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# 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 been 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 and it was not an easy task. 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 with  $N \geq 2$  and  $L$  fixed nuclei. While the distinct vectors  $R_1, \dots, R_L \in \mathbb{R}^3$  denote the positions of the nuclei, the positions of the electrons are given by  $x_1, \dots, x_N \in \mathbb{R}^3$ . The charges of the nuclei are given by the positive  $Z_1, \dots, Z_L$  and the electronic charge is  $-1$ . In this picture, the Hamiltonian of the system is

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

$$+ \sum_{1 \leq k < k' \leq L} \frac{Z_k Z_{k'}}{|R_k - R_{k'}|},$$

where  $-\Delta_{x_j}$  stands for the Laplacian in the variable  $x_j$ . We denote the last term in (1.1) by  $E_0$ . Setting  $\Delta := \sum_{j=1}^N \Delta_{x_j}$ , the potential  $V$  of the system is the multiplication operator defined by  $H = -\Delta + V$ . Since the  $V$  is  $\Delta$ -bounded with relative bound 0 by Hardy inequality,  $H$  is self-adjoint on the domain of the Laplacian  $\Delta$ , namely  $W^{2,2}(\mathbb{R}^{3N})$  (see Kato's theorem in [RS], p. 166-167). Let  $\psi \in W^{2,2}(\mathbb{R}^{3N}) \setminus \{0\}$  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  $\psi$  is the following  $L^1(\mathbb{R}^3)$ -function

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

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

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

**Remark 1.2.** *In [FHHS1], it is proved that  $\rho$  is smooth on  $\mathbb{R}^3 \setminus \{R_1, \dots, R_L\}$ . 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 is given in Section 2. We consider the almost everywhere defined  $W^{2,2}$ -function

$$\tilde{\psi} : \mathbb{R}^3 \ni x \mapsto \psi(x, \cdot, \dots, \cdot) \in W^{2,2}(\mathbb{R}^{3(N-1)}) \quad (1.2)$$

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

$$V = V_0 + V_1 \quad \text{with} \quad V_0(x) = E_0 - \sum_{k=1}^L \frac{Z_k}{|x - R_k|}. \quad (1.3)$$

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

$$-\Delta_x \tilde{\psi} + Q(x) \tilde{\psi} = 0, \quad (1.4)$$

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

$$Q(x) = -\Delta_{x'} + V_0 - E + V_1 \quad \text{with} \quad \Delta_{x'} = \sum_{j=2}^N \Delta_{x_j}. \quad (1.5)$$

Considering (1.4) in a small enough neighbourhood  $\Omega$  of some  $x_0 \in \mathbb{R}^3 \setminus \{R_1, \dots, R_L\}$ , we pick from [KMSW] a  $x$ -dependent unitary operator  $U_{x_0}(x)$  on  $\mathbb{L}^2(\mathbb{R}^{3(N-1)})$  such that the map

$$W : \Omega \ni x \mapsto U_{x_0}(x) V_1(x) U_{x_0}(x)^{-1} \in \mathcal{B} \quad (1.6)$$

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 a differential operator in  $x$  with analytic, differential coefficients in  $\mathcal{B}$ , and, as differential operator in all variables, it is elliptic. Applying  $U_{x_0}$  to (1.4) and setting  $\varphi = U_{x_0} \tilde{\psi}$ , we obtain

$$(P_0 + W(x) + V_0(x) - E) \varphi = 0. \quad (1.7)$$

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

The main idea in the construction of the unitary operator  $U_{x_0}$  is to change, locally in  $x$ , the variables  $x_2, \dots, x_N$  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  $x_2, \dots, x_N$  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. Sordani 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 that, as function of all variables, the eigenfunction  $\psi \in \mathbb{W}^{2,2}(\mathbb{R}^{3N})$ . In [FHHS1, FHHS2], the authors used much more precise and involved regularity results on  $\psi$  and also its strong decay at infinity. 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.

This section is devoted to the completion of the proof of Theorem 1.1, sketched in Section 1. We first introduce some notation and recall some well-known, basic facts.

