Defining the symbols q_k in $S(m^{-k}, g; \mathcal{B}')$ by $q_k(x, D_x) = q(x, D_x)^k \cdot (C + p)^{-1}(x, D_x)$ and denoting by q_∞ an asymptotic sum of the symbols q_k, we have

$$Q(P_0 + W + V_0 + C) = 1 + R \quad \text{with} \tag{2.19}$$

$$Q := q_\infty(x, D_x) \in \mathcal{L}\Big(\mathrm{W}^{k,2}(\Omega; \mathcal{B}'); \mathrm{W}^{k+2,2}(\Omega; \mathcal{B}')\Big)\,, \tag{2.20}$$

$$R \in \mathcal{L}\Big(\mathrm{W}^{k,2}(\Omega; \mathcal{B}_2); \mathrm{W}^{k+\ell,2}(\Omega; \mathcal{B}_2)\Big)\,, \tag{2.21}$$

for all $k, \ell \in \mathbb{N}$ (cf. [H2]).
Starting with $\varphi \in \mathrm{W}^{0,2}(\Omega; \mathcal{W}_2)$ and applying Q to (1.8), we see that $\varphi = (E + C)Q\varphi - R\varphi$ and actually belongs to $\mathrm{W}^{2,2}(\Omega; \mathcal{W}_2)$, by (2.19), (2.20), and (2.21). By induction and by (2.1), we get that $\varphi \in C^\infty(\Omega; \mathcal{W}_2)$. We have recovered the result in [FHHS1]. Note that, to get it, we need neither the refined bounds (2.16) nor the power series mentioned above but just use the fact that the functions f, g, F, G are smooth w.r.t. x.

Analyticity. To show that $\varphi \in C^\omega(\Omega; \mathcal{W}_2)$, we adapt the proof of Theorem 7.5.1 in [H1] for equation (1.8). So we view the latter as $P\varphi = 0$ where $P = \sum_{|\alpha| \leq 2} a_\alpha D_x^\alpha$ with analytic coefficients $a_\alpha \in \mathcal{B}$ (cf. Lemma 2.1, (1.4), and (2.10)). Applying D_x^α to (2.19) with $|\alpha| \leq 2$ and using (2.20) and (2.21), we find $C > 0$ such that, for all $v \in C_c^\infty(\Omega; \mathcal{W}_2)$ and $\alpha \in \mathbb{N}^3$,

$$|\alpha| \leq 2 \implies \|D_x^\alpha v\|_{\mathrm{L}^2(\Omega; \mathcal{W}_2)} \leq C\|Pv\|_{\mathrm{L}^2(\Omega; \mathcal{W}_0)} + C\|v\|_{\mathrm{L}^2(\Omega; \mathcal{W}_2)}\,. \tag{2.22}$$

For $\epsilon > 0$, let $\Omega_\epsilon := \{x \in \Omega;\ d(x; \mathbb{R}^3 \setminus \Omega) > \epsilon\}$ and, for $r \in \mathbb{N}$, denote the $\mathrm{L}^2(\Omega_\epsilon; \mathcal{W}_r)$-norm of v by $N_\epsilon^r(v)$. As in [H1] (Lemma 7.5.1), we use an appropriate cut-off function, Leibniz' formula, and (2.22), to find $C > 0$ such that, for all $v \in C_c^\infty(\Omega; \mathcal{W}_2)$, for all $\epsilon, \epsilon_1 > 0$, for all $\alpha \in \mathbb{N}^3$ such that $|\alpha| \leq 2$,

$$\epsilon^{|\alpha|} N_{\epsilon+\epsilon_1}^2\Big(D_x^\alpha v\Big) \leq C\epsilon^2 N_{\epsilon_1}^0\Big(Pv\Big) + C \sum_{|\alpha'| < 2} \epsilon^{|\alpha'|} N_{\epsilon_1}^2\Big(D_x^{\alpha'} v\Big)\,. \tag{2.23}$$

We used the fact that (2.23) holds true for ϵ large enough since the l.h.s. is zero. Next we show that there exists $B > 0$ such that, for all $\epsilon > 0$, $j \in \mathbb{N}^*$, and $\alpha \in \mathbb{N}^3$,

$$|\alpha| < 2 + j \implies \epsilon^{|\alpha|} N_{j\epsilon}^2 \Big(D_x^\alpha \varphi \Big) \;\leq\; B^{|\alpha|+1} \,. \tag{2.24}$$

This is done by induction on j following the arguments in [H1]. As explained in [H1], $\varphi \in C^\omega(\Omega; \mathcal{W}_2)$ follows from (2.24) and (2.2).

A Appendix

Using Cauchy integral formula for analytic functions in several variables (cf. [H3]), we prove here the following extension of (2.16). For $d \in \mathbb{N}^*$, there exists $K > 0$ such that

$$\forall \alpha \in \mathbb{N}^d \,,\, \forall y \in \mathbb{R}^d \setminus \{0\} \,, \quad \Big| D^\alpha \frac{1}{|\cdot|} \Big| (y) \;\leq\; \frac{K^{|\alpha|+1} (\alpha!)}{|y|^{|\alpha|+1}} \,. \tag{A.1}$$

In dimension $d = 1$, one can show (A.1) with $K = 1$ by induction. To treat the general case, we use Cauchy inequalities for an appropriate analytic function.
Let $\sqrt{\cdot}$ denote the analytic branch of the square root that is defined on $\mathbb{C} \setminus \mathbb{R}^-$. Take $y \in \mathbb{R}^d \setminus \{0\}$. On the polydisc

$$\mathcal{D} \;=\; \Big\{ z = (z_1, \cdots, z_d) \in \mathbb{C}^d \,; \forall j \,,\, |z_j| < |y|/(4\sqrt{d}) \Big\} \,,\, \Re \sum_{j=1}^d (y_j + z_j)^2 \;\geq\; (7/16)|y|^2 \;>\; 0 \,.$$

Thus the function $u : \mathcal{D} \longrightarrow \mathbb{C}$ given by

$$u(z) \;=\; \frac{1}{\sqrt{\sum_{j=1}^d (y_j + z_j)^2}}$$

is well defined and analytic. Its modulus is bounded above by $|y|^{-1} 4/\sqrt{7}$. By Cauchy inequalities (cf. Theorem 2.2.7, p. 27, in [H3]),

$$\forall \alpha \in \mathbb{N}^d \,,\, |\partial_z^\alpha u(0)| \;\leq\; \frac{4}{|y|\sqrt{7}} \cdot (\alpha!) \cdot \Big(|y|/(4\sqrt{d}) \Big)^{-|\alpha|} \;\leq\; \frac{(4\sqrt{d})^{|\alpha|+1} (\alpha!)}{|y|^{|\alpha|+1}} \,. \tag{A.2}$$

Here $\partial_{z_j} := (1/2)(\partial_{\Re z_j} + i \partial_{\Im z_j})$ but it can be replaced by $\partial_{\Re z_j}$ in the formula since u is analytic. Now (A.1) follows from (A.2) since, for all α,

$$\Big(\partial_{\Re z}^\alpha u \Big)(0) \;=\; i^{|\alpha|} \Big(D^\alpha \frac{1}{|\cdot|} \Big)(y) \,.$$

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