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THE RELATION BETWEEN THE (N) AND (N-1) ELECTRONS
ATOMIC GROUND STATE

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ABSTRACT : The relations between the ground state of an N and (N-1) electrons atomic system are studied. We show that in some directions of the configuration space, the ratio of the N electrons atomic ground state to the one particle density is asymptotically equivalent to the (N-1) electrons atomic ground state.

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I - INTRODUCTION

We consider the Schrodinger operator associated to an atomic system with N electrons and infinitely heavy nucleus with charge Z :

$$1.1 \quad H^N = -\sum_{i=1}^{N} \Delta_i - \sum_{i=1}^{N} \frac{Z}{|x_i|} + \sum_{i\neq j}^{N} \frac{1}{|x_i - x_j|}$$

The asymptotic behaviour of the ground state ρ_0^N associated to H^N has been studied by many authors [1] ; [2] ; [3] ; [4] . Recently Agmon [5] , Carmona-Simon [6] obtained the following bounds :

$$1.2 \quad \forall \delta > 0 ; \forall x \in \mathbb{R}^{3N} ; \quad C e^{-(1+\delta)\gamma(x)} \leq \rho_0^N(x) \leq D e^{-(1-\delta)\gamma(x)}$$

Here $\gamma(x)$ is the Agmon metric's associated to (1.1) ; it gives a non isotropic asymptotic behaviour for ρ_0^N depending on the direction along which X goes to infinity in the configuration space of electrons. Along this line of result, we want to show that for large $|x_1|$ one can obtain ρ_0^N as a product of the (N-1) particles ground state ρ_0^{N-1} and the one particle density :

$$\rho^{1/2}(x_1) = \left(\int |\rho_0^N|^2 dx^{3(N-1)} \right)^{1/2}$$

More precisely we prove the conjecture of J. Morgan and T.Hoffman-Ostenof :

$$1.3 \quad \lim_{|x_1| \to \infty} \left\| \frac{\rho_0^N}{\rho^{1/2}} - \rho_0^{N-1} \right\|_{L^2(\mathbb{R}^{3(N-1)})} = 0$$

We shall show also a stronger version of (1.3) :

$$1.4 \quad \lim_{|x_1| \to \infty} \left(\frac{\rho_0^N}{\rho^{1/2}} , \left(H^{N-1} - E_0^{N-1} \right) \frac{\rho_0^N}{\rho^{1/2}} \right)_{L^2(\mathbb{R}^{3(N-1)})} = 0$$

The formulas (1.3) and (1.4) were obtained by Combes-Hoffman-Ostenof [7] for helium like systems. For N-body systems Lieb-Simon [8] proved (1.3) in the special case where the potentials have compact support.

To prove (1.3) and (1.4) we extend the Combes-Hoffman-Ostenof's method with the help of the bounds (1.2). An essential ingredient of this approach is the fundamental density associated to ρ_0^N :

$$u(x_1) = \left(\rho_0^N , \rho_0^{N-1} \right)_{L^2(\mathbb{R}^{3(N-1)})} (x_1),$$

The function u possesses some interesting properties for our problem : on the one hand u is a lower bound asymptotically equal to $\rho^{1/2}$ and on the other hand u is the solution of a one particle Schrodinger equation with a potential V_e of the form :

$$1.5 \quad V_e(|x_1|) \sim \frac{Z-(N-1)}{|x_1|} \quad \text{for large } |x_1|$$

This provides us the detailed information required for the proof of (1.3) and (1.4). This proof involves some slight modifications of the complex boost method as used in [1] ; [3] . As in this last paper we will also use the so called geometrical technics in the operator form developped e.g. in [2] , [17] , [14] .

In chapter II, we recall the results obtained in [7] and adapt them to our problem, properties on function u are *described in chapter III. The chapter IV is devoted to the* spectral analysis of operators that we shall need in chapter IV to prove the formulas (1.3) and (1.4).

II - PRELIMINARS - RESULTS

The proof of formulas (1.3) and (1.4) requires the generalization of some results obtained by Combes-Hoffman-Ostenof [7] namely theorem 2-1 below for its proof we need no more supplementary material than in [7] and we shall describe here only the relevant part.

Let P be the orthogonal projection operator on $L^2(\mathbb{R}^{3N})$ defined by :

$$2.1 \quad \forall \Psi \in L^2(\mathbb{R}^{3(N)}) ; \quad (P\Psi)(x) = (\Psi, \rho_0^{N-1})_{L^2(\mathbb{R}^{3(N-1)})}(x_1) \cdot \rho_0^{N-1}(x_2, \dots x_N)$$

and $Q = \mathbb{1} - P$

If $\Psi = \rho_0^N$ we set $u = (\rho_0^N, \rho_0^{N-1})_{L^2(\mathbb{R}^{3(N-1)})}$. From its definitions and properties of ρ_0^N [10] u is continuous, strictly positive and spherically symmetric.