For a function  $f : \mathbb{R}^d \times \mathbb{R}^n \ni (x, y) \mapsto f(x, y) \in \mathbb{R}^p$ , we denote by  $d_x f$  the total derivative of  $f$  w.r.t.  $x$ , by  $\partial_x^\alpha f$  with  $\alpha \in \mathbb{N}^d$  the corresponding partial derivatives, and we set  $D_x^\alpha = -i\partial_x^\alpha$  and  $D_x = -i\nabla_x$ . For  $\alpha \in \mathbb{N}^d$  and  $x \in \mathbb{R}^d$ ,  $x^\alpha := x_1^{\alpha_1} \cdots x_d^{\alpha_d}$ ,  $|\alpha| := \alpha_1 + \cdots + \alpha_d$ . 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). We use the traditional notation  $W^{k,2}(O; \mathcal{A})$  for the Sobolev spaces of  $L^2(O; \mathcal{A})$ -functions with  $k$  derivatives in  $L^2(O; \mathcal{A})$ ,  $k \in \mathbb{N}$ . 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  $A \in \mathcal{L}(\mathcal{A})$ ,  $A^T$  denotes the transpose of  $A$  and  $\text{Det}A$  its determinant. By the Sobolev injections,

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

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  $K \subset O$ , one can find some constant  $C$  such that

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

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

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

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

$$\forall x \in \Omega, \quad \sup_s \|(d_s f)(x, s) - I_3\|_{\mathcal{L}(\mathbb{R}^3)} \leq 1/2, \quad (2.4)$$

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

$$\left( (d_s f)(x, s) \right)^{-1} = I_3 + \left( \sum_{n=1}^{\infty} \left( -\langle \nabla \tau(s), (x - x_0) \rangle \right)^{n-1} \right) \langle \nabla \tau(s), \cdot \rangle (x - x_0).$$

Notice that the power serie converges uniformly w.r.t.  $s$ . This is still true for the serie of the derivatives  $\partial_s^\beta$ , for  $\beta \in \mathbb{N}^3$ . Since

$$(d_s g)(x, f(x, s)) = \left( (d_s f)(x, s) \right)^{-1} \text{ and } (d_x g)(x, f(x, s)) = -(d_s g)(x, f(x, s)) \cdot (d_x f)(x, s),$$

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

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

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  $\tau$ .

For  $x \in \mathbb{R}^3$  and  $y = (y_2, \dots, y_N) \in \mathbb{R}^{3(N-1)}$ , let  $F(x, y) = (f(x, y_2), \dots, f(x, y_N))$ . For  $x \in \Omega$ ,  $F(x, \cdot)$  is a  $C^\infty$ -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  $y, y' \in \mathbb{R}^{3(N-1)}$ ,

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

$$|\partial_x^\alpha F(x, y) - \partial_x^\alpha F(x, y')| \leq C_0 |y - y'|, \quad (2.7)$$

$$\text{and, for } |\alpha| \geq 1, |\partial_x^\alpha F(x, y)| \leq C_0. \quad (2.8)$$

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

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

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

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

The conjugated terms in (1.7) has been computed in [KMSW, MS]. Consider the functions

$$\Omega \ni x \mapsto J_1(x, \cdot) \in C_c^\infty(\mathbb{R}^{3(N-1)}; \mathcal{L}(\mathbb{R}^{3(N-1)}; \mathbb{R}^3)),$$

$$\Omega \ni x \mapsto J_2(x, \cdot) \in C_c^\infty(\mathbb{R}^{3(N-1)}; \mathbb{R}^3),$$

$$\Omega \ni x \mapsto J_3(x, \cdot) \in C_b^\infty(\mathbb{R}^{3(N-1)}; \mathcal{L}(\mathbb{R}^{3(N-1)})),$$

$$\Omega \ni x \mapsto J_4(x, \cdot) \in C_c^\infty(\mathbb{R}^{3(N-1)}; \mathbb{R}^{3(N-1)}),$$

defined by

$$J_1(x, y) = (d_x G(x, y'))^T(x, y' = F(x, y)),$$

$$J_2(x, y) = \left| \text{Det } d_y F(x, y) \right|^{1/2} D_x \left( \left| \text{Det } d_{y'} G(x, y') \right|^{1/2} \right) \Big|_{y'=F(x, y)},$$

$$J_3(x, y) = (d_{y'} G(x, y'))^T(x, y' = F(x, y)),$$

$$J_4(x, y) = \left| \text{Det } d_y F(x, y) \right|^{1/2} D_{y'} \left( \left| \text{Det } d_{y'} G(x, y') \right|^{1/2} \right) \Big|_{y'=F(x, y)}.$$

