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On the analyticity  
of electronic reduced densities  
for molecules.

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**Abstract**

We consider an electronic bound state of the usual, non-relativistic, molecular Hamiltonian with Coulomb interactions and fixed nuclei. Away from appropriate collisions, we prove the real analyticity of all the reduced densities and density matrices, that are associated to this bound state. We provide a similar result for the associated reduced current density.

**Keywords:** Analytic elliptic regularity, molecular Hamiltonian, electronic reduced densities, electronic reduced density matrices, Coulomb potential, twisted differential calculus.

## 1 Introduction.

The notions of density and density matrices are quite old tools in the treatment of physical  $N$ -body problems. For instance, the Thomas-Fermi theory goes back to the year 1927 (cf. [Li]). Nowadays these tools do play a central rôle in one important approach of the  $N$ -body problem, namely the Density Functional Theory (DFT) (cf. [E, LiSe]). Regularity properties of the related reduced density and density matrices are useful to develop the DFT. For instance, the real analyticity of a density was recently used for Hohenberg-Kohn Theorems in [G]. The purpose of the present paper is to prove, in a large region of the configuration space, the real analyticity of all reduced densities and density matrices of a pure state for a molecular Hamiltonian with fixed nuclei.

We consider a molecule with  $N$  moving electrons, with  $N > 1$ , and  $L$  fixed nuclei, with  $L \geq 1$  (Born-Oppenheimer idealization). While the  $L$  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 respectively given by the positive  $Z_1, \dots, Z_L$  and the electronic charge is  $-1$ . In this picture, the Hamiltonian of the electronic system is

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

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

and  $-\Delta_{x_j}$  stands for the Laplacian in the variable  $x_j$ . Here we denote by  $|\cdot|$  the euclidian norm on  $\mathbb{R}^3$ . Setting  $\Delta := \sum_{j=1}^N \Delta_{x_j}$ , we define the potential  $V$  of the system as the multiplication operator satisfying  $H = -\Delta + V$ . Thanks to Hardy's inequality

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

one can show that  $V$  is  $\Delta$ -bounded with relative bound 0. Therefore the Hamiltonian  $H$  is self-adjoint on the domain of the Laplacian  $\Delta$ , namely  $W^{2,2}(\mathbb{R}^{3N})$  (see Kato's theorem in [RS2], p. 166-167).

From now on, we fix an electronic bound state  $\psi \in W^{2,2}(\mathbb{R}^{3N}) \setminus \{0\}$  such that, for some real  $E$ ,  $H\psi = E\psi$ . We point out (cf. [CFKS, FH, RS4]) that such a bound state exists at least if  $E \leq E_0$  and

$$N < L - 1 + 2 \sum_{k=1}^L Z_k.$$

Associated to that bound state  $\psi$ , we consider the following objects. Let  $k$  be an integer such that  $0 < k < N$ . Let  $\rho_k : (\mathbb{R}^3)^k \rightarrow \mathbb{R}$  be the almost everywhere defined,  $L^1(\mathbb{R}^{3k})$ -function given by, for  $\underline{x} = (x_1; \dots; x_k) \in \mathbb{R}^{3k}$ ,

$$\rho_k(\underline{x}) = \int_{\mathbb{R}^{3(N-k)}} |\psi(\underline{x}; y)|^2 dy. \quad (1.3)$$

Define  $\gamma_k : (\mathbb{R}^3)^{2k} \rightarrow \mathbb{C}$  as the almost everywhere defined function given by, for  $\underline{x} = (x_1; \dots; x_k) \in \mathbb{R}^{3k}$  and  $\underline{x}' = (x'_1; \dots; x'_k) \in \mathbb{R}^{3k}$ ,

$$\gamma_k(\underline{x}; \underline{x}') = \int_{\mathbb{R}^{3(N-k)}} \overline{\psi(\underline{x}; y)} \psi(\underline{x}'; y) dy. \quad (1.4)$$

Note that, almost everywhere,  $\rho_k(\underline{x}) = \gamma_k(\underline{x}; \underline{x})$ . It turns out that  $\gamma_k$  may be seen as the kernel (“Green function”) of a trace class operator (see [Le, LiSe]). We call the function  $\rho_k$  the *k-particle reduced density* and the kernel  $\gamma_k$  the *k-particle reduced density matrix*. When  $k = 1$ ,  $\rho := \rho_1$  is often simply called the (electronic) density. In this case, we also introduce the *reduced current density*, defined as the almost everywhere defined,  $L^1(\mathbb{R}^3)$ -function  $C : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  given by, for  $x \in \mathbb{R}^3$ , the following imaginary part

$$C(x) = \Im \int_{\mathbb{R}^{3(N-1)}} \overline{\nabla_x \psi(x; y)} \psi(x; y) dy. \quad (1.5)$$

From a physical point of view, the previous objects differ from the true physical ones by some prefactor (see [E, Le, LiSe]).

It is useful to introduce the following subsets of  $\mathbb{R}^{3k}$ . The closed set

$$\mathcal{C}_k := \{ \underline{x} = (x_1; \dots; x_k) \in \mathbb{R}^{3k}; \exists (j; j') \in ([1; k] \cap \mathbb{N})^2; j \neq j' \text{ and } x_j = x_{j'} \}$$

gathers all possible collisions between the first  $k$  electrons while the closed set

$$\mathcal{R}_k := \{ \underline{x} = (x_1; \dots; x_k) \in \mathbb{R}^{3k}; \exists j \in [1; k] \cap \mathbb{N}, \exists \ell \in [1; L] \cap \mathbb{N}; x_j = R_\ell \}$$

groups together all possible collisions of these  $k$  electrons with the nuclei. We set  $\mathcal{U}_k^{(1)} := \mathbb{R}^{3k} \setminus (\mathcal{C}_k \cup \mathcal{R}_k)$ , which is an open subset of  $\mathbb{R}^{3k}$ .

Now, we consider two sets of positions for the first  $k$  electrons and introduce the set of all possible collisions between positions of different sets, namely

$$\mathcal{C}_k^{(2)} := \left\{ \begin{array}{l} (\underline{x}; \underline{x}') \in (\mathbb{R}^{3k})^2; \underline{x} = (x_1; \dots; x_k), \underline{x}' = (x'_1; \dots; x'_k), \\ \exists (j; j') \in ([1; k] \cap \mathbb{N})^2; x_j = x'_{j'} \end{array} \right\}.$$

We introduce the open subset of  $(\mathbb{R}^{3k})^2$  defined by

$$\mathcal{U}_k^{(2)} = (\mathcal{U}_k^{(1)} \times \mathcal{U}_k^{(1)})^2 \setminus \mathcal{C}_k^{(2)}.$$

In the  $k = 1$  case, we note that  $\mathcal{C}_1 = \emptyset$ ,  $\mathcal{U}_1^{(1)} = \mathbb{R}^3 \setminus \{R_1, \dots, R_L\}$  and

$$\mathcal{U}_1^{(2)} = (\mathbb{R}^3 \setminus \{R_1, \dots, R_L\})^2 \setminus D,$$

where  $D = \{(x; x') \in (\mathbb{R}^3)^2; x = x'\}$  is the diagonal of  $(\mathbb{R}^3)^2$ . We have the following

**Theorem 1.1.** [FHHS1, FHHS2, J].

*The one-particle reduced density  $\rho := \rho_1$  is real analytic on  $\mathcal{U}_1^{(1)} = \mathbb{R}^3 \setminus \{R_1, \dots, R_L\}$ .*

The original proof was given in [FHHS1, FHHS2] and relies on a clever decomposition of the integration domain of the integral defining  $\rho$  into pieces, on which one can perform an appropriate change of variables. A different proof of Theorem 1.1 is provided in [J]. We refer to [FHHS2, FS] for a refined information on  $\rho$ . In [FHHS2], a similar analyticity result on  $\gamma_1$  was announced, without proof. More precisely, it was claimed there that  $\gamma_1$  should be real analytic on  $\mathcal{U}_1^{(1)} \times \mathcal{U}_1^{(1)}$ . Adapting the method of [FHHS2], a slightly weaker result on  $\gamma_1$  was proved in [HS], namely

**Theorem 1.2.** [HS].

*The one-particle reduced density matrix  $\gamma_1$  is real analytic on  $\mathcal{U}_1^{(2)}$ .*

Note that  $\mathcal{U}_1^{(2)}$  is indeed a strict subset of  $\mathcal{U}_1^{(1)} \times \mathcal{U}_1^{(1)}$ .

In [FHHS2], it was also announced without proof that the real analyticity of  $\rho_2$  should be granted on

$$\mathcal{U}_2^{(1)} = \mathbb{R}^6 \setminus (\mathcal{C}_2 \cup \mathcal{R}_2) = (\mathbb{R}^3 \setminus \{R_1, \dots, R_L\})^2 \setminus D = \mathcal{U}_1^{(2)}.$$

In the present paper, we work with the tools and the method, used in [J] to get Theorem 1.1, to prove the following three results.

**Theorem 1.3.** *The reduced current density  $C$  is real analytic on  $\mathcal{U}_1^{(1)} = \mathbb{R}^3 \setminus \{R_1, \dots, R_L\}$ .*

**Theorem 1.4.** *For all integer  $k$  with  $0 < k < N$ , the  $k$ -particle reduced density  $\rho_k$  is real analytic on  $\mathcal{U}_k^{(1)}$ .*

**Theorem 1.5.** *For all integer  $k$  with  $0 < k < N$ , the  $k$ -particle reduced density matrix  $\gamma_k$  is real analytic on  $\mathcal{U}_k^{(2)} = (\mathcal{U}_k^{(1)} \times \mathcal{U}_k^{(1)}) \setminus \mathcal{C}_k^{(2)}$ .*

Theorem 1.4 for  $k = 1$  coincides with Theorem 1.1. The proof of Theorem 1.4 is, when restricted to the  $k = 1$  case, just a rewriting of the proof of Theorem 1.1 in [J] and provides a direct justification of Theorem 1.3. We note that Theorem 1.5 for  $k = 1$  is exactly Theorem 1.2 and that Theorem 1.4 with  $k = 2$  fits precisely to the announced result on  $\rho_2$  in [FHHS2].

The set of all possible collisions between particles is  $\mathcal{C}_N \cup \mathcal{R}_N$  and the potential  $V$  is real analytic precisely on  $\mathbb{R}^{3N} \setminus (\mathcal{C}_N \cup \mathcal{R}_N)$ . Classical elliptic regularity applied to the equation  $H\psi = E\psi$  shows that  $\psi$  is also real analytic on  $\mathbb{R}^{3N} \setminus (\mathcal{C}_N \cup \mathcal{R}_N)$ . We refer to [ACN, FHHS4, FS] for more information on the behaviour of  $\psi$  near collisions. It turns out that, at least at some places in  $\mathcal{C}_N \cup \mathcal{R}_N$ ,  $\psi$  is not real analytic (cf. [FHHS4]). Thus, in the definition (1.3) of  $\rho_k$ , for an integer  $k$  with  $0 < k < N$ , the domain of integration does contain such singularities. Therefore it is not clear a priori that  $\rho_k$  is real analytic somewhere. This is however true, by Theorem 1.4, on the complement of the set of all possible collisions of the ‘‘external’’ electrons, namely on  $\mathcal{U}_k^{(1)}$ .

The proofs of Theorems 1.1 and 1.2 do not directly use the analyticity of  $\psi$ . This is also the case of the proofs of Theorems 1.3, 1.4, and 1.5, below.

It turns out that our proofs of Theorems 1.4 and 1.5 have a common structure that we want to describe now. Using an appropriate,  $\underline{x}$ -dependent, unitary operator  $U_{\underline{x}}$ , that acts on  $L^2(\mathbb{R}^{3(N-k)})$ , we locally transform the equation  $H\psi = E\psi$  into an elliptic differential

equation  $(U_{\underline{x}} H U_{\underline{x}}^{-1}) U_{\underline{x}} \psi = E U_{\underline{x}} \psi$  (the “twisted” equation), the coefficients of which have nice analytic properties. Applying elliptic regularity to the latter equation, we obtain the real analyticity of  $\underline{x} \mapsto U_{\underline{x}} \psi \in L^2(\mathbb{R}^{3(N-k)})$  that yields the real analyticity of  $\rho_k : \underline{x} \mapsto \|U_{\underline{x}} \psi\|^2$  ( $\|\cdot\|$  being the norm on  $L^2(\mathbb{R}^{3(N-k)})$ ). For  $\gamma_k$ , we follow the same lines but with a  $(\underline{x}; \underline{x}')$ -dependent, unitary operator  $U_{(\underline{x}; \underline{x}')}$ , and two “twisted” differential equations in the variables  $(\underline{x}; \underline{x}'; y)$ . These proofs are performed in Section 4.

Let us now compare the two available methods to prove such results, namely the one mentioned just above and the one used in [FHHS2, HS] to get Theorems 1.1 and 1.2. We point out that elliptic regularity was also an important tool in [FHHS2, HS]. Another common tool is the use of a  $\underline{x}$ -dependent change of variables on the “internal” variables  $y \in \mathbb{R}^{3(N-k)}$ , since the above unitary operators are both the implementation in  $L^2(\mathbb{R}^{3(N-k)})$  of such a change of variables. However, we use here global changes of variables in contrast to the local ones in [FHHS2, HS]. While, there, the integrals on  $\mathbb{R}^{3(N-1)}$  defining  $\rho_1$  and  $\gamma_1$  are split in several pieces, on which an appropriate change of variables is performed to make the real analyticity apparent, we view here  $\rho_k$  (resp.  $\gamma_k$ ) as the  $L^2(\mathbb{R}^{3(N-k)})$ -norm (resp. the  $L^2(\mathbb{R}^{3(N-k)})$ -scalar product) of one (resp. two)  $L^2(\mathbb{R}^{3(N-k)})$ -valued, real analytic function(s).

In view of the behaviour of  $\psi$  near some points in  $\mathcal{C}_N \cup \mathcal{R}_N$ , that was established in [FHHS4], it is quite natural to expect that, for an integer  $k$  with  $0 < k < N$ , neither  $\rho_k$  nor  $\gamma_k$  is real analytic everywhere. Their exact domain of real analyticity is still an open question. The domains obtained in Theorems 1.4 and 1.5 are the largest ones that can be reached by the method used in this paper, as explained in Remarks 4.2 and 4.4.

As already pointed out in [J], the twisted calculus, that we use here, allows us to treat more general Hamiltonian than  $H$ . We introduce, in Section 5, a class of elliptic, second order differential operators with Coulomb singularities. We observe that the conjugation by the twist actually preserves the ellipticity. Assuming that there exists a bound state for such an operator, we show in Theorem 5.1 that our previous, main results hold true for it. Moreover, we expect that this should extend to a class of elliptic, *pseudo*-differential operators with Coulomb singularities, since the used tools are available for such operators. We refer to [MS] for more information on the twisted (pseudo-)differential calculus.

Maybe it would be useful for the DFT to extend the present results on pure states to general states (see Sections 3.1.4 and 3.1.5 in [LiSe] for details). We expect that Theorem 3.9 below could be a good starting point for this purpose.

The paper is organized as follow. In Section 2, we provide a general notation, basic facts on real analyticity, and a result on elliptic regularity, that was essentially present in [J]. In Section 3, we review the twisted calculus based on Hunziker’s twist, show how it can be used to “desingularize” a differential equation with Coulomb singularities, and apply elliptic regularity to the corresponding twisted equation. Section 4 is devoted to the proof of our main results, namely Theorems 1.3, 1.4, and 1.5. The extension of these results to a larger class of Hamiltonians is performed in Section 5. Finally, we gathered in an Appendix some computations that are used in the main text.

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## 2 Basic tools and elliptic regularity.

To prepare the proof of the main results, we recall basic tools and state a general result on the analytic regularity of solutions of some elliptic equations.

### 2.1 Notation and basic tools.

We start with a general notation. We denote by  $\mathbb{N}$  the set of nonnegative integers. Let  $p$  be a positive integer (i.e.  $p \in \mathbb{N} \setminus \{0\}$ ). Recall that, for  $u \in \mathbb{R}^p$ , we write  $|u|$  for the euclidian norm of  $u$ . Given such a vector  $u \in \mathbb{R}^p$  and a nonnegative real number  $r$ , we denote by  $B(u; r[$  (resp.  $B(u; r]$ ) the open (resp. closed) ball of radius  $r$  and centre  $u$ , for the euclidian norm  $|\cdot|$ .

In the one dimensional case, we use the following convention for (possibly empty) intervals: for  $(a; b) \in \mathbb{R}^2$ , let  $[a; b] = \{t \in \mathbb{R}; a \leq t \leq b\}$ ,  $[a; b[ = \{t \in \mathbb{R}; a \leq t < b\}$ ,  $]a; b] = \{t \in \mathbb{R}; a < t \leq b\}$ , and  $]a; b[ = \{t \in \mathbb{R}; a < t < b\}$ .

Given an open subset  $O$  of  $\mathbb{R}^p$  and  $n \in \mathbb{N}$ , we denote by  $W^{n,2}(O)$  the standard Sobolev space of those  $L^2$ -functions on  $O$  such that, for  $n' \in [0; n] \cap \mathbb{N}$ , their distributional derivatives of order  $n'$  belong to  $L^2(O)$ . We denote by  $\langle \cdot, \cdot \rangle_n$  (resp.  $\|\cdot\|_n$ ) the right linear scalar product (resp. the norm) on  $\mathcal{A}$ . In particular,  $W^{0,2}(O) = L^2(O)$ . Without reference to  $p$  and  $O$ , we denote by  $\|\cdot\|$  (resp.  $\langle \cdot, \cdot \rangle$ ) the  $L^2$ -norm (resp. the right linear scalar product) on  $L^2(O)$ .

For two Banach spaces  $(\mathcal{A}, \|\cdot\|_{\mathcal{A}})$  and  $(\mathcal{B}, \|\cdot\|_{\mathcal{B}})$ , the space  $\mathcal{L}(\mathcal{A}; \mathcal{B})$  of continuous linear maps from  $\mathcal{A}$  to  $\mathcal{B}$  is also a Banach space for the operator norm  $\|\cdot\|_{\mathcal{L}(\mathcal{A}; \mathcal{B})}$  defined by

$$\forall M \in \mathcal{L}(\mathcal{A}; \mathcal{B}), \quad \|M\|_{\mathcal{L}(\mathcal{A}; \mathcal{B})} := \sup_{a \in \mathcal{A} \setminus \{0\}} \frac{\|M(a)\|_{\mathcal{B}}}{\|a\|_{\mathcal{A}}}.$$

We simply denote  $\mathcal{L}(\mathcal{A}; \mathcal{A})$  by  $\mathcal{L}(\mathcal{A})$ .

Let  $p$  be a positive integer and  $O$  an open subset of  $\mathbb{R}^p$ . Let  $(\mathcal{A}, \|\cdot\|_{\mathcal{A}})$  be a Banach space and  $\theta : O \ni x = (x_1; \dots; x_p) \mapsto \theta(x) \in \mathcal{A}$ . For  $j \in [1; p] \cap \mathbb{N}$ , we denote by  $\partial_j \theta$  or  $\partial_{x_j} \theta$  the  $j$ 'th first partial derivative of  $\theta$ . For  $\alpha \in \mathbb{N}^p$  and  $x \in \mathbb{R}^d$ , we set  $D_x^\alpha := (-i\partial_x)^\alpha := (-i\partial_{x_1})^{\alpha_1} \dots (-i\partial_{x_p})^{\alpha_p}$ ,  $D_x = -i\nabla_x$ ,  $x^\alpha := x_1^{\alpha_1} \dots x_p^{\alpha_p}$ ,  $|\alpha| := \alpha_1 + \dots + \alpha_p$ ,  $\alpha! := (\alpha_1!) \dots (\alpha_p!)$ ,  $|x|^2 = x_1^2 + \dots + x_p^2$ , and  $\langle x \rangle := (1 + |x|^2)^{1/2}$ .

We choose the same notation for the length  $|\alpha|$  of a multiindex  $\alpha \in \mathbb{N}^p$  and for the euclidian norm  $|x|$  of a vector  $x \in \mathbb{R}^p$  but the context should avoid any confusion.

We denote by  $\mathcal{C}^\infty(O; \mathcal{A})$  (resp.  $\mathcal{C}_b^\infty(O; \mathcal{A})$ , resp.  $\mathcal{C}_c^\infty(O; \mathcal{A})$ , resp.  $\mathcal{C}^\omega(O; \mathcal{A})$ ) the vector

space of functions from  $O$  to  $\mathcal{A}$  which are smooth (resp. smooth with bounded derivatives, resp. smooth with compact support, resp. real analytic). If  $\mathcal{A} = \mathbb{C}$ , we simply write  $\mathcal{C}^\infty(O)$  (resp.  $\mathcal{C}_b^\infty(O)$ , resp.  $\mathcal{C}_c^\infty(O)$ , resp.  $\mathcal{C}^\omega(O)$ ).

Now we recall basic facts on analytic functions. Take again a Banach space  $(\mathcal{A}, \|\cdot\|_{\mathcal{A}})$ , a positive integer  $p$ , and an open subset  $O$  of  $\mathbb{R}^p$ . For a smooth function  $\theta : O \rightarrow \mathcal{A}$ , the following properties are equivalent:  $\theta \in \mathcal{C}^\omega(O; \mathcal{A})$ ;

$$\exists A > 0, \forall \text{ compact } K \subset O, \forall \alpha \in \mathbb{N}^p, \quad \sup_{x \in K} \|(D_x^\alpha \theta)(x)\|_{\mathcal{A}} \leq A^{|\alpha|+1} \cdot (|\alpha|!); \quad (2.1)$$

$$\exists A > 0, \forall \text{ compact } K \subset O, \forall \alpha \in \mathbb{N}^p, \quad \sup_{x \in K} \|(D_x^\alpha \theta)(x)\|_{\mathcal{A}} \leq A^{|\alpha|+1} \cdot (|\alpha|!); \quad (2.2)$$

$$\exists A > 0, \forall \text{ compact } K \subset O, \forall \alpha \in \mathbb{N}^p, \quad \sup_{x \in K} \|(D_x^\alpha \theta)(x)\|_{\mathcal{A}} \leq A^{|\alpha|+1} \cdot (1 + |\alpha|)^{|\alpha|}. \quad (2.3)$$

We refer to [Hö3, HS, J] for details.

Let  $(\mathcal{B}, \|\cdot\|_{\mathcal{B}})$  be another Banach space and  $f : \mathcal{A}^2 \rightarrow \mathcal{B}$  be a continuous bilinear map. Then, for any  $(\theta_1; \theta_2) \in (\mathcal{C}^\omega(O; \mathcal{A}))^2$ , the map  $f(\theta_1; \theta_2) : O \ni x \mapsto f(\theta_1(x); \theta_2(x)) \in \mathcal{B}$  is real analytic.

Consider the case where  $\mathcal{A} = W^{n,2}(O)$ , for some integer  $n$ , and recall that  $\langle \cdot, \cdot \rangle_n$  (resp.  $\|\cdot\|_n$ ) is the right linear scalar product (resp. the norm) on  $\mathcal{A}$ . Take  $(\theta_1; \theta_2) \in (\mathcal{C}^\omega(O; \mathcal{A}))^2$ . Then the map  $\langle \theta_1, \theta_2 \rangle_n : O \rightarrow \mathbb{C}$ , defined by  $\langle \theta_1, \theta_2 \rangle_n(x) = \langle \theta_1(x), \theta_2(x) \rangle_n$ , is real analytic. So is also the real valued map  $\|\theta_1\|_n^2 : O \ni x \mapsto \|\theta_1(x)\|_n^2$ . In particular, taking  $n = 0$ , the maps  $\langle \theta_1, \theta_2 \rangle : O \ni x \mapsto \langle \theta_1(x), \theta_2(x) \rangle \in \mathbb{C}$  and  $\|\theta_1\|^2 : O \ni x \mapsto \|\theta_1(x)\|^2 \in \mathbb{R}^+$  are also real analytic.

Finally we need some specific notation to describe the structure of the considered Hamiltonian and of our results.

For a  $\mathcal{A}$ -valued function  $\theta : \mathbb{R}^3 \ni z = (z^{(1)}; z^{(2)}; z^{(3)}) \mapsto \theta(z) \in \mathcal{A}$ , we denote by  $d\theta$  or  $d_z\theta$  the total derivative of  $\theta$ . According to the previous notation, we denote, for  $j \in \{1; 2; 3\}$ , by  $\partial_j\theta$  or  $\partial_{z^{(j)}}\theta$  the  $j$ 'th first partial derivative. For a multiindex  $\alpha = (\alpha_1; \alpha_2; \alpha_3) \in \mathbb{N}^3$ , we set  $D_z^\alpha := (-i\partial_z)^\alpha := (-i\partial_1)^{\alpha_1}(-i\partial_2)^{\alpha_2}(-i\partial_3)^{\alpha_3}$ ,  $D_z = -i\nabla_z$ ,  $z^\alpha = (z^{(1)})^{\alpha_1}(z^{(2)})^{\alpha_2}(z^{(3)})^{\alpha_3}$ , and  $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$ .

Let  $m$  be a positive integer. We write a point  $x \in \mathbb{R}^{3m}$  as  $x = (x_1; \dots; x_m)$ . For any multiindex  $\alpha = (\alpha_1; \dots; \alpha_m) \in \mathbb{N}^{3m}$ , we set  $D_x^\alpha := (-i\partial_x)^\alpha := (-i\partial_{x_1})^{\alpha_1} \dots (-i\partial_{x_m})^{\alpha_m}$ ,  $D_x = -i\nabla_x$ ,  $x^\alpha = x_1^{\alpha_1} \dots x_m^{\alpha_m}$ , and  $|\alpha| = |\alpha_1| + \dots + |\alpha_m|$ .

Let  $m$  and  $p$  be positive integers. We write  $x \in \mathbb{R}^{3m}$  (resp.  $y \in \mathbb{R}^{3p}$ ) as  $x = (x_1; \dots; x_m)$  (resp.  $y = (y_1; \dots; y_p)$ ). For a  $\mathcal{A}$ -valued function  $\theta : \mathbb{R}^{3m} \times \mathbb{R}^{3p} \ni (x; y) \mapsto \theta(x; y) \in \mathcal{A}$ , let  $d_x\theta$  (resp.  $d_y\theta$ ) be the total derivative of  $\theta$  w.r.t.  $x$  (resp.  $y$ ).

For  $n \in \mathbb{N}$ ,  $W^{n,2}(\mathbb{R}^{3p})$  denotes the standard Sobolev space of  $L^2$ -functions on  $\mathbb{R}^{3p}$  admitting, up to order  $n$ ,  $L^2$  distributional derivatives. In particular,  $W^{0,2}(\mathbb{R}^{3p}) = L^2(\mathbb{R}^{3p})$ . We set  $\mathcal{W}_n = W^{n,2}(\mathbb{R}^{3p})$  and let  $\mathcal{B}_n = \mathcal{L}(\mathcal{W}_n; \mathcal{W}_0)$  be the Banach space of linear continuous maps from  $\mathcal{W}_n$  to  $\mathcal{W}_0$ .



## 2.2 Elliptic regularity.

In this subsection, we extend, with the same proof, a regularity result that was proved but not stated in [J].

Let  $(m; p) \in (\mathbb{N}^*)^2$ . Let  $\Omega$  be an open subset of  $\mathbb{R}^{3m}$ . We consider second order differential operators  $P$  on  $\Omega \times \mathbb{R}^{3p}$  given by

$$P = \sum_{\substack{(\alpha; \beta) \in \mathbb{N}^{3m} \times \mathbb{N}^{3p} \\ |\alpha| + |\beta| \leq 2}} c_{\alpha\beta}(\mathbf{x}; \mathbf{y}) D_{\mathbf{x}}^{\alpha} D_{\mathbf{y}}^{\beta}, \quad (2.4)$$

where the coefficients  $c_{\alpha\beta}$  belong to  $\mathcal{C}_b^{\infty}(\Omega \times \mathbb{R}^{3p}; \mathbb{C})$ . In particular, for  $\mathbf{x} \in \Omega$ , the multiplication operator  $C_{\alpha\beta}(\mathbf{x}; \cdot)$  by  $c_{\alpha\beta}(\mathbf{x}; \cdot)$  belongs to  $\mathcal{L}(\mathcal{W}_n)$ , for all  $n \in \mathbb{N}$ .

The principal symbol of those operators  $P$  is the smooth, complex-valued function  $\sigma_P$ , that is defined on  $\Omega \times \mathbb{R}^{3p} \times \mathbb{R}^{3m} \times \mathbb{R}^{3p}$  by

$$\sigma_P(\mathbf{x}; \mathbf{y}; \xi; \eta) = \sum_{\substack{(\alpha; \beta) \in \mathbb{N}^{3m} \times \mathbb{N}^{3p} \\ |\alpha| + |\beta| = 2}} c_{\alpha\beta}(\mathbf{x}; \mathbf{y}) \xi^{\alpha} \eta^{\beta}.$$

We assume that  $P$  is (globally) elliptic. This means that there exists  $C > 0$  such that, for all  $(\mathbf{x}; \mathbf{y}; \xi; \eta) \in \Omega \times \mathbb{R}^{3p} \times \mathbb{R}^{3m} \times \mathbb{R}^{3p}$ ,

$$|\xi|^2 + |\eta|^2 \geq 1 \implies |\sigma_P(\mathbf{x}; \mathbf{y}; \xi; \eta)| \geq C(|\xi|^2 + |\eta|^2). \quad (2.5)$$

Furthermore, we require that, for  $(\alpha; \beta) \in \mathbb{N}^m \times \mathbb{N}^p$  with  $|\alpha| + |\beta| \leq 2$ , the map  $\Omega \ni \mathbf{x} \mapsto C_{\alpha\beta}(\mathbf{x}; \cdot) \in \mathcal{B}_0$  is well-defined and real analytic.