Actually, the support of  $J_k(x, \cdot)$ , for  $k \neq 3$ , is contained in the  $x$ -independent, compact support of the function  $\tau$  (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 serie in  $x$  with smooth coefficients depending on  $y$ . Now

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

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

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

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 colonn 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  $\Omega$  by a power serie of  $x$  with coefficients in  $\mathcal{B}$  and therefore are analytic functions on  $\Omega$  with values in  $\mathcal{B}$  (cf. [H3]). Furthermore, one can check that (2.10) is an elliptic operator as differential operator in all variables, in the sense that its symbol  $p_0(x; \xi; y; \eta)$  does not vanish for  $(\xi; \eta) \neq (0; 0)$ . In fact,  $p_0$  belongs to the Hörmander class  $S(m, g)$  on  $\Omega \times \mathbb{R}^{3(N-1)}$ , where

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

Thus (see [H2] for instance) we can find two pseudodifferential operators  $P_1$  and  $R$  with symbols  $p_1, r \in S(m^{-1}, g)$  such that  $P_1 P_0 = I + R$  ( $I$  being the identity operator) and, for all  $(k, \ell) \in \mathbb{Z}^2$ ,

$$P_1, R \in \mathcal{L} \left( W^{k,2}(\Omega; W^{\ell,2}(\mathbb{R}^{3(N-1)})); W^{k+2,2}(\Omega; W^{\ell+2,2}(\mathbb{R}^{3(N-1)})) \right). \quad (2.11)$$

Next, we look at  $W$  defined in (1.6). For  $j, j' \in \{2; \dots; N\}$  with  $j \neq j'$ , for  $k \in \{1; \dots; L\}$ , for  $x \in \Omega$ ,

$$U_{x_0}(x) \left( |x - x_j|^{-1} \right) U_{x_0}^{-1}(x) = |f(x; x_0) - f(x; y_j)|^{-1}, \quad (2.12)$$

$$U_{x_0}(x) \left( |x_j - R_k|^{-1} \right) U_{x_0}^{-1}(x) = |f(x; y_j) - f(x; R_k)|^{-1}, \quad (2.13)$$

$$U_{x_0}(x) \left( |x_j - x_{j'}|^{-1} \right) U_{x_0}^{-1}(x) = |f(x; y_j) - f(x; y_{j'})|^{-1}. \quad (2.14)$$

**Lemma 2.1.** *The potential  $W$  in (1.6) is an analytic function from  $\Omega$  to  $\mathcal{B}$ .*

**Proof:** We follow the arguments in [KMSW] where the  $C^\infty$  regularity of  $W$  is already proved. We just add the following (known?) fact, that we prove in appendix below, to show the analyticity. There exists  $K > 0$  such that

$$\forall \alpha \in \mathbb{N}^3, \forall y \in \mathbb{R}^3 \setminus \{0\}, \quad \left| D^\alpha \frac{1}{|\cdot|} \right| (y) \leq \frac{K^{|\alpha|+1} (|\alpha|!)}{|y|^{|\alpha|+1}}. \quad (2.15)$$

Recall that  $W$  is a sum of terms of the form (2.12), (2.13), and (2.14). We show the regularity of (2.12). Similar arguments apply for the other terms.