Under these assumptions on  $P$ , we note that, for all  $\alpha \in \mathbb{N}^{3m}$  with  $|\alpha| \leq 2$ , the function  $a_{\alpha} : \Omega \longrightarrow \mathcal{B}_{2-|\alpha|}$ , which maps each  $\mathbf{x} \in \Omega$  to the differential operator

$$a_{\alpha}(\mathbf{x}) = \sum_{\substack{\beta \in \mathbb{N}^{3p} \\ |\beta| \leq 2 - |\alpha|}} c_{\alpha\beta}(\mathbf{x}; \cdot) D_{\mathbf{y}}^{\beta}$$

on  $\mathbb{R}^{3p}$ , is well-defined and real analytic.

**Definition 2.1.** For  $(m; p) \in (\mathbb{N}^*)^2$  and  $\Omega$  an open subset of  $\mathbb{R}^{3m}$ . We denote by  $\text{Diff}_2(\Omega)$  the set of all the differential operators  $P$  on  $\Omega \times \mathbb{R}^{3p}$  satisfying the previous requirements.

**Theorem 2.2.** [J]. Let  $P$  be differential operator in the class  $\text{Diff}_2(\Omega)$ . Let  $W : \Omega \longrightarrow \mathcal{B}_1$  be a real analytic map. Take  $\varphi \in W^{2,2}(\Omega \times \mathbb{R}^{3p})$  such that  $(P + W)\varphi = 0$ . Then, the map  $\Omega \ni \mathbf{x} \mapsto \varphi(\mathbf{x}; \cdot) \in \mathcal{W}_2$  is real analytic.

**Proof:** It suffices to follow the arguments of the paragraphs ‘‘Smoothness’’ and ‘‘Analyticity’’ in [J]. They make use of the basic, global pseudo-differential calculus (cf. Chapter XVIII in [Hö2]).  $\square$

**Remark 2.3.** *If, in Theorem 2.2, one replace  $3m$  by some positive interger  $n$  and one sets  $p = 0$  and  $w = 0$  with the convention that  $\Omega \times \mathbb{R}^0 = \Omega$  and  $\mathcal{W}_2 = \mathbb{C}$ , then one recovers exactly Hörmander’s Theorem 7.5.1 in [Hö1]. We assign Theorem 2.2 to [J] since, although it was not stated there, it was proved in a particular case and the corresponding proof directly extends to the present, general case. In [FHHS1, FHHS2, HS], one can find similar results in a slightly narrower framework. Therefore, Theorem 2.2 is more or less known in the literature.*

**Remark 2.4.** *As already pointed out in [J], the above proof of Theorem 2.2 does not use the most powerful tools of microlocal analysis, such as the analytic wave front set, which could shorten some parts of the proof. We chose to use a global pseudodifferential calculus, which is more accessible. However, we point out that one can prove Theorem 2.2 without pseudodifferential technics. In fact, the arguments used in [FHHS2] (see the proof of Lemma 3.1) and in [HS] (see Section 3.3) can be extended to get a proof of Theorem 2.2.*

### 3 Twisted differential calculus.

In this section, we recall the notion of “twist” used in [Hu, KMSW, MS] to “desingularize” a class of Hamiltonians with Coulomb-like singularities.

#### 3.1 Framework.

We need some more notation. Denoting by  $\mathbb{S}^2$  the unit euclidian sphere of  $\mathbb{R}^3$ , let  $\tilde{v}_0 : \mathbb{S} \rightarrow \mathbb{C}$  and  $\eta : ]0; +\infty[ \rightarrow \mathbb{R}^+$  be two functions such that, for some  $\eta_0 \in ]0; 1[$  and  $B_0 > 0$ ,  $(1/B_0) \leq |\tilde{v}_0| \leq B_0$  and

$$\forall t > 0, \quad \sup_{t(1-\eta_0) \leq s \leq t(1+\eta_0)} \eta(s) \leq B_0 \cdot \eta(t). \quad (3.1)$$

We assume further that the multiplication operator by the function  $\eta(|\cdot|) : \mathbb{R}^3 \ni z \mapsto \eta(|z|) \in \mathbb{R}^+$  belongs to  $\mathcal{L}(\mathcal{W}^{1,2}(\mathbb{R}^3); L^3(\mathbb{R}^3))$ . The multiplication operator by the function  $v_0 : \mathbb{R}^3 \setminus \{0\} \rightarrow \mathbb{C}$ , defined by  $v_0(z) = \eta(|z|)\tilde{v}_0(z/|z|)$ , also belongs to  $\mathcal{L}(\mathcal{W}^{1,2}(\mathbb{R}^3); L^3(\mathbb{R}^3))$ .

**Definition 3.1.** *Let  $\mathcal{V}$  be the class of functions  $v : \mathbb{R}^3 \rightarrow \mathbb{C}$  such that  $v \in C^\omega(\mathbb{R}^3 \setminus \{0\})$  and there exists  $C > 0$  such that*

$$\forall \alpha \in \mathbb{N}^3, \forall z \in \mathbb{R}^3 \setminus \{0\}, |z|^{|\alpha|} \cdot |D^\alpha v(z)| \leq C^{1+|\alpha|} \cdot (|\alpha|!) \cdot |v_0(z)|. \quad (3.2)$$

We observe that, if  $v \in \mathcal{V}$ , then the multiplication operator by  $v$  belongs to the space  $\mathcal{L}(\mathcal{W}^{1,2}(\mathbb{R}^3); L^3(\mathbb{R}^3))$ .

We consider a system of  $m + p$  electrons, interacting to one another and moving under the influence of  $L$  fixed nuclei. Let  $\mathcal{I}_e := \{1; \dots; m\}$  be the set of indices for the “external” electronic variables  $x \in \mathbb{R}^{3m}$ , let  $\mathcal{I}_i := \{1; \dots; p\}$  be the one of “internal” electronic

variables  $y \in \mathbb{R}^{3p}$ , and let  $\mathcal{I}_n := \{1; \dots; L\}$  be the one of the nuclear variables  $R_\ell \in \mathbb{R}^3$ . It is convenient to introduce the distinct union of those sets, namely

$$\mathcal{I}_e \sqcup \mathcal{I}_i \sqcup \mathcal{I}_n := \{(a; j); a \in \{e; i; n\}, j \in \mathcal{I}_a\}.$$

For  $c = (a; j) \in \mathcal{I}_e \sqcup \mathcal{I}_i \sqcup \mathcal{I}_n$ , let  $\pi_1(c) = a$  and  $\pi_2(c) = j$ . We define  $X_c = x_j$  if  $\pi_1(c) = e$ ,  $X_c = y_j$  if  $\pi_1(c) = i$ , and  $X_c = R_j$  if  $\pi_1(c) = n$ . Let

$$\mathcal{P} := \{\{c; c'\}; (c; c') \in (\mathcal{I}_e \sqcup \mathcal{I}_i \sqcup \mathcal{I}_n)^2 \text{ and } c \neq c'\}$$

be the set of all possible particle pairings. Let  $\underline{\Omega}$  be an open subset of  $\mathbb{R}^{3m}$ . We consider potentials  $\underline{V}$  where

$$\forall (x; y) \in \underline{\Omega} \times \mathbb{R}^{3p}, \quad \underline{V}(x; y) = \sum_{\{c; c'\} \in \mathcal{P}} V_{\{c; c'\}}(X_c - X_{c'}), \quad (3.3)$$

with  $V_{\{c; c'\}} \in \mathcal{V}$  (cf. Definition 3.1), for all  $\{c; c'\} \in \mathcal{P}$ .

Recall that  $\mathcal{W}_n = W^{n,2}(\mathbb{R}^{3p})$ , for  $n \in \mathbb{N}$ , and  $\mathcal{B}_1 = \mathcal{L}(\mathcal{W}_1; \mathcal{W}_0)$ . We note that, if  $v \in \mathcal{V}$  and  $\{c; c'\} \in \mathcal{P}$ , then, for any fixed  $x$ , the multiplication by the almost everywhere defined function  $v(X_c - X_{c'})$  of  $y$  belongs to  $\mathcal{B}_1$ , thanks to (3.2) and the assumption on  $v_0$ .

Recall that we introduced in Definition 2.1 a class of differential operators. The class of Hamiltonians, that we want to treat, is defined in the following:

**Definition 3.2.** For  $(m; p) \in (\mathbb{N}^*)^2$  and  $\underline{\Omega}$  an open subset of  $\mathbb{R}^{3m}$ . We denote by  $\text{Ham}_2(\underline{\Omega})$  the set of all the Hamiltonians  $\underline{H}$  on  $\underline{\Omega} \times \mathbb{R}^{3p}$  such that  $\underline{H} = \underline{P} + \underline{V}$ , where  $\underline{P} \in \text{Diff}_2(\underline{\Omega})$  (cf. Definition 2.1) and  $\underline{V}$  satisfies (3.3).

### 3.2 Heuristic.

In this subsection, we want to motivate the notion of “twist”, that is going to play a crucial rôle in the proof of the main results. To explain the basic idea, let us consider the following situation.

Take the Hamiltonian  $H$  in (1.1) with  $N = 2$ . We are not able to apply Theorem 2.2 with  $x = x_1$  and  $y = x_2$  to the equation  $H\psi = E\psi$ , since the map  $x_1 \mapsto (x_2 \mapsto |x_1 - x_2|^{-1}) \in \mathcal{B}_1 = \mathcal{L}(W^{1,2}(\mathbb{R}^3); L^2(\mathbb{R}^3))$  is admittedly well defined by (1.2) but is not analytic. The problem lies in the dependency of the Coulomb singularity on  $x_1$ .

Assume that, for some open subset  $\Omega$  of  $\mathbb{R}^3$  and some  $x^0 \in \mathbb{R}^3$ , we have a smooth map  $f : \Omega \times \mathbb{R}^3 \rightarrow \mathbb{R}^3$  such that, for all  $x_1 \in \Omega$ ,  $f(x_1; \cdot)$  is a smooth diffeomorphism of  $\mathbb{R}^3$  satisfying  $f(x_1; x^0) = x_1$ . For such  $x_1$ , let  $U_{x_1}$  be the unitary implementation of  $f(x_1; \cdot)$  on  $L^2(\mathbb{R}^3)$  (the “twist”). For any function  $\varphi \in W^{1,2}(\mathbb{R}^3)$  and for  $x_1 \in \Omega$ ,

$$U_{x_1}(|x_1 - \cdot|^{-1}\varphi)(y) = |f(x_1; x^0) - f(x_1; y)|^{-1} \cdot (U_{x_1}\varphi)(y).$$

Now, since  $f(x_1; \cdot)$  is a diffeomorphism, the singularity occurs when  $y = x^0$ . Therefore, it does not depend on  $x_1$  anymore. We can write

$$(U_{x_1}|x_1 - \cdot|^{-1}U_{x_1}^{-1}\varphi)(y) = |x^0 - y| \cdot |f(x_1; x^0) - f(x_1; y)|^{-1} \cdot |x^0 - y|^{-1} \cdot \varphi(y).$$

Assuming further that the map

$$\Omega \ni x_1 \mapsto |x^0 - \cdot| \cdot |f(x_1; x^0) - f(x_1; \cdot)|^{-1} \in L^\infty(\mathbb{R}^3) \quad (3.4)$$

is smooth, we see that  $\Omega \ni x_1 \mapsto U_{x_1}|x_1 - \cdot|^{-1}U_{x_1}^{-1} \in \mathcal{B}_1 = \mathcal{L}(W^{1,2}(\mathbb{R}^3); L^2(\mathbb{R}^3))$  is also smooth, thanks to (1.2).

What can we do with the other singular terms in  $H$ ? Since the terms  $|x_1 - R_\ell|^{-1}$  do not depend on  $x_2$ , the previous conjugation has no effect on them. But, if  $x_1$  stays far away from all  $R_\ell$ , they are not singular. We are left with the terms  $|x_2 - R_\ell|^{-1}$ , which are a constant function of  $x_1$  with values in  $\mathcal{B}_1$  by (1.2). Since we want to perform the above conjugation to treat the term  $|x_1 - x_2|^{-1}$ , we need to verify that this conjugation does not destroy the nice property of these terms. If we require that, for all  $\ell$  and all  $x_1 \in \Omega$ ,  $f(x_1; R_\ell) = R_\ell$ , and the smoothness of the map (3.4) with  $x^0$  replaced by  $R_\ell$ , the above computation shows that the map  $\Omega \ni x_1 \mapsto U_{x_1}|x_2 - R_\ell|^{-1}U_{x_1}^{-1} \in \mathcal{B}_1$  is also smooth.

We just have seen that the “twisted” potential  $U_{x_1}VU_{x_1}^{-1}$  is a smooth,  $\mathcal{B}_1$ -valued function. What about the “twisted” kinetic energy? A simple computation shows that the operators  $\nabla_{x_1}$  and  $\nabla_{x_2}$  are transformed by the twist into differential operators in the  $(x_1; x_2)$  variables with explicit coefficients in terms of the derivatives of  $f$  (cf. (3.16) and (3.18)). As we shall see below, the ellipticity of  $H$  is preserved by the “twist”.

Coming back to the original problem, we do not apply Theorem 2.2 with  $x = x_1$  and  $y = x_2$  to the equation  $H\psi = E\psi$  but to the “twisted” equation  $(U_{x_1}HU_{x_1}^{-1})U_{x_1}\psi = EU_{x_1}\psi$ . Therefore, we obtain some analytic regularity of the “twisted” bound state, namely  $U_{x_1}\psi$ , not on  $\psi$  itself. But, if we are interested in the regularity of  $\rho_1$ , we are done. Indeed, since we can write  $\rho_1(x_1) = \|\psi(x_1; \cdot)\|^2$  ( $\|\cdot\|$  being the  $L^2$ -norm on  $\mathbb{R}^3$ ) and since  $U_{x_1}$  is unitary on  $L^2(\mathbb{R}^3)$ ,  $\rho_1(x_1) = \|U_{x_1}\psi(x_1; \cdot)\|^2$  and  $\rho_1$  is smooth on  $\Omega$  by composition.

We just have sketched, in the  $N = 2$  case, the proof of the smoothness of  $\rho_1$ , which was performed in [J], provided there exists a map  $f$  satisfying the above requirements. Actually it does (see Subsection 3.3 below). Now, if we further assume some appropriate analyticity property of the function  $f$  w.r.t.  $x_1$ , it is reasonable to expect that  $\rho_1$  is analytic, and, again, it is the case.

### 3.3 Hunziker’s twist.

With the above strategy in mind, we recall Hunziker’s twist (cf. [Hu, KMSW]) and provide basic properties of it.

We take a real-valued cut-off function  $\tau \in C_c^\infty(\mathbb{R}^3)$  such that  $\tau(x) = 0$  if  $|x| \geq 1$ , and  $\tau(0) = 1$ . Let  $\mathcal{U}$  be the open subset of  $\mathbb{R}^{3m}$  defined by

$$\begin{aligned} \mathcal{U} &= \{x \in \mathbb{R}^{3m}; \forall (c; c') \in \mathcal{P}; \pi_1(c) = e \text{ and } \pi_1(c') \in \{e; n\}, X_c \neq X_{c'}\} \\ &= \{x \in \mathbb{R}^{3m}; \forall 1 \leq j \leq m, \forall 1 \leq j' \leq m, \forall 1 \leq \ell \leq L, x_j \neq R_\ell \\ &\quad \text{and } j \neq j' \implies x_j \neq x_{j'}\}. \end{aligned} \quad (3.5)$$

Let  $x^0 = (x_1^0; \dots; x_m^0) \in \mathcal{U}$ . We can find some  $r_0 > 0$  such that, for  $(j; j') \in ([1; m] \cap \mathbb{N})^2$ , for  $\ell \in [1; L] \cap \mathbb{N}$ ,

$$|x_j^0 - R_\ell| \geq r_0 \quad \text{and} \quad j \neq j' \implies |x_j^0 - x_{j'}^0| \geq r_0. \quad (3.6)$$

Let  $f : \mathbb{R}^{3m} \times \mathbb{R}^3 \longrightarrow \mathbb{R}^3$  be the smooth function defined by

$$f(\mathbf{x}; z) = z + \sum_{j=1}^m \tau(r_0^{-1}(z - \mathbf{x}_j^0)) \cdot (\mathbf{x}_j - \mathbf{x}_j^0). \quad (3.7)$$

Notice that, by (3.6), we have, for all  $\mathbf{x} \in \mathbb{R}^{3m}$ ,

$$\forall j \in [1; m] \cap \mathbb{N}, \ell \in [1; L] \cap \mathbb{N}, \quad f(\mathbf{x}; \mathbf{x}_j^0) = \mathbf{x}_j \quad \text{and} \quad f(\mathbf{x}; R_\ell) = R_\ell. \quad (3.8)$$

For all  $(\mathbf{x}; z) \in \mathbb{R}^{3m} \times \mathbb{R}^3$ , the total differential of  $f$  w.r.t.  $\mathbf{x}$  is given by

$$(d_{\mathbf{x}}f)(\mathbf{x}; z) = \sum_{j=1}^m \tau(r_0^{-1}(z - \mathbf{x}_j^0)) \, d\mathbf{x}_j \quad (3.9)$$

where  $d\mathbf{x}_j : \mathbb{R}^{3m} \ni \mathbf{x}' \mapsto \mathbf{x}'_j \in \mathbb{R}^3$ , for  $1 \leq j \leq m$ . In particular, the map  $\mathbb{R}^{3m} \ni \mathbf{x} \mapsto (d_{\mathbf{x}}f)(\mathbf{x}; \cdot) \in \mathcal{C}_b^\infty(\mathbb{R}^3; \mathcal{L}(\mathbb{R}^{3m}; \mathbb{R}^3))$  is well-defined and constant. Using (3.9) and setting

$$C(\tau) = \sup_{z \in \mathbb{R}^3} \|d\tau(z)\|_{\mathcal{L}(\mathbb{R}^3)} < +\infty,$$

we can write, for all  $j \in [1; m] \cap \mathbb{N}$ , for all  $(z; z') \in (\mathbb{R}^3)^2$ , and for all  $\mathbf{x} \in \mathbb{R}^{3m}$ ,

$$\begin{aligned} \|(d_{\mathbf{x}_j}f)(\mathbf{x}; z) - (d_{\mathbf{x}_j}f)(\mathbf{x}; z')\|_{\mathcal{L}(\mathbb{R}^{3m}; \mathbb{R}^3)} &= \left| \tau(r_0^{-1}(z - \mathbf{x}_j^0)) - \tau(r_0^{-1}(z' - \mathbf{x}_j^0)) \right| \\ &\leq r_0^{-1} C(\tau) |z - z'|. \end{aligned} \quad (3.10)$$

For all  $(\mathbf{x}; z) \in \mathbb{R}^{3m} \times \mathbb{R}^3$ , the total differential of  $f$  w.r.t.  $z$  is given by, for  $z^\epsilon \in \mathbb{R}^3$ ,

$$(d_z f)(\mathbf{x}; z) \cdot z^\epsilon = z^\epsilon + r_0^{-1} \sum_{j=1}^m ((d\tau)(r_0^{-1}(z - \mathbf{x}_j^0)) \cdot z^\epsilon)(\mathbf{x}_j - \mathbf{x}_j^0). \quad (3.11)$$

For  $\delta > 0$ , set  $\Omega(\delta) := B(\mathbf{x}_1^0; \delta] \times \cdots \times B(\mathbf{x}_m^0; \delta[$ . Recall that the class  $\mathcal{V}$  (cf. Definition 3.1) depends on a parameter  $\eta_0$  (see (3.1)). By (3.11), we can find some  $\delta_0 \in ]0; r_0/2[$ , depending on  $C(\tau)$  and  $r_0$ , such that

$$\forall \mathbf{x} \in \Omega(\delta_0), \quad \sup_{z \in \mathbb{R}^3} \|(d_z f)(\mathbf{x}; z) - I_3\|_{\mathcal{L}(\mathbb{R}^3)} \leq \min(\eta_0; 1 - \eta_0) < 1. \quad (3.12)$$

We note that the requirement  $\delta_0 \in ]0; r_0/2[$  yields  $\Omega(\delta_0) \subset \mathcal{U}$ , by (3.6) and the triangle inequality. Thanks to (3.12), for each  $\mathbf{x} \in \Omega(\delta_0)$ ,  $f(\mathbf{x}; \cdot)$  is a  $\mathcal{C}^\infty$ -diffeomorphism of  $\mathbb{R}^3$ . We denote by  $f^{(-1)}(\mathbf{x}; \cdot)$  its inverse. Furthermore, for all  $\mathbf{x} \in \Omega(\delta_0)$ , for all  $(z; z') \in (\mathbb{R}^3)^2$ ,

$$(1 - \eta_0) |z - z'| \leq |f(\mathbf{x}; z) - f(\mathbf{x}; z')| \leq (1 + \eta_0) |z - z'|. \quad (3.13)$$

By a direct computation using (3.9) and (3.11), one can express the derivative  $d_z f^{(-1)}$  and  $d_{\mathbf{x}} f^{(-1)}$  in terms of  $d_z f$  (see the Appendix for details). In particular, one can check that  $f \in \mathcal{C}_b^\infty(\Omega(\delta_0) \times \mathbb{R}^3; \mathbb{R}^3)$  and  $f^{(-1)} \in \mathcal{C}_b^\infty(\Omega(\delta_0) \times \mathbb{R}^3; \mathbb{R}^3)$ .

Consider the map  $F : \Omega(\delta_0) \times \mathbb{R}^{3p} \longrightarrow \mathbb{R}^{3p}$ , defined by  $F(\mathbf{x}; \mathbf{y}) = (f(\mathbf{x}; \mathbf{y}_1); \cdots; f(\mathbf{x}; \mathbf{y}_p))$ . For each  $\mathbf{x} \in \Omega(\delta_0)$ ,  $F(\mathbf{x}; \cdot)$  is a  $\mathcal{C}^\infty$ -diffeomorphism of  $\mathbb{R}^{3p}$  and we denote its inverse map

by  $F^{(-1)}(\mathbf{x}; \cdot)$ . Explicit expressions for  $d_x F$ ,  $d_y F$ ,  $d_x F^{(-1)}$ , and  $d_y F^{(-1)}$ , are provided in the Appendix. In particular, we observe that  $F \in \mathcal{C}_b^\infty(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{R}^{3p})$  and  $F^{(-1)} \in \mathcal{C}_b^\infty(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{R}^{3p})$ .

We introduce the map  $U : \Omega(\delta_0) \ni \mathbf{x} \mapsto U_x \in \mathcal{B}_0$  (with  $\mathcal{B}_0 = \mathcal{L}(\mathcal{W}_0)$  and  $\mathcal{W}_0 = L^2(\mathbb{R}^{3p})$ ), with values in the set of unitary operators on  $\mathcal{W}_0$ , defined by, for  $\theta \in \mathcal{W}_0$ ,

$$(U_x \theta)(y) = |\text{Det}(d_y F)(x; y)|^{1/2} \cdot \theta(F(x; y)). \quad (3.14)$$

For  $\mathbf{x} \in \Omega(\delta_0)$ , the map  $U_x$  is the unitary implementation of  $F(\mathbf{x}; \cdot)$  on  $L^2(\mathbb{R}^{3p})$  and

$$(U_x^{-1} \theta)(y) = \left| \text{Det}(d_y F^{(-1)})(x; y) \right|^{1/2} \cdot \theta(F^{(-1)}(x; y)). \quad (3.15)$$

Denoting by  $A^T$  the transposed of a linear map  $A$  and by  $\text{Det} A$  its determinant, we see by a direct computation that, as differential operators on  $\Omega(\delta_0) \times \mathbb{R}^{3p}$ ,

$$U_x^{-1} D_x U_x = D_x + J_1(F) D_y + J_2(F), \quad (3.16)$$

$$U_x D_x U_x^{-1} = D_x + J_1(F^{(-1)}) D_y + J_2(F^{(-1)}), \quad (3.17)$$

$$U_x^{-1} D_{y'} U_x = J_3(F) D_y + J_4(F), \quad (3.18)$$

$$U_x D_{y'} U_x^{-1} = J_3(F^{(-1)}) D_y + J_4(F^{(-1)}), \quad (3.19)$$

where, for  $\mathbf{x} \in \Omega(\delta_0)$  and  $\mathbf{y} \in \mathbb{R}^{3p}$ , with  $G = F$  and  $G^{(-1)} = F^{(-1)}$  or with  $G = F^{(-1)}$  and  $G^{(-1)} = F$ ,

$$J_1(G)(\mathbf{x}; \mathbf{y}) := \left( (d_x G)(\mathbf{x}; \mathbf{y}') \right)^T (\mathbf{x}; \mathbf{y}' = G^{(-1)}(\mathbf{x}; \mathbf{y})),$$

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

$$J_3(G)(\mathbf{x}; \mathbf{y}) := \left( (d_{y'} G)(\mathbf{x}; \mathbf{y}') \right)^T (\mathbf{x}; \mathbf{y}' = G^{(-1)}(\mathbf{x}; \mathbf{y})),$$

$$J_4(G)(\mathbf{x}; \mathbf{y}) := -i \left| \text{Det}(d_y G^{(-1)})(\mathbf{x}; \mathbf{y}) \right|^{1/2} D_{y'} \left( \left| \text{Det}(d_{y'} G)(\mathbf{x}; \mathbf{y}') \right|^{1/2} \right) \Big|_{\mathbf{y}' = G^{(-1)}(\mathbf{x}; \mathbf{y})}.$$

Thanks to the computation written in the Appendix, we note that, on one hand, for  $G \in \{F; F^{(-1)}\}$ ,

$$J_1(G) \in \mathcal{C}_b^\infty\left(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathcal{L}(\mathbb{R}^{3p}; \mathbb{R}^{3m})\right), \quad iJ_2(G) \in \mathcal{C}_b^\infty\left(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{R}^{3m}\right), \quad (3.20)$$

$$J_3(G) \in \mathcal{C}_b^\infty\left(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathcal{L}(\mathbb{R}^{3p})\right), \quad iJ_4(G) \in \mathcal{C}_b^\infty\left(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{R}^{3p}\right), \quad (3.21)$$

and, on the other hand, if we denote by  $J$  the multiplication operator by any component of  $J_k(G)$ ,  $k \in \{1; 2; 3; 4\}$  and  $G \in \{F; F^{(-1)}\}$ ,

$$J \in \mathcal{C}^\omega(\Omega(\delta_0); \mathcal{B}_0). \quad (3.22)$$

Furthermore (cf. Appendix), there exists  $C > 0$  such that, for  $G \in \{F; F^{(-1)}\}$ , for all  $(\mathbf{x}; \mathbf{y}) \in \Omega(\delta_0) \times \mathbb{R}^{3p}$ ,  $J_3(G)(\mathbf{x}; \mathbf{y})$  is invertible and

$$C^{-1} \geq \left\| J_3(G)(\mathbf{x}; \mathbf{y}) \right\|_{\mathcal{L}(\mathbb{R}^{3p})} + \left\| (J_3(G)(\mathbf{x}; \mathbf{y}))^{-1} \right\|_{\mathcal{L}(\mathbb{R}^{3p})} \geq C. \quad (3.23)$$

Now, using (3.18),

$$D_{y'}U_x = U_x(J_3(F)D_y - J_4(F))$$

thus, for all  $x \in \Omega(\delta_0)$ , we see, by induction and by (3.21), that  $U_x$  leaves  $\mathcal{W}_n$  invariant, for all  $n \in \mathbb{N}$ . Similarly, we can show, using (3.19) and (3.21), that, for all  $x \in \Omega(\delta_0)$ ,  $U_x^{-1}$  also leaves  $\mathcal{W}_n$  invariant, for all  $n \in \mathbb{N}$ . By the same arguments, we can check, starting from (3.16) and (3.18), that  $U$  preserves the space  $W^{2,2}(\Omega(\delta_0) \times \mathbb{R}^{3p})$ .

### 3.4 Potential regularization by a twist.

We first consider the action by conjugation of the twist  $U$  on the potential part  $\underline{V}$  of Hamiltonians  $\underline{H}$  in the class  $\text{Ham}_2(\Omega)$ .