Using the fact that  $d_x(f(x, x_0) - f(x, y_j))$  does not depend on  $x$ ,

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

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

$$\begin{aligned} D_x^\alpha \left( |f(x, x_0) - f(x, y_j)|^{-1} \right) &\leq C_0^{2|\alpha|} |f(x, x_0) - f(x, y_j)|^{|\alpha|} \left| D_x^\alpha \frac{1}{|\cdot|} \right| (f(x, x_0) - f(x, y_j)) \\ &\leq C_0^{2|\alpha|} K^{|\alpha|+1} (|\alpha|!) \cdot |f(x, x_0) - f(x, y_j)|^{-1}, \end{aligned}$$

thanks to (2.15). Since  $|x'|^{-1}$  is  $\Delta_{x'}$ -bounded and since  $U(x_0)(x)$  is unitary,  $|f(x, x_0) - f(x, y_j)|^{-1}$  is  $U(x_0)(x)\Delta_{x'}(U(x_0)(x))^{-1}$ -bounded with the same bounds. But, by (2.9),

$$U(x_0)(x)\Delta_{x'}U(x_0)(x)^{-1}(-\Delta_y + 1)^{-1}$$

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

$$\left\| D_x^\alpha \left( |f(x, x_0) - f(x, y_j)|^{-1} \right) \right\|_{\mathcal{B}} \leq C_1 C_0^{2|\alpha|} K^{|\alpha|+1} (|\alpha|!) \leq K_1^{|\alpha|+1} (|\alpha|!)$$

uniformly w.r.t.  $\alpha \in \mathbb{N}^3$  and  $x \in \Omega$ . This yields the result by (2.2).  $\square$

Now we come back to (1.7). Let  $\mathcal{W} := W^{2,2}(\mathbb{R}^{3(N-1)})$  and  $\mathcal{W}_0 := L^2(\mathbb{R}^{3(N-1)})$ . By (2.9) and the properties of the functions  $J$ 's,  $\varphi \in W^{2,2}(\Omega; \mathcal{W})$  since  $\psi \in W^{2,2}(\Omega; \mathcal{W})$  (cf. (1.2)). Applying  $P_1$  to (1.7), we get

$$R\varphi + P_1W\varphi + P_1(V_0 - E)\varphi = -\varphi. \quad (2.16)$$

By Lemma 2.1,  $W\varphi \in W^{2,2}(\Omega; \mathcal{W}_0)$ . By (2.11),  $P_1W\varphi \in W^{4,2}(\Omega; \mathcal{W})$ . Using again (2.11) and the smoothness of  $V_0$  on  $\Omega$ , we derive from (2.16) that  $\varphi \in W^{4,2}(\Omega; \mathcal{W})$ . Inserting this information in (2.16) again, we get in the same way that  $\varphi \in W^{6,2}(\Omega; \mathcal{W})$ . By induction, we show that  $\varphi \in W^{k,2}(\Omega; \mathcal{W})$ , for all  $k \in \mathbb{N}$ . Thus  $\varphi \in C^\infty(\Omega; \mathcal{W})$  by (2.1). We have recovered the result in [FHHS1]. Note that, to get it, we do not need the power series mentioned above but just use the fact that the functions  $f, g, F, G$  are smooth w.r.t.  $x$ .

To show that  $\varphi \in C^\omega(\Omega; \mathcal{W}_0)$ , we shall use the proof of Theorem 7.5.1 in [H1], the equation (7.5.1) there being replaced here by (1.7). So we view the latter as  $P(x; D_x)\varphi = 0$  where  $P(x; D_x)$  is a differential operator with analytic differential coefficients in  $\mathcal{B} = \mathcal{L}(\mathcal{W}; \mathcal{W}_0)$ . We first show that, for some  $C > 0$ ,

$$\begin{aligned} \forall v \in C_c^\infty(\Omega; \mathcal{W}), \forall \alpha \in \mathbb{N}^3 \text{ with } |\alpha| \leq 2, \\ \|D_x^\alpha v\|_{L^2(\Omega; \mathcal{W}_0)} \leq C \|P(x; D_x)v\|_{L^2(\Omega; \mathcal{W}_0)} + C \|v\|_{L^2(\Omega; \mathcal{W}_0)}. \end{aligned} \quad (2.17)$$