**Proposition 3.3.** *Take  $x^0 \in \mathcal{U} \subset \mathbb{R}^{3m}$ . We choose  $r_0 > 0$  and  $\delta_0 \in ]0; r_0/2]$  such that (3.6) and (3.12) hold true. Recall that the neighbourhood  $\Omega(\delta_0) := B(x_1^0; \delta_0) \times \cdots \times B(x_m^0; \delta_0)$  of  $x^0$  is included in  $\mathcal{U}$ .*

*Then, for any  $v \in \mathcal{V}$  and any  $\{c; c'\} \in \mathcal{P}$ , the map  $\Omega(\delta_0) \ni x \mapsto U_x v(X_c - X_{c'}) U_x^{-1} \in \mathcal{B}_1$  is well-defined and real analytic.*

**Remark 3.4.** *We point out that the Coulomb potential  $|\cdot|^{-1}$  does belong to  $\mathcal{V}$ . Indeed, (3.2), for  $v = v_0 = |\cdot|^{-1}$ , was proved in [J] and the multiplication by this  $v_0$  belongs to  $\mathcal{L}(\mathcal{W}^{1,2}(\mathbb{R}^3); \mathcal{L}^3(\mathbb{R}^3))$  by Hardy's inequality (1.2).*

**Remark 3.5.** *A proof of Proposition 3.3 is essentially available in [Hu, J]. However, the proof in [Hu] is restricted to Coulomb interactions. We provide below a more transparent version of the proof in [J].*

**Proof of Proposition 3.3:** Let  $x \in \Omega(\delta_0)$ . Recall that, for  $k \in \{0; 1\}$ ,  $U_x$  and  $U_x^{-1}$  leave  $\mathcal{W}_k$  invariant. Recall that, for all  $\{c; c'\} \in \mathcal{P}$ , the multiplication by  $v(X_c - X_{c'})$  belongs to  $\mathcal{B}_1$ . Therefore the map  $w : \Omega(\delta_0) \ni x \mapsto U_x v(X_c - X_{c'}) U_x^{-1} \in \mathcal{B}_1$  is well-defined. We treat all possible cases for  $\{c; c'\} \in \mathcal{P}$ .

If  $\pi_1(c) = \pi_1(c') = n$ , then  $w : \Omega(\delta_0) \ni x \mapsto v(X_c - X_{c'})$  is a constant.

Assume that  $\pi_1(c) = e$  and  $\pi_1(c') \in \{e; n\}$  or that  $\pi_1(c') = e$  and  $\pi_1(c) \in \{e; n\}$ . Since  $\Omega(\delta_0) \subset \mathcal{U}$ ,  $X_c - X_{c'}$  does not vanish on  $\Omega(\delta_0)$ . Thus  $w : \Omega(\delta_0) \ni x \mapsto v(X_c - X_{c'})$  is real analytic, by composition.

Assume that  $\pi_1(c) = e$  and  $\pi_1(c') = i$ . Let  $j = \pi_2(c)$  and  $k = \pi_2(c')$ . Then, for  $x \in \Omega(\delta_0)$ ,  $U_x v(X_c - X_{c'}) U_x^{-1}$  is the multiplication operator on  $\mathcal{W}_1$  by the function

$$y \mapsto v(x_j - f(x; y_k)) = v(f(x; x_j^0) - f(x; y_k)),$$

by (3.8). Let  $j' \in \mathcal{I}_e$ . Using the fact that  $d_x f$  does not depend on  $x$  (see (3.9)), we have, for  $\alpha \in \mathbb{N}^3$  and  $y_k \neq x_j^0$ ,

$$\begin{aligned} & \partial_{x_{j'}}^\alpha \left( v(f(x; x_j^0) - f(x; y_k)) \right) \\ &= (\partial^\alpha v)(f(x; x_j^0) - f(x; y_k)) \cdot \left( \tau(r_0^{-1}(x_j^0 - x_{j'}^0)) - \tau(r_0^{-1}(y_k - x_{j'}^0)) \right)^{|\alpha|}. \end{aligned} \quad (3.24)$$

Using successively (3.10), (3.13), and (3.2), we obtain

$$\begin{aligned}
& \left| \partial_{x_j'}^\alpha \left( v(f(\mathbf{x}; \mathbf{x}_j^0) - f(\mathbf{x}; y_k)) \right) \right| \\
& \leq |(\partial^\alpha v)(f(\mathbf{x}; \mathbf{x}_j^0) - f(\mathbf{x}; y_k))| \cdot \left( r_0^{-1} C(\tau) |\mathbf{x}_j^0 - y_k| \right)^{|\alpha|}, \\
& \leq |(\partial^\alpha v)(f(\mathbf{x}; \mathbf{x}_j^0) - f(\mathbf{x}; y_k))| \cdot \left( (r_0(1 - \eta_0))^{-1} C(\tau) |f(\mathbf{x}; \mathbf{x}_j^0) - f(\mathbf{x}; y_k)| \right)^{|\alpha|}, \\
& \leq C_1^{1+|\alpha|} \cdot (|\alpha|!) \cdot \left| v_0(f(\mathbf{x}; \mathbf{x}_j^0) - f(\mathbf{x}; y_k)) \right|,
\end{aligned}$$

for some  $C_1 > 0$ . Now, by the structure of  $v_0$  and by (3.13) and (3.1), we derive that, for some positive constants  $C_2$  and  $C_3$ ,

$$\begin{aligned}
\left| \partial_{x_j'}^\alpha \left( v(f(\mathbf{x}; \mathbf{x}_j^0) - f(\mathbf{x}; y_k)) \right) \right| & \leq C_2^{1+|\alpha|} \cdot (|\alpha|!) \cdot \eta(f(\mathbf{x}; \mathbf{x}_j^0) - f(\mathbf{x}; y_k)), \\
& \leq C_3^{1+|\alpha|} \cdot (|\alpha|!) \cdot \eta(|\mathbf{x}_j^0 - y_k|). \tag{3.25}
\end{aligned}$$

Now, one can check, by induction on  $|\alpha|$  and by the fact that the multiplication by  $\eta(|\cdot|)$  belongs to  $\mathcal{B}_1$ , that, on  $\Omega(\delta_0)$ , the  $\partial_{x_j'}^\alpha$  partial derivative of  $w$  exists and maps each  $\mathbf{x} \in \Omega(\delta_0)$  to the multiplication operator on  $\mathcal{W}_1$  by the almost everywhere defined function (3.24) of  $y$ . Thus,  $w \in \mathcal{C}^\infty(\Omega(\delta_0); \mathcal{B}_1)$ . Using (3.25) again, we obtain that

$$\sup_{\mathbf{x} \in \Omega(\delta_0)} \left\| (D_{x_j'}^\alpha w)(\mathbf{x}) \right\|_{\mathcal{B}_1} \leq C_4^{1+|\alpha|} \cdot (|\alpha|!), \tag{3.26}$$

for some  $C_4 > 0$ . By (2.2),  $w$  is real analytic w.r.t.  $x_j'$ . Since this holds true for all  $j'$ ,  $w$  is real analytic.

Similarly, we can treat the case  $\pi_1(c) = i$  and  $\pi_1(c') = e$ .

Assume that  $\pi_1(c) = n$  and  $\pi_1(c') = i$ . Let  $\ell = \pi_2(c)$  and  $k = \pi_2(c')$ . For  $\mathbf{x} \in \Omega(\delta_0)$ ,  $w(\mathbf{x})$  is the multiplication operator in  $\mathcal{B}_1$  by the function

$$y \mapsto v(R_\ell - f(\mathbf{x}; y_k)) = v(f(\mathbf{x}; R_\ell) - f(\mathbf{x}; y_k)), \tag{3.27}$$

by (3.8). We redo the computation (3.24) - (3.25), with  $\mathbf{x}_j^0$  replaced by  $R_\ell$ . Furthermore, we also can check that the  $\partial_{x_j'}^\alpha$  partial derivative of  $w$  exists and maps each  $\mathbf{x} \in \Omega(\delta_0)$  to the multiplication operator on  $\mathcal{W}_1$  by the almost everywhere defined  $\partial_{x_j'}^\alpha$  partial derivative of (3.27). Using the new estimate (3.25), we derive a bound like (3.26). As above, we conclude that  $w$  is real analytic.

Again, we have a similar treatment of the case  $\pi_1(c) = i$  and  $\pi_1(c') = n$ .

We are left with the case  $\pi_1(c) = i$  and  $\pi_1(c') = i$ . We set  $k = \pi_2(c)$  and  $k' = \pi_2(c')$ . By assumption,  $k \neq k'$ . Using (3.8) again, we see that, for  $\mathbf{x} \in \Omega(\delta_0)$ ,  $w(\mathbf{x})$  is the multiplication operator in  $\mathcal{B}_1$  by the function

$$y \mapsto v(f(\mathbf{x}; y_k) - f(\mathbf{x}; y_{k'})). \tag{3.28}$$

Once again, we perform the computation (3.24) - (3.25) and follow the above arguments, using this time that the multiplication by  $y \mapsto \eta(|y_k - y_{k'}|)$  belongs to  $\mathcal{B}_1$ . This yields the real analyticity of  $w$ .  $\square$



### 3.5 Twisted regular differential calculus.

Next, we let act the twist  $U$  by conjugation on the regular, differential part  $\underline{P} \in \text{Diff}_2(\underline{\Omega})$  of Hamiltonians  $\underline{H}$  in the class  $\text{Ham}_2(\underline{\Omega})$  (cf. Definitions 2.1 and 3.2). It turns out that this action preserves this class  $\text{Diff}_2(\underline{\Omega})$ .

**Proposition 3.6.** *Let  $\mathbf{x}^0 \in \mathcal{U} \cap \underline{\Omega} \subset \mathbb{R}^{3m}$ . Take  $r_0 > 0$  and  $\delta_0 \in ]0; r_0/2]$  such that (3.6) and (3.12) hold true, and such that  $\Omega(\delta_0) := B(\mathbf{x}_1^0; \delta_0] \times \cdots \times B(\mathbf{x}_m^0; \delta_0] \subset \underline{\Omega}$ . We recall that  $\Omega(\delta_0) \subset \mathcal{U}$ . Let us define  $U^* : \Omega(\delta_0) \ni \mathbf{x} \mapsto U_{\mathbf{x}}^{-1} \in \mathcal{B}_0$ .*

*Let  $\underline{P} \in \text{Diff}_2(\underline{\Omega})$  (see Definition 2.1). Then the operator composition  $P = U\underline{P}U^*$  defines a differential operator on  $\Omega(\delta_0) \times \mathbb{R}^{3p}$  that belongs to  $\text{Diff}_2(\Omega(\delta_0))$ .*

**Remark 3.7.** *In [Hu, J], it was proven that the twisted Laplacian  $U\Delta U^*$  is elliptic, when  $m = 1$ . Proposition 3.6 shows that the conjugation by the twist of an elliptic operator is also elliptic. This property is actually used in [KMSW, MS] in a semiclassical framework.*

**Remark 3.8.** *In the proof of Proposition 3.6 below, we essentially follow [Hu, J]. Observing that  $U$  is a Fourier integral operator (cf. [GS, Hö4]), one can use composition rules for such operators to derive the relationship between the principal symbols of  $\underline{P}$  and  $P$ , given in (3.30) below.*

**Proof of Proposition 3.6:** Take  $\underline{P} \in \text{Diff}_2(\underline{\Omega})$ , that is of the form (2.4). We first observe that, for  $(\alpha; \beta) \in \mathbb{N}^{3m} \times \mathbb{N}^{3p}$  with  $|\alpha| + |\beta| \leq 2$ ,  $U c_{\alpha\beta} U^*$  is, as differential operator, the multiplication operator by the function

$$\Omega(\delta_0) \times \mathbb{R}^{3p} \ni (\mathbf{x}; \mathbf{y}) \mapsto c_{\alpha\beta}(\mathbf{x}; F(\mathbf{x}; \mathbf{y})),$$

which belongs to  $\mathcal{C}_b^\infty(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{C})$ . Using (3.17) and (3.19) componentwise and taking advantage of (3.20) and (3.21) for  $G = F^{(-1)}$ , we see that  $P = U\underline{P}U^*$  has the form (2.4) on  $\Omega(\delta_0) \times \mathbb{R}^{3p}$  with coefficients in  $\mathcal{C}_b^\infty(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{C})$ .

We are left with the proof of the ellipticity of  $P$ . To this end, we compute its principal symbol  $\sigma_P$ . Let us denote by “ $\cdot$ ” the scalar product in  $\mathbb{R}^d$ , for any  $d \in \mathbb{N}^*$ . It is well-known that the total symbol of  $P$  is the map  $S_P : \Omega(\delta_0) \times \mathbb{R}^{3p} \times \mathbb{R}^{3m} \times \mathbb{R}^{3p} \rightarrow \mathbb{C}$  defined by

$$S_P(\mathbf{x}; \mathbf{y}; \xi; \eta) = e^{-i\mathbf{x} \cdot \xi - i\mathbf{y} \cdot \eta} P(e^{i\mathbf{x} \cdot \xi + i\mathbf{y} \cdot \eta}). \quad (3.29)$$

Using this, we obtain in the Appendix that, for  $(\mathbf{x}; \mathbf{y}; \xi; \eta) \in \Omega(\delta_0) \times \mathbb{R}^{3p} \times \mathbb{R}^{3m} \times \mathbb{R}^{3p}$ ,

$$\sigma_P(\mathbf{x}; \mathbf{y}; \xi; \eta) = \sigma_{\underline{P}}(\mathbf{x}; F(\mathbf{x}; \mathbf{y}); \xi + J_1(F^{(-1)})(\mathbf{x}; \mathbf{y})\eta; J_3(F^{(-1)})(\mathbf{x}; \mathbf{y})\eta). \quad (3.30)$$

Since  $\underline{P}$  is elliptic, there exists  $\underline{C} > 0$  such that (2.5) holds true with  $P$  replaced by  $\underline{P}$  and  $C$  replaced by  $\underline{C}$ . Take  $(\xi; \eta)$  satisfying  $|\xi|^2 + |\eta|^2 \geq 1$ . Then

$$\underline{C}^{-1} \sigma_P(\mathbf{x}; \mathbf{y}; \xi; \eta) \geq |\xi + J_1(F^{(-1)})(\mathbf{x}; \mathbf{y})\eta|^2 + |J_3(F^{(-1)})(\mathbf{x}; \mathbf{y})\eta|^2. \quad (3.31)$$

By (3.20), we can find  $M > 0$  such that, for all  $(\mathbf{x}; \mathbf{y}) \in \Omega(\delta_0) \times \mathbb{R}^{3p}$ ,

$$\|J_1(F^{(-1)})(\mathbf{x}; \mathbf{y})\|_{\mathcal{L}(\mathbb{R}^{3p}; \mathbb{R}^{3m})} \leq M.$$

Now let  $S = \sqrt{1 + 4M^2}$ . Consider first the case where  $S|\eta| \leq (|\xi|^2 + |\eta|^2)^{1/2}$ . We have  $2M|\eta| \leq |\xi|$ . Thus

$$|\xi + J_1(F^{(-1)})(\mathbf{x}; \mathbf{y})\eta|^2 \geq \frac{|\xi|^2}{4}$$

and, using (3.23), we obtain from (3.31) the lower bound

$$\underline{C}^{-1}\sigma_P(\mathbf{x}; \mathbf{y}; \xi; \eta) \geq \min(1/4; C^2)(|\xi|^2 + |\eta|^2).$$

If, now,  $S|\eta| \geq (|\xi|^2 + |\eta|^2)^{1/2}$ , it follows from (3.23) and (3.31) that

$$\underline{C}^{-1}\sigma_P(\mathbf{x}; \mathbf{y}; \xi; \eta) \geq C^2S^{-2}(|\xi|^2 + |\eta|^2).$$

This yields (2.5). Thus  $P \in \text{Diff}_2(\Omega(\delta_0))$ .  $\square$

### 3.6 Elliptic regularity for twisted Hamiltonians.

Now, we conjugate by the twist  $U$  any Hamiltonians  $\underline{H}$  of the class  $\text{Ham}_2(\underline{\Omega})$  (cf. Definition 3.2) and show that we can apply Theorem 2.2 to the twisted operator.

**Theorem 3.9.** *Let  $\underline{\Omega}$  be an open subset of  $\mathbb{R}^{3m}$  and  $\mathbf{x}^0 \in \mathcal{U} \cap \underline{\Omega}$ . Then, one can find a neighbourhood  $\Omega_0$  of  $\mathbf{x}^0$  and a unitary operators valued map  $U : \Omega_0 \ni \mathbf{x} \mapsto U_{\mathbf{x}} \in \mathcal{B}_0$  such that the following holds true:*

*For any Hamiltonian  $\underline{H} \in \text{Ham}_2(\underline{\Omega})$  on  $\underline{\Omega} \times \mathbb{R}^{3p} \subset \mathbb{R}^{3(m+p)}$ , for any  $\Psi \in W^{2,2}(\underline{\Omega} \times \mathbb{R}^{3p})$  such that  $\underline{H}\Psi = 0$ , the map  $U\Psi : \Omega_0 \ni \mathbf{x} \mapsto U_{\mathbf{x}}\Psi(\mathbf{x}; \cdot) \in \mathcal{W}_2$  is well-defined and real analytic. Furthermore, for any  $\alpha \in \mathbb{N}^{3m}$  with  $1 \leq |\alpha| \leq 2$ , the map  $U(D_{\mathbf{x}}^{\alpha}\Psi) : \Omega_0 \ni \mathbf{x} \mapsto U_{\mathbf{x}}(D_{\mathbf{x}}^{\alpha}\Psi)(\mathbf{x}; \cdot) \in \mathcal{W}_{2-|\alpha|}$  is well-defined and real analytic.*

**Proof:** Given  $\mathbf{x}^0 \in \mathcal{U} \cap \underline{\Omega}$ , take  $\Omega_0 = \Omega(\delta_0)$  satisfying the assumptions of Proposition 3.6 and consider the twist  $U : \Omega_0 \rightarrow \mathcal{B}_0$  defined by (3.14). Recall that  $U^* : \Omega_0 \ni \mathbf{x} \mapsto U_{\mathbf{x}}^{-1} \in \mathcal{B}_0$ . Take  $\underline{H} = \underline{P} + \underline{V} \in \text{Ham}_2(\underline{\Omega})$  and  $\Psi \in W^{2,2}(\underline{\Omega} \times \mathbb{R}^{3p})$  such that  $\underline{H}\Psi = 0$ . Applying Proposition 3.3 to each term of  $\underline{V}$  and Proposition 3.6 to  $\underline{P}$ , we see that  $P = U\underline{P}U^*$  and  $W = U\underline{V}U^*$  satisfy the assumptions of Theorem 2.2 on  $\Omega_0$ , yielding the real analyticity of the map  $U\Psi : \Omega_0 \ni \mathbf{x} \mapsto U_{\mathbf{x}}\Psi(\mathbf{x}; \cdot) \in \mathcal{W}_2$ .

By (3.17), we have, for  $\mathbf{x} \in \Omega_0$ , setting  $J_1 := J_1(F^{(-1)})$  and  $J_2 := J_2(F^{(-1)})$ ,

$$\begin{aligned} U_{\mathbf{x}}(D_{\mathbf{x}}\Psi)(\mathbf{x}; \cdot) &= U_{\mathbf{x}}D_{\mathbf{x}}U_{\mathbf{x}}^{-1} \cdot U_{\mathbf{x}}\Psi(\mathbf{x}; \cdot) \\ &= D_{\mathbf{x}}(U_{\mathbf{x}}\Psi(\mathbf{x}; \cdot)) + J_1(\mathbf{x}; \cdot) \cdot D_{\mathbf{y}}(U_{\mathbf{x}}\Psi(\mathbf{x}; \cdot)) + J_2(\mathbf{x}; \cdot)(U_{\mathbf{x}}\Psi(\mathbf{x}; \cdot)). \end{aligned}$$

By (3.20), this implies that, for  $\alpha \in \mathbb{N}^{3m}$  with  $|\alpha| = 1$ ,  $U(D_{\mathbf{x}}^{\alpha}\Psi) : \Omega_0 \ni \mathbf{x} \mapsto U_{\mathbf{x}}(D_{\mathbf{x}}^{\alpha}\Psi)(\mathbf{x}; \cdot) \in \mathcal{W}_1$  is well-defined and real analytic. Letting act  $U_{\mathbf{x}}D_{\mathbf{x}}U_{\mathbf{x}}^{-1}$  on the above equality and using (3.17), (3.20), and (3.21), we obtain that, for  $\alpha \in \mathbb{N}^{3m}$  with  $|\alpha| = 2$ ,  $U(D_{\mathbf{x}}^{\alpha}\Psi) : \Omega_0 \ni \mathbf{x} \mapsto U_{\mathbf{x}}(D_{\mathbf{x}}^{\alpha}\Psi)(\mathbf{x}; \cdot) \in \mathcal{W}_0$  is well-defined and real analytic.  $\square$

**Remark 3.10.** *We observe that the present framework (the one in Theorem 3.9) is closer to the one in [KMSW] than the one in Hunziker's original paper [Hu]. This comes from the fact that, here and in [KMSW], the considered Hamiltonian contains derivatives w.r.t. the "external" variable  $\mathbf{x}$ , whereas it is not the case in [Hu]. We further point out that a variant of Hunziker's twist is used in a similar way in [MM].*

## 4 Proof of the main results.

In this section, we provide a proof for our main results, namely Theorem 1.3, Theorem 1.4, and Theorem 1.5. We first prove the result on the current density  $C$ .

**Proof of Theorem 1.3:** Let  $x^0 \in \mathbb{R}^3 \setminus \{R_1, \dots, R_L\}$ . Notice that, if we set  $m = 1$  and  $p = N - 1$ , then  $\mathcal{U} = \mathbb{R}^3 \setminus \{R_1, \dots, R_L\}$ , by (3.5). Note that  $\underline{H} := H - E \in \text{Ham}(\mathbb{R}^3)$  and  $\underline{H}\psi = 0$ . Applying Theorem 3.9 to  $\underline{\Omega} = \mathbb{R}^{3m} = \mathbb{R}^3$  and  $\mathbf{x}^0 = x^0 \in \mathcal{U} \cap \underline{\Omega}$ , there exists some neighbourhood  $\Omega_0$  of  $x^0$  and a map  $U : \Omega_0 \ni x \mapsto U_x \in \mathcal{B}_0$ , the values of which are unitary operator on  $\mathcal{W}_0$ , such that, for all  $\alpha \in \mathbb{N}^3$  with  $|\alpha| \leq 1$ , the map  $U(D_x^\alpha \psi) : \Omega_0 \ni x \mapsto U_x(D_x^\alpha \psi)(x; \cdot) \in \mathcal{W}_{2-|\alpha|}$  is well-defined and real analytic.

Let  $\alpha \in \mathbb{N}^3$  with  $|\alpha| = 1$ . For  $x \in \Omega_0$ , we can write, since  $U_x$  is unitary,

$$\langle (D_x^\alpha \psi)(x; \cdot), \psi(x; \cdot) \rangle = \langle U_x(D_x^\alpha \psi)(x; \cdot), U_x \psi(x; \cdot) \rangle.$$

As the scalar product of real analytic,  $\mathcal{W}_0$ -valued maps, the map  $\Omega_0 \ni x \mapsto \langle (D_x^\alpha \psi), \psi \rangle$  is also real analytic. This gives the desired result by (1.5).  $\square$

Next we come to the proof of Theorem 1.4 on the densities  $\rho_k$ . We also comment on the limitation on the analyticity domain in this result (cf. Remark 4.2).

**Proof of Theorem 1.4:** Take an integer  $k$  such that  $0 < k < N$ . Let  $\underline{x}^0 = (x_1^0; \dots; x_k^0) \in \mathcal{U}_k^{(1)}$ . Setting  $m = k$  and  $p = N - k$ , we observe that  $\mathcal{U}_k^{(1)}$  coincide with the set  $\mathcal{U}$ , defined in (3.5). Since  $-\Delta = -\Delta_x - \Delta_y \in \text{Diff}_2(\mathbb{R}^{3m})$  and  $V - E$  is a potential of the type  $\underline{V}$  in (3.3) on  $\mathbb{R}^{3m} \times \mathbb{R}^{3p}$ , by Remark 3.4, we may apply Theorem 3.9 to  $\underline{H} = H - E$ ,  $\underline{\Omega} = \mathbb{R}^{3m}$ ,  $\Psi = \psi$ , and  $\mathbf{x}^0 = \underline{x}^0 \in \mathcal{U} \cap \underline{\Omega}$ . Thus there exist some neighbourhood  $\Omega_0$  of  $\underline{x}^0$  and a map  $U : \Omega_0 \rightarrow \mathcal{B}_0$ , with values in the set of unitary operators on  $\mathcal{W}_0$ , such that the map  $U\psi : \Omega_0 \ni \underline{x} \mapsto U_{\underline{x}}\psi(\underline{x}; \cdot) \in \mathcal{W}_2$  is well-defined and real analytic. For  $\underline{x} \in \Omega_0$ , the density  $\rho_k(\underline{x})$  is, by definition (see (1.3)), the squared  $\mathcal{W}_0$ -norm of  $\psi(\underline{x}; \cdot)$ , which is also the one of  $U_{\underline{x}}\psi(\underline{x}; \cdot)$ , since  $U_{\underline{x}}$  is unitary on  $\mathcal{W}_0$ . Thus,  $\rho_k$  is real analytic on  $\Omega_0$ .  $\square$

**Remark 4.1.** *In the  $k = 1$  case, the above proof reproduces the one of [J] on the density  $\rho = \rho_1$ . Thanks to Hunziker's twist, the proof in the general case is essentially identical.*

**Remark 4.2.** *Theorem 1.4 ensures the real analyticity of  $\rho_k$  on  $\mathcal{U}_k^{(1)}$ . We actually can give two obstacles to the extension of this property to a larger set by the method used in Section 3.*

*If we try to apply this method near a point  $\underline{x}^0 \in \mathcal{C}_k \cup \mathcal{R}_k$ , we have to work near the singularity of a term of the form  $|x_j - R_\ell|^{-1}$  or  $|x_j - x_{j'}|^{-1}$  with  $1 \leq j \neq j' \leq k$  and such a singular term would be unaffected by any twist. Thus, we cannot apply Theorem 2.2 to the twisted equation to get the result of Theorem 3.9.*

*The second obstacle takes place in the construction of the twist near such a point  $\underline{x}^0 \in \mathcal{C}_k \cup \mathcal{R}_k$ . To explain this, let us use the notation of Subsection 3.3 and consider a point  $\mathbf{x}^0$  such that, either  $x_j^0 = R_\ell$  or  $x_j^0 = x_{j'}^0$ , for  $j \neq j'$ . Assume that we have a function  $f$  defined on a neighbourhood of such  $\mathbf{x}^0$  times  $\mathbb{R}^3$  such that, for  $\mathbf{x}$  close to  $\mathbf{x}^0$ ,  $f(\mathbf{x}; \cdot)$  is a diffeomorphism on  $\mathbb{R}^3$  that satisfies (3.8). If  $x_j^0 = x_{j'}^0$ , then, for  $\mathbf{x}$  close to  $\mathbf{x}^0$  with different*

$x_j$  and  $x_{j'}$ , we would have  $x_j = f(x; x_j^0) = f(x; x_{j'}^0) = x_{j'}$ , which is a contradiction. If  $x_j^0 = R_\ell$ , then, for  $x$  close to  $x^0$  with  $x_j \neq R_\ell$ , we would have  $x_j = f(x; x_j^0) = f(x; R_\ell) = R_\ell$ , which is again a contradiction.

Finally, we prove Theorem 1.5 concerning the density matrices  $\gamma_k$ . Again we provide a comment on the limitation on the analyticity domain in this result (cf. Remark 4.4).

**Proof of Theorem 1.5:** Let  $k$  be an integer between 0 and  $N$ . Let  $\underline{x}^0 = (x_1^0; \dots; x_k^0)$  and  $\underline{x}'^0 = (x_1'^0; \dots; x_k'^0)$  two points in  $(\mathbb{R}^3)^k$  such that  $(\underline{x}^0; \underline{x}'^0) \in \mathcal{U}_k^{(2)}$ . Setting  $m = 2k$  and  $p = N - k$ , we note that  $\mathcal{U} = \mathcal{U}_k^{(2)}$ . Denoting by  $y$  the variable in  $\mathbb{R}^{3(N-2k)} = \mathbb{R}^{3p}$ , we consider the Hamiltonians  $H_1$  and  $H_2$  on  $(\mathbb{R}^{3k})^2 \times \mathbb{R}^{3(N-2k)} = \mathbb{R}^{3m} \times \mathbb{R}^{3p}$  defined by

$$H_1 = -\Delta_{\underline{x}} - \Delta_{\underline{x}'} - \Delta_y + V(\underline{x}; y) \quad \text{and} \quad H_2 = -\Delta_{\underline{x}} - \Delta_{\underline{x}'} - \Delta_y + V(\underline{x}'; y)$$

and the almost everywhere defined functions  $\Psi_1 : \mathbb{R}^{3m} \times \mathbb{R}^{3p} \ni (\underline{x}; \underline{x}'; y) \mapsto \psi(\underline{x}; y)$  and  $\Psi_2 : \mathbb{R}^{3m} \times \mathbb{R}^{3p} \ni (\underline{x}; \underline{x}'; y) \mapsto \psi(\underline{x}'; y)$ . We note that  $H_1 \in \text{Ham}_2(\mathbb{R}^{3m})$  and  $H_2 \in \text{Ham}_2(\mathbb{R}^{3m})$ . From  $H\psi = E\psi$ , we derive that  $H_1\Psi_1 = E\Psi_1$  and  $H_2\Psi_1 = E\Psi_2$ , in the distributional sense. Furthermore, for any bounded subset  $B$  of  $\mathbb{R}^{3m}$ , we observe that

$$\Psi_1 \in W^{2,2}(B \times \mathbb{R}_y^{3p}) \quad \text{and} \quad \Psi_2 \in W^{2,2}(B \times \mathbb{R}_y^{3p}).$$

Let  $B_0$  be a bounded neighbourhood of  $(\underline{x}^0; \underline{x}'^0)$ .