This is true if  $P(x; D_x)$  is replaced by  $-\Delta_x - \Delta_{x'}$ . Recall (2.10). Note that, for  $v \in C_c^\infty(\Omega; \mathcal{W})$ ,

$$\|(-\Delta_x - \Delta_{x'})v\|_{L^2(\Omega; \mathcal{W}_0)} = \|P_0U_{x_0}v\|_{L^2(\Omega; \mathcal{W}_0)} \quad \text{and} \quad \|v\|_{L^2(\Omega; \mathcal{W}_0)} = \|U_{x_0}v\|_{L^2(\Omega; \mathcal{W}_0)},$$



since, for all  $x \in \Omega$ ,  $U_{x_0}(x)$  is unitary on  $\mathcal{W}_0$  and preserves  $\mathcal{W}$ . This implies that (2.17) is true for  $\alpha = 0$  with  $P(x; D_x)$  replaced by  $P_0$ . Writing, for  $v \in C_c^\infty(\Omega; \mathcal{W})$  and  $|\alpha| \leq 2$ ,  $D_x^\alpha v = D_x^\alpha P_1 \cdot P_0 v - D_x^\alpha Rv$ , we see, thanks to (2.11), that (2.17) holds true with  $P(x; D_x)$  replaced by  $P_0$  and for  $|\alpha| \leq 2$ . Since  $V$  is  $(\Delta_x + \Delta_{x'})$ -bounded with relative bound 0,  $W$  is  $P_0$ -bounded with relative bound 0, by the properties of  $U_{x_0}$ . Thus (2.17) holds true.

Now we follow the proof of Theorem 7.5.1 in [H1], replacing the estimate (7.5.2) in [H1] by the weaker estimate (2.17) and keeping in mind that the coefficients  $a^\beta$  of our operator  $P(x; D_x)$  are differential operators in  $\mathcal{B}$ . One can check that (2.17) is sufficient to get the estimate (7.5.3) in [H1]. In the estimates (7.5.5) and (7.5.6) in [H1], we just have to replace the absolute value of each  $D_x^\alpha a^\beta$  by its norm in  $\mathcal{B}$  and use Lemma 2.1. Then the arguments in [H1] gives the desired result.

## A Appendix

Using the multidimensional Faà di Bruno formula (cf. [Ha] and [Fe] p. 222), we prove here the following estimate that generalizes (2.15) we used above. For  $d \in \mathbb{N}^*$ , there exists  $K > 0$  such that

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

In dimension one, it is elementary. We did not find in the litterature a reference for the multidimensional case.

We see the function  $|\cdot|^{-1}$  as the composition of  $f : (0; +\infty) \ni t \mapsto t^{1/2} \in \mathbb{R}$  with  $g : \mathbb{R}^d \setminus \{0\} \ni y \mapsto |y|^2 \in (0; +\infty)$ . Given  $\alpha \in \mathbb{N}^d$ , let  $n = |\alpha|$  and introduce  $n$  variables  $x_1, \dots, x_n$  such that, for  $j \in \{1, \dots, d\}$ ,

$$|\alpha_1| + \dots + |\alpha_{j-1}| < \ell \leq |\alpha_1| + \dots + |\alpha_j| \implies x_\ell = y_j.$$

By  $x_\ell = y_j$ , we mean that the variable  $x_\ell$  is actually (a copy of) the variable  $y_j$ . Thus

$$\left( D^\alpha \frac{1}{|\cdot|} \right)(y) = \left( D^\alpha (f \circ g) \right)(y) = \frac{\partial^n (f \circ g)}{\partial x_1 \dots \partial x_n}(y).$$

Now the multidimensional Faà di Bruno formula in [Ha] tells us that

$$\frac{\partial^n (f \circ g)}{\partial x_1 \dots \partial x_n}(y) = \sum_{\pi \in \mathcal{P}_n} f^{(|\pi|)}(g(y)) \cdot \prod_{b \in \pi} \frac{\partial^{|b|} g}{(\partial x)^b}(y). \quad (\text{A.2})$$

Here  $\mathcal{P}_n$  denotes the set of partitions of  $\{1, \dots, n\}$ ,  $|\pi|$  denotes the number of subsets of  $\{1, \dots, n\}$  present in the partition  $\pi$ , and  $|b|$  denotes the cardinal of a subset  $b$  of the partition  $\pi$ . For  $p \in \mathbb{N}$ ,  $f^{(p)}$  is the  $p$ -th derivative of  $f$  and, for  $b \in \pi$  with  $\pi \in \mathcal{P}_n$ ,  $\partial^{|b|} g / (\partial x)^b$  is the  $|b|$ -th derivative of  $g$  w.r.t. the variables  $x_j$ , for  $j \in b$ . Since  $g$  is a quadratic polynomial, we note that  $\partial^{|b|} g / (\partial x)^b$  vanishes if  $|b| > 2$ . Furthermore, for  $|b| \leq 2$ ,

$$\left| \frac{\partial^{|b|} g}{(\partial x)^b}(y) \right| \leq 2 |y|^{2-|b|}. \quad (\text{A.3})$$

Let  $\mathcal{Q}_n$  be the set of partitions  $\pi \in \mathcal{P}_n$  such that  $|\pi| \leq 2$ . Then

$$\mathcal{Q}_n = \bigsqcup_{p \in \{0, \dots, E(n/2)\}} \mathcal{Q}_{n,p} \quad \text{with} \quad \mathcal{Q}_{n,p} = \left\{ \pi \in \mathcal{Q}_n; |\{b \in \pi; |b| = 2\}| = p \right\},$$

where  $E(n/2)$  denotes the integer part of  $n/2$ . Denoting by

$$C_n^p = \frac{n!}{(p!) \cdot ((n-p)!)}$$

the binomial coefficients, the cardinal  $|\mathcal{Q}_{n,p}|$  of  $\mathcal{Q}_{n,p}$  is given by:

$$\frac{1}{p!} \cdot \prod_{k=0}^{p-1} C_{n-2k}^2 = \frac{n!}{((n-2p)! \cdot (p!))} \cdot \frac{1}{2^p}.$$

We also note that, for  $\pi \in \mathcal{Q}_{n,p}$ ,  $\pi$  contains  $p$  pairs thus  $n = (|\pi| - p) + 2p$  and  $|\pi| = n - p$ . So, we can rewrite (A.2) as

$$\frac{\partial^n (f \circ g)}{\partial x_1 \cdots \partial x_n}(y) = \sum_{p=0}^{E(n/2)} f^{(n-p)}(g(y)) \sum_{\pi \in \mathcal{Q}_{n,p}} \prod_{b \in \pi} \frac{\partial^{|b|} g}{(\partial x)^b}(y)$$

and, using (A.3), get the bound

$$\left| \left( D^\alpha \frac{1}{|\cdot|} \right) (y) \right| \leq \sum_{p=0}^{E(n/2)} \left| f^{(n-p)}(g(y)) \right| \cdot (2|y|)^{n-2p} \cdot 2^p \cdot |\mathcal{Q}_{n,p}|.$$

Since, for all  $k \in \mathbb{N}$  and all  $t > 0$ ,

$$f^{(k)}(t) = \frac{(-1)^k}{4^k} \cdot \frac{(2k)!}{k!} \cdot t^{-1/2-k},$$

$$\begin{aligned} \left| \left( D^\alpha \frac{1}{|\cdot|} \right) (y) \right| &\leq \sum_{p=0}^{E(n/2)} \frac{1}{2^{n-p}} \frac{(2n-2p)!}{(n-p)!} \cdot \frac{n!}{((n-2p)! \cdot (p!))} \frac{1}{2^p} \cdot \frac{1}{|y|^{n+1}} \\ &\leq \frac{n!}{2^n |y|^{n+1}} \sum_{p=0}^{E(n/2)} \frac{(2n-2p)!}{((n-p)!)^2} \cdot C_{n-p}^p. \end{aligned}$$

Using the Stirling formula:  $n! \sim e^{-n} n^n \sqrt{2\pi n}$ , we can find some constant  $L > 0$  such that, for all  $p \in \{0, \dots, E(n/2)\}$ ,

$$\frac{(2n-2p)!}{((n-p)!)^2} \leq L^n \quad \text{and} \quad C_{n-p}^p \leq L^n \cdot C_n^p.$$

This yields

$$\left| \left( D^\alpha \frac{1}{|\cdot|} \right) (y) \right| \leq \frac{L^{2n}}{2^n} \cdot \frac{n!}{|y|^{n+1}} \sum_{p=0}^{E(n/2)} C_n^p \leq \frac{L^{2n}}{2^n} \cdot \frac{n!}{|y|^{n+1}} \cdot 2^n = \frac{L^{2n} n!}{|y|^{n+1}},$$

which gives (A.1).

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