Now we apply Theorem 3.9 to  $\Omega = B_0$  and  $\underline{x}^0 = (\underline{x}^0; \underline{x}'^0) \in \mathcal{U} \cap \Omega$ . Therefore there exist a bounded neighbourhood  $\Omega_0$  of  $(\underline{x}^0; \underline{x}'^0)$  and a map  $U : \Omega_0 \rightarrow \mathcal{B}_0$ , with values in the set of unitary operators on  $\mathcal{W}_0$ , such that the maps  $U\Psi_1 : \Omega_0 \ni (\underline{x}; \underline{x}') \mapsto U_{\underline{x}; \underline{x}'}\Psi_1(\underline{x}; \underline{x}'; \cdot) \in \mathcal{W}_2$  and  $U\Psi_2 : \Omega_0 \ni (\underline{x}; \underline{x}') \mapsto U_{\underline{x}; \underline{x}'}\Psi_2(\underline{x}; \underline{x}'; \cdot) \in \mathcal{W}_2$  are well-defined and real analytic. Now, by definition of  $\gamma_k$  (see (1.4)), we have, for  $(\underline{x}; \underline{x}') \in \Omega_0$ ,

$$\gamma_k(\underline{x}; \underline{x}') = \langle \Psi_1(\underline{x}; \underline{x}'; \cdot), \Psi_2(\underline{x}; \underline{x}'; \cdot) \rangle = \langle U_{\underline{x}; \underline{x}'}\Psi_1(\underline{x}; \underline{x}'; \cdot), U_{\underline{x}; \underline{x}'}\Psi_2(\underline{x}; \underline{x}'; \cdot) \rangle,$$

since  $U_{\underline{x}; \underline{x}'}$  is unitary. As the scalar product of real analytic,  $\mathcal{W}_0$ -valued maps on  $\Omega_0$ ,  $\gamma_k$  is also real analytic on  $\Omega_0$ .  $\square$

**Remark 4.3.** We note that our proofs of Theorems 1.3, 1.4, and 1.5, have a common structure. They all use an appropriate twist and Theorem 3.9. Differences between them occur in the used set of variables.

**Remark 4.4.** According to the first obstacle mentioned in Remark 4.2, the method of Section 3 requires to work on  $\mathcal{U}_k^{(1)} \times \mathcal{U}_k^{(1)}$ . Now, because of the second obstacle mentioned there, we also need to exclude the set  $\mathcal{C}_k^{(2)}$  and, therefore, work on  $\mathcal{U}_k^{(2)} = (\mathcal{U}_k^{(1)} \times \mathcal{U}_k^{(1)}) \setminus \mathcal{C}_k^{(2)}$ .

## 5 Extensions.

In Section 3, we worked in a larger framework than the one that would be needed to treat the physical operator  $H$  in (1.1). It is thus natural to expect that our main results on  $H$  extend to a larger class of Hamiltonians. This is the case, as we shall see in this Section.

We consider again a system of  $N$  electrons, interacting to one another and moving under the influence of  $L$  fixed nuclei. Let  $\mathcal{I} := \{1; \dots; N\}$  be the set of indices for the electronic variables  $x \in \mathbb{R}^{3N}$  and let  $\mathcal{I}_n := \{1; \dots; L\}$  be the one of the nuclear variables  $R_\ell \in \mathbb{R}^3$ . It is convenient to introduce the distinct union of those sets, namely

$$\mathcal{I} \sqcup \mathcal{I}_n := \{(a; j); a \in \{e; n\}, j \in \mathcal{I}_a\}.$$

For  $c = (a; j) \in \mathcal{I}_e \sqcup \mathcal{I}_n$ , let  $\pi_1(c) = a$  and  $\pi_2(c) = j$ . We define  $X_c = x_j$  if  $\pi_1(c) = e$  and  $X_c = R_j$  if  $\pi_1(c) = n$ . Let

$$\tilde{\mathcal{P}} := \{\{c; c'\}; (c; c') \in (\mathcal{I}_e \sqcup \mathcal{I}_n)^2 \text{ and } c \neq c'\}$$

be the set of all possible particle pairings. We consider a potential  $\tilde{V}$  where

$$\forall x \in \mathbb{R}^{3N}, \quad \tilde{V}(x) = \sum_{\{c; c'\} \in \tilde{\mathcal{P}}} V_{\{c; c'\}}(X_c - X_{c'}), \quad (5.1)$$

with  $V_{\{c; c'\}} \in \mathcal{V}$  (cf. Definition 3.1), for all  $\{c; c'\} \in \tilde{\mathcal{P}}$ .

Now, let  $\tilde{P} = \tilde{P}(x; D_x)$  a differential operator on  $\mathbb{R}^{3N}$  of the form

$$\tilde{P} = \sum_{\substack{\alpha \in \mathbb{N}^{3N} \\ |\alpha| \leq 2}} \tilde{c}_\alpha(x) D_x^\alpha, \quad (5.2)$$

where the coefficients  $\tilde{c}_\alpha$  belong to  $\mathcal{C}_b^\infty(\mathbb{R}^{3N}; \mathbb{C})$ . Let  $\tilde{H} = \tilde{P} + \tilde{V}$  and assume that there exists  $\tilde{\psi} \in W^{2,2}(\mathbb{R}^{3N})$  such that  $\tilde{H}\tilde{\psi} = 0$ . For  $0 < k < N$ , we still denote by  $\rho_k$ ,  $\gamma_k$ , and  $C$  the objects that are respectively defined by (1.3), (1.4), and (1.5), with  $\psi$  replaced by  $\tilde{\psi}$ .

**Theorem 5.1.** *Under the above assumptions on  $\tilde{H}$  and  $\tilde{\psi}$ , the results of Theorems 1.3, 1.4, and 1.5, are valid.*

**Proof:** We can follow the above proofs of Theorems 1.3, 1.4, and 1.5. In the later, we use the elliptic operators

$$H_1 = -\Delta_{\underline{x}'} - \tilde{P}(\underline{x}; y; D_{\underline{x}}; D_y) + \tilde{V}(\underline{x}; y) \quad \text{and} \quad H_2 = -\Delta_{\underline{x}} - \tilde{P}(\underline{x}'; y; D_{\underline{x}'}; D_y) + \tilde{V}(\underline{x}'; y)$$

and the almost everywhere defined functions  $\Psi_1 : \mathbb{R}^{3m} \times \mathbb{R}^{3p} \ni (\underline{x}; \underline{x}'; y) \mapsto \tilde{\psi}(\underline{x}; y)$  and  $\Psi_2 : \mathbb{R}^{3m} \times \mathbb{R}^{3p} \ni (\underline{x}; \underline{x}'; y) \mapsto \tilde{\psi}(\underline{x}'; y)$ .  $\square$

**Remark 5.2.** *We point out that the present class of operators includes Laplace-Beltrami operators associated to appropriate metrics. One can also replace  $D_x$  by  $D_x - A(x)$ , where  $A$  is a real analytic vector potential in  $\mathcal{C}_b^\infty(\mathbb{R}^{3N}; \mathbb{R}^3)$ , and add an external electric potential  $V_e$  in  $\mathcal{C}_b^\infty(\mathbb{R}^{3N}; \mathbb{C})$ , that is also real analytic.*

*Notice that the class  $\mathcal{V}$  in Definition 3.1 contains non-radial pair potentials. Among the admissible functions  $\eta$  used to define  $\mathcal{V}$ , we have  $0 < t \mapsto t^{-1}$  but we can also choose  $0 < t \mapsto t^{-1}(\ln(t))^{-\epsilon}$ , with  $\epsilon > 0$ . We observe that this class  $\mathcal{V}$  is contained in the class of pair potentials used in [FS].*

## A Appendix

In this Appendix, we provide explicit formulae for several objects related to the twist  $U$  in Subsection 3.3 and the computation of the principal symbol of some differential operator, that is needed in Subsection 3.5.

First of all, let us notice that, from the expressions of  $d_x f$  and  $d_z f$ , there exists some  $\tau$ ,  $r_0$ , and  $x^0$  dependent constant  $M$ , such that, denoting by  $I_3$  the identity on  $\mathbb{R}^3$ ,

$$\forall \mathbf{x} \in \mathbb{R}^{3m}, \forall z \in \mathbb{R}^3, |z| \geq M \implies ((d_x f)(\mathbf{x}; z) = 0 \text{ and } (d_z f)(\mathbf{x}; z) - I_3 = 0). \quad (\text{A.1})$$

Using (3.12), we can find some  $c > 0$  such that

$$\forall (\mathbf{x}; z) \in \Omega(\delta_0) \times \mathbb{R}^3, c^{-1} \leq \|((d_z f)(\mathbf{x}; z))^{-1}\|_{\mathcal{L}(\mathbb{R}^3)} + \|(d_z f)(\mathbf{x}; z)\|_{\mathcal{L}(\mathbb{R}^3)} \leq c. \quad (\text{A.2})$$

For  $\mathbf{x} \in \Omega(\delta_0)$ ,  $j \in \mathbb{N} \cap [1; m]$ , and  $z \in \mathbb{R}^3$ , we have

$$f^{(-1)}(\mathbf{x}; f(\mathbf{x}; z)) = z.$$

By differentiation of this equality and by using (3.9), we obtain, with equalities in  $\mathcal{L}(\mathbb{R}^3)$ , in  $\mathcal{L}(\mathbb{R}^3)$ , and in  $\mathcal{L}(\mathbb{R}^{3m}; \mathbb{R}^3)$ , respectively,

$$(d_z f^{(-1)})(\mathbf{x}; f(\mathbf{x}; z)) = ((d_z f)(\mathbf{x}; z))^{-1}, \quad (\text{A.3})$$

$$(d_{x_j} f^{(-1)})(\mathbf{x}; f(\mathbf{x}; z)) = -\tau(r_0^{-1}(z - x_j^0))(d_z f^{(-1)})(\mathbf{x}; f(\mathbf{x}; z)), \quad (\text{A.4})$$

$$(d_x f^{(-1)})(\mathbf{x}; f(\mathbf{x}; z)) = -(d_z f^{(-1)})(\mathbf{x}; f(\mathbf{x}; z)) \circ \sum_{j'=1}^m \tau(r_0^{-1}(z - x_{j'}^0)) dx_{j'}. \quad (\text{A.5})$$

Now, using (A.1), (A.2), (A.3), (A.4), and (A.5), it is straightforward to check that

$$f \in \mathcal{C}_b^\infty(\Omega(\delta_0) \times \mathbb{R}^3; \mathbb{R}^3) \quad \text{and} \quad f^{(-1)} \in \mathcal{C}_b^\infty(\Omega(\delta_0) \times \mathbb{R}^3; \mathbb{R}^3). \quad (\text{A.6})$$

From the very definition of  $F$ , we note that, for  $\mathbf{x} \in \Omega(\delta_0)$ ,  $x^\epsilon \in \mathbb{R}^{3m}$ , and  $y \in \mathbb{R}^{3p}$ ,

$$(d_x F)(\mathbf{x}; y) \cdot x^\epsilon = ((d_x f)(\mathbf{x}; y_1) \cdot x^\epsilon; \dots; (d_x f)(\mathbf{x}; y_p) \cdot x^\epsilon) \in \mathbb{R}^{3p}$$

and the  $k$ -th component (with  $k \in \mathbb{N} \cap [1; p]$ ) in the latter expression is given by

$$(d_x f)(\mathbf{x}; y_k) \cdot x^\epsilon = \sum_{j=1}^m \tau(r_0^{-1}(y_k - x_j^0)) x_j^\epsilon \in \mathbb{R}^3,$$

by (3.9). For  $\mathbf{x} \in \Omega(\delta_0)$ ,  $y \in \mathbb{R}^{3p}$ ,  $z \in \mathbb{R}^3$ , and  $k \in \mathbb{N} \cap [1; p]$ , we have

$$(d_{y_k} F)(\mathbf{x}; y) \cdot z = (0; \dots; 0; (d_z f)(\mathbf{x}; y_k) \cdot z; 0; \dots; 0) \in \mathbb{R}^{3p}$$

(the term containing  $z$  being in the  $k$ th position) and, for  $y^\epsilon \in \mathbb{R}^{3p}$ ,

$$(d_y F)(\mathbf{x}; y) \cdot y^\epsilon = \sum_{k=1}^p (0; \dots; 0; (d_z f)(\mathbf{x}; y_k) \cdot y_k^\epsilon; 0; \dots; 0) \in \mathbb{R}^{3p}$$

$$= y^\epsilon + r_0^{-1} \sum_{k=1}^p \sum_{j=1}^m \left( 0; \dots; 0; ((d\tau)(r_0^{-1}(y_k - x_j^0)) \cdot y_k^\epsilon)(x_j - x_j^0); 0; \dots; 0 \right),$$

by (3.11), each term containing  $d\tau$  being in the  $k$ th position. Since we can write, for  $x \in \Omega(\delta_0)$  and  $y \in \mathbb{R}^{3p}$ ,

$$F^{(-1)}(x; y) = (f^{(-1)}(x; y_1); \dots; f^{(-1)}(x; y_p)) \in \mathbb{R}^{3p},$$

we have, for  $x^\epsilon \in \mathbb{R}^{3m}$ ,

$$\begin{aligned} & (d_x F^{(-1)})(x; F(x; y)) \cdot x^\epsilon \\ &= ((d_x f^{(-1)})(x; f(x; y_1)) \cdot x^\epsilon; \dots; (d_x f^{(-1)})(x; f(x; y_p)) \cdot x^\epsilon) \in \mathbb{R}^{3p}, \end{aligned}$$

where  $d_x f^{(-1)}$  is given by (A.5). Finally, for  $y^\epsilon \in \mathbb{R}^{3p}$ , we have

$$\begin{aligned} & (d_y F^{(-1)})(x; F(x; y)) \cdot y^\epsilon \\ &= \sum_{k=1}^p (0; \dots; 0; (d_z f^{(-1)})(x; f(x; y_k)) \cdot y_k^\epsilon; 0; \dots; 0) \in \mathbb{R}^{3p}, \end{aligned}$$

where  $d_z f^{(-1)}$  is explicited in (A.3).

We derive from (A.6) that

$$F \in \mathcal{C}_b^\infty(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{R}^{3p}) \quad \text{and} \quad F^{(-1)} \in \mathcal{C}_b^\infty(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{R}^{3p}). \quad (\text{A.7})$$

Next, we compute the terms  $J_k(G)$ , for  $1 \leq k \leq 4$  and  $G \in \{F; F^{(-1)}\}$ , that appear in (3.16), (3.17), (3.18), and (3.19).

Let  $G \in \{F; F^{(-1)}\}$ . Let us consider the smooth functions  $\rho_\pm \in \mathcal{C}^\infty(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{R})$  defined by

$$\rho_+(x; y) = |\text{Det}(d_y G)(x; y)|^{1/2} \quad \text{and} \quad \rho_-(x; y) = |\text{Det}(d_y G^{(-1)})(x; y)|^{1/2}.$$

From the identity  $G^{(-1)}(x; G(x; y)) = (x; y)$ , we derive that  $\rho_+(x; y)\rho_-(x; G(x; y)) = 1$ . Let  $\varphi \in \mathcal{C}^\infty(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{R})$ . We set

$$(U_G \varphi)(x; y) = \rho_+(x; y) \varphi(x; G(x; y)) \quad \text{and} \quad (U_G^{(-1)} \varphi)(x; y) = \rho_-(x; y) \varphi(x; G^{(-1)}(x; y)).$$

Since

$$\begin{aligned} d_x (U_G^{(-1)} \varphi)(x; y) &= \varphi(x; G^{(-1)}(x; y)) d_x \rho_-(x; y) \\ &\quad + \rho_-(x; y) (d_x \varphi)(x; G^{(-1)}(x; y)) \\ &\quad + \rho_-(x; y) (d_y \varphi)(x; G^{(-1)}(x; y)) (d_x G^{(-1)})(x; y), \end{aligned}$$

we have, for  $x_\epsilon \in \mathbb{R}^{3m}$ ,

$$\begin{aligned} d_x (U_G^{(-1)} \varphi)(x; y) x_\epsilon &= \varphi(x; G^{(-1)}(x; y)) \nabla_x \rho_-(x; y) \cdot x_\epsilon \\ &\quad + \rho_-(x; y) (\nabla_x \varphi)(x; G^{(-1)}(x; y)) \cdot x_\epsilon \\ &\quad + \rho_-(x; y) (\nabla_y \varphi)(x; G^{(-1)}(x; y)) \cdot (d_x G^{(-1)})(x; y) x_\epsilon, \end{aligned}$$

with scalar products in  $\mathbb{R}^{3m}$ ,  $\mathbb{R}^{3m}$ , and  $\mathbb{R}^{3p}$ , respectively. This yields

$$\begin{aligned}\nabla_{\mathbf{x}}(U_G^{(-1)}\varphi)(\mathbf{x}; \mathbf{y}) &= \varphi(\mathbf{x}; G^{(-1)}(\mathbf{x}; \mathbf{y})) \nabla_{\mathbf{x}}\rho_{-}(\mathbf{x}; \mathbf{y}) \\ &\quad + \rho_{-}(\mathbf{x}; \mathbf{y}) (\nabla_{\mathbf{x}}\varphi)(\mathbf{x}; G^{(-1)}(\mathbf{x}; \mathbf{y})) \\ &\quad + \rho_{-}(\mathbf{x}; \mathbf{y}) (d_{\mathbf{x}}G^{(-1)})^T(\mathbf{x}; \mathbf{y})(\nabla_{\mathbf{y}}\varphi)(\mathbf{x}; G^{(-1)}(\mathbf{x}; \mathbf{y})) .\end{aligned}$$

Thus, using  $\rho_{+}(\mathbf{x}; \mathbf{y})\rho_{-}(\mathbf{x}; G(\mathbf{x}; \mathbf{y})) = 1$ ,

$$\begin{aligned}(U_G\nabla_{\mathbf{x}}U_G^{(-1)}\varphi)(\mathbf{x}; \mathbf{y}) &= \rho_{+}(\mathbf{x}; \mathbf{y})\varphi(\mathbf{x}; \mathbf{y}) (\nabla_{\mathbf{x}}\rho_{-})(\mathbf{x}; G(\mathbf{x}; \mathbf{y})) + (\nabla_{\mathbf{x}}\varphi)(\mathbf{x}; \mathbf{y}) \\ &\quad + (d_{\mathbf{x}}G^{(-1)})^T(\mathbf{x}; G(\mathbf{x}; \mathbf{y}))(\nabla_{\mathbf{y}}\varphi)(\mathbf{x}; \mathbf{y}) .\end{aligned}$$

Since

$$\begin{aligned}d_{\mathbf{y}}(U_G^{(-1)}\varphi)(\mathbf{x}; \mathbf{y}) &= \varphi(\mathbf{x}; G^{(-1)}(\mathbf{x}; \mathbf{y})) d_{\mathbf{y}}\rho_{-}(\mathbf{x}; \mathbf{y}) \\ &\quad + \rho_{-}(\mathbf{x}; \mathbf{y}) (d_{\mathbf{y}}\varphi)(\mathbf{x}; G^{(-1)}(\mathbf{x}; \mathbf{y})) (d_{\mathbf{y}}G^{(-1)})(\mathbf{x}; \mathbf{y}) ,\end{aligned}$$

we have, for  $\mathbf{y}_{\epsilon} \in \mathbb{R}^{3p}$ ,

$$\begin{aligned}d_{\mathbf{y}}(U_G^{(-1)}\varphi)(\mathbf{x}; \mathbf{y})\mathbf{y}_{\epsilon} &= \varphi(\mathbf{x}; G^{(-1)}(\mathbf{x}; \mathbf{y})) \nabla_{\mathbf{y}}\rho_{-}(\mathbf{x}; \mathbf{y}) \cdot \mathbf{y}_{\epsilon} \\ &\quad + \rho_{-}(\mathbf{x}; \mathbf{y}) (\nabla_{\mathbf{y}}\varphi)(\mathbf{x}; G^{(-1)}(\mathbf{x}; \mathbf{y})) \cdot (d_{\mathbf{y}}G^{(-1)})(\mathbf{x}; \mathbf{y})\mathbf{y}_{\epsilon} ,\end{aligned}$$

with scalar products in  $\mathbb{R}^{3p}$ . This yields

$$\begin{aligned}\nabla_{\mathbf{y}}(U_G^{(-1)}\varphi)(\mathbf{x}; \mathbf{y}) &= \varphi(\mathbf{x}; G^{(-1)}(\mathbf{x}; \mathbf{y})) \nabla_{\mathbf{y}}\rho_{-}(\mathbf{x}; \mathbf{y}) \\ &\quad + \rho_{-}(\mathbf{x}; \mathbf{y}) (d_{\mathbf{y}}G^{(-1)})^T(\mathbf{x}; \mathbf{y})(\nabla_{\mathbf{y}}\varphi)(\mathbf{x}; G^{(-1)}(\mathbf{x}; \mathbf{y})) .\end{aligned}$$

Thus, using  $\rho_{+}(\mathbf{x}; \mathbf{y})\rho_{-}(\mathbf{x}; G(\mathbf{x}; \mathbf{y})) = 1$ ,

$$\begin{aligned}(U_G\nabla_{\mathbf{y}}U_G^{(-1)}\varphi)(\mathbf{x}; \mathbf{y}) &= \rho_{+}(\mathbf{x}; \mathbf{y})\varphi(\mathbf{x}; \mathbf{y}) (\nabla_{\mathbf{y}}\rho_{-})(\mathbf{x}; G(\mathbf{x}; \mathbf{y})) \\ &\quad + (d_{\mathbf{x}}G^{(-1)})^T(\mathbf{x}; G(\mathbf{x}; \mathbf{y}))(\nabla_{\mathbf{y}}\varphi)(\mathbf{x}; \mathbf{y}) .\end{aligned}$$

This proves (3.16), (3.17), (3.18), and (3.19). Now, taking into account (A.7), we obtain (3.20) and (3.21). Using (A.2) and (A.3), we see that (3.23) holds true.

Finally, we compute the principal symbol  $\sigma_P$  appearing in the proof of Proposition 3.6. In the vector space of polynomials in  $\mathbb{R}^{3m} \times \mathbb{R}^{3p}$  with  $\mathcal{C}_b^{\infty}(\Omega(\delta_0) \times \mathbb{R}^{3p}; \mathbb{C})$ -coefficients, we denote by  $\equiv$  the equality of polynomials modulo polynomials of degree less than 2. Then, for  $(\mathbf{x}; \mathbf{y}; \xi; \eta) \in \Omega(\delta_0) \times \mathbb{R}^{3p} \times \mathbb{R}^{3m} \times \mathbb{R}^{3p}$ , we have, by (3.29), (3.17), and (3.19),

$$\begin{aligned}&\sigma_P(\mathbf{x}; \mathbf{y}; \xi; \eta) \\ &\equiv S_P(\mathbf{x}; \mathbf{y}; \xi; \eta) \\ &\equiv \sum_{\substack{(\alpha; \beta) \in \mathbb{N}^{3m} \times \mathbb{N}^{3p} \\ |\alpha| + |\beta| = 2}} c_{\alpha\beta}(\mathbf{x}; F(\mathbf{x}; \mathbf{y})) \left( \xi + J_1(F^{(-1)})(\mathbf{x}; \mathbf{y}) \eta + J_2(F^{(-1)})(\mathbf{x}; \mathbf{y}) \right)^{\alpha} \\ &\quad \times \left( J_3(F^{(-1)})(\mathbf{x}; \mathbf{y}) \eta + J_4(F^{(-1)})(\mathbf{x}; \mathbf{y}) \right)^{\beta} \\ &\equiv \sum_{\substack{(\alpha; \beta) \in \mathbb{N}^{3m} \times \mathbb{N}^{3p} \\ |\alpha| + |\beta| = 2}} c_{\alpha\beta}(\mathbf{x}; F(\mathbf{x}; \mathbf{y})) \left( \xi + J_1(F^{(-1)})(\mathbf{x}; \mathbf{y}) \eta \right)^{\alpha} \left( J_3(F^{(-1)})(\mathbf{x}; \mathbf{y}) \eta \right)^{\beta}\end{aligned}$$



and the last term is actually  $\sigma_P(\mathbf{x}; y; \xi; \eta)$ , since it is homogeneous of degree 2. Thus

$$\sigma_P(\mathbf{x}; y; \xi; \eta) = \sigma_P\left(\mathbf{x}; F(\mathbf{x}; y); \xi + J_1(F^{(-1)})(\mathbf{x}; y) \eta; J_3(F^{(-1)})(\mathbf{x}; y) \eta\right),$$

yielding (3.30).

## References

- [ACN] B. Ammann, C. Carvalho, V. Nistor: *Regularity for eigenfunctions of Schrödinger operators*. Lett. Math. Phys. **101**, (2012), no. **1**, 49-84.
- [CFKS] H.L. Cycon, R.G. Froese, W. Kirsch, B. Simon: *Schrödinger operators with applications to quantum mechanics and global geometry*. Springer, 1987.
- [E] H. Eschrig: *The fundamentals of density functional theory*. B.G. Teubner Verlagsgesellschaft Stuttgart-Leipzig 1996.
- [FHHS1] S. Fournais, M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, T. Østergaard Sørensen: *The electron density is smooth away from the nuclei*. Comm. Math. Phys. **228**, no. **3** (2002), 401-415.
- [FHHS2] S. Fournais, M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, T. Østergaard Sørensen: *Analyticity of the density of electronic wave functions*. Ark. Mat. **42**, no. **1** (2004), 87-106.
- [FHHS3] S. Fournais, M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, T. Østergaard Sørensen: *Non-isotropic cusp conditions and regularity of the electron density of molecules at the nuclei*. Ann. Henri Poincaré **8** (2007), 731-748.
- [FHHS4] S. Fournais, M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, T. Østergaard Sørensen: *Analytic structure of many-body coulombic wave functions*. Comm. Math. Phys. **289**, no. (2009), 291-310.
- [FS] S. Fournais, T. Østergaard Sørensen: *Pointwise estimates on derivatives of Coulombic wave functions and their electron densities*. . Accepted for publication in J. Reine Angew. Math.  
arXiv: arXiv:1803.03495.
- [FH] R.G. Froese, I. Herbst: *Exponential bounds and absence of positive eigenvalues for N-body Schrödinger operators*. Comm. Math. Phys. **87**, no. **3**, 429-447 (1982).
- [G] L. Garrigue: *Hohenberg-Kohn Theorems for interactions, spins, and temperature*. J. Stat. Phys. (2019). DOI: “<https://doi.org/10.1007/s10955-019-02365-6>”.
- [GS] A. Grigis, J. Sjöstrand: *Microlocal analysis for differential operators. An introduction*. Cambridge university press (1994).

- [HS] P. Hearnshaw, A.V. Sobolev: *Analyticity of the one-particle density matrix*. Preprint arxiv 2006.  
“ <https://arxiv.org/abs/2006.11785> ”.
- [Hö1] L. Hörmander: *Linear partial differential operators*. Fourth printing Springer Verlag, 1976.
- [Hö2] L. Hörmander: *The analysis of linear partial differential operators III*. Springer Verlag, 1985.
- [Hö3] L. Hörmander: *An introduction to complex analysis in several variables*. Elsevier science publishers B.V., 1990.
- [Hö4] L. Hörmander: *The analysis of linear partial differential operators IV*. Springer Verlag, 1985.
- [Hu] W. Hunziker: *Distortion analyticity and molecular resonance curves*. Ann. Inst. H. Poincaré, section A, tome **45**, no **4**, p. 339-358 (1986).
- [J] Th. Jecko: *A new proof of the analyticity of the electronic density of molecules*. Lett. Math. Phys. (2010), **93**, pp. 73-83.
- [K] T. Kato: *On the eigenfunctions of many-particle systems in Quantum Mechanics*. Comm. Pure Appl. Maths, vol. **10**, 151-177 (1957).
- [KMSW] M. Klein, A. Martinez, R. Seiler, X.P. Wang: *On the Born-Oppenheimer expansion for polyatomic molecules*. Comm. Math. Phys. **143**, no. **3**, 607-639 (1992).
- [Le] M. Lewin: *Geometric methods for non-linear many-body quantum systems*. J. Funct. Ana. **260** (2011), pp. 3535-3595.
- [Li] E. H. Lieb: *Thomas-Fermi and related theories of atoms and molecules*. in *Rigorous atomic and molecular Physics*. Ed. G. Velo and A.S. Wightman, Plenum Press (1980), pp. 213-308.
- [LSc] E.H. Lieb, R. Seiringer: *Current Densities in Density Functional Theory*. Physical Review A, **88**, 10.1103/PhysRevA.88.032516 (2013).
- [LiSe] E.H. Lieb, R. Seiringer: *The stability of matter in quantum mechanics*. Cambridge university press (2010).
- [MM] A. Martinez, B. Messirdi: *Resonances of diatomic molecules in the Born-Oppenheimer approximation*. CPDE **19** (7&8), pp. 1139-1162, (1994).
- [MS] A. Martinez, V. Sordani: *Twisted pseudodifferential calculus and application to the quantum evolution of molecules*. Memoirs Am. Math. Soc., Vol. **200**, n. **936** (2009).
- [RS2] M. Reed, B. Simon: *Methods of Modern Mathematical Physics, Vol. II : Fourier Analysis, Self-adjointness*. Academic Press, 1979.
- [RS4] M. Reed, B. Simon: *Methods of Modern Mathematical Physics, Vol. IV : Analysis of operators*. Academic Press, 1979.