For $\alpha \in \mathbb{R}$ consider the unitary group on $L^2(\mathbb{R}^{3N})$ defined by :

$$2.2 \quad \forall \Psi \in L^2(\mathbb{R}^{3N}) ; \quad (V(\alpha)\Psi)(x) = (e^{-i\alpha \ln(u)} \cdot \Psi)(x)$$

One has :

2.3 $$H^N(\alpha) = V(\alpha) H^N V(\alpha)^{-1} = \left(i\nabla_1 + \alpha \frac{\nabla u}{u}\right)^2 - \sum_{i=2}^{N} \Delta_i - \sum_{i=1}^{N} \frac{2}{|x_i|} + \sum_{i\neq j}^{N} \frac{1}{|x_i - x_j|}$$

Under the conditions (*) on u (cf. §3, remark 3.3), $\{H^N(\alpha) ; \alpha \in \mathbb{R}\}$ can be analytically continued to the whole complex plane into a self adjoint holomorphic family of type A.

Let $W^{2,2}(\mathbb{R}^{3N})$ denote the usual Sobolev-space, and Ω the unit ball in $\mathbb{C}$, we have the following result :

<u>Theorem 2.1</u> : $V(\alpha) Q \rho_0^N = u^{-i\alpha} Q \rho_0^N \in W^{2,2}(\mathbb{R}^{3N})$ as long as $E_0^N \notin \sigma_{ess}(H^N(\alpha) + \delta P)$ for some $\delta > 0$ and $\alpha \in \Omega$.

<u>Sketch of proof</u>

By using the well known partionning technic [18] one gets :

2.4 $$\forall \alpha \in \mathbb{R} ;\ u^{-i\alpha} Q \rho_0^N = (E_0^N - Q H^N(\alpha) Q)^{-1} \left(\sum_{j>1} Q \frac{1}{|x_1 - x_j|} u^{1-i\alpha} \rho_0^{N-1} \right)$$

Now it is sufficient to show that under the conditions of theorem 2.1, the rhs of 2.4 has a $L^2(\mathbb{R}^{3N})$ - continuous continuation in Ω. But this is true if $(E_0^N - Q H(\alpha) Q)^{-1}$ is a bounded family of operators in Ω, in other words if $E_0^N \notin \sigma(Q H(\alpha) Q)$

On the one hand $E_0^N \notin \sigma_{ess}(H^N(\alpha) + \delta P)$ *by assumption, then*

$E_0^N \notin \sigma_{ess}(P H^N(\alpha) P + \delta P + Q H^N(\alpha) Q)$ since $\sum_{j>1} P \frac{1}{|x_1 - x_j|} Q + Q \frac{1}{|x_1 - x_j|} P$ is $H^N(\alpha)$ -compact [19] .

On the other hand, by some standards analyticity arguments [1] , $E_0^N \notin \sigma_d(P H^N(\alpha) P + \delta P + Q H^N(\alpha) Q)$ if $E_0^N \notin \sigma_d(P H^N P + \delta P + Q H^N Q)$ Suppose that $E_0^N \in \sigma_d(P H^N P + \delta P)$ then $\inf_{\psi} (\psi, H^N \psi) \geq E_0^N + \delta$. This is a contradiction. Now if $E_0^N \in \sigma_d(Q H^N Q)$ then $P \rho_0^N = 0$ and $u = 0$ which contradicts the positivity of u . We conclude $E_0^N \notin \sigma(P H^N(\alpha) P + \delta P + Q H^N(\alpha) Q)$ therefore $E_0^N \notin \sigma(Q H^N(\alpha) Q)$

To complete this proof, we must show that $\left(\sum_{j>1} Q \frac{1}{|x_1 - x_j|} u^{1-i\alpha} \rho_0^N\right)$ is a family of $L^2(\mathbb{R}^{3N})$ vectors continuous in Ω ,which can be seen in [7] .

<u>III - The fondamental density associated to</u>

The analysis of the essential spectrum of the operators family $\{H^N(\alpha) ; \alpha \in \mathbb{C}\}$ is a subtle point because the operators are non-self-adjoint. It will require some *results on the fundamental density* u *and in particular on the* asymptotic behaviour of $\nabla u / u$. This is the purpose of this present section.

The study of u is based on the following one particle Schrodinger equation [4] ; [8] :

$$3.1 \quad \left[-\Delta_1 - \frac{Z}{|x_1|} + (N-1)V_e\right]u = -\mathcal{E}u$$

Here $\mathcal{E}$ is the ionisation energy $\mathcal{E} = E_0^{N-1} - E_0^N$ and $V_e(|x_1|)$ is a screened potential :

$$3.2 \quad V_e(|x_1|) = u^{-1}(|x_1|) \cdot \int \frac{\rho_0^N \cdot \rho_0^{N-1}}{|x_1 - x_j|} dy^{3(N-1)} \quad ; \text{ for some } j \neq 1$$

The equation 3.1 is easily obtained from the identity : $\left([H^N - E_0^N]\rho_0^N , \rho_0^{N-1} \right)_{L^2(\mathbb{R}^{3(N-1)})} = 0$. The "effective" potential $V_e(|x_1|)$ is continuous, strictly positive and spherically symmetric function, and we have the following :

<u>Lemma 3.1</u>: V_e satisfies the pointwise estimate:

$$3.3 \quad V_e(|x_1|) \leq C \cdot \frac{N-1}{|x_1|} + O\left(|x_1| e^{-\alpha|x_1|}\right) \qquad \text{for } C>1 \text{ and } \alpha > 0$$

<u>Proof</u>

Let us recall that u is a bounded function ; more precisely we have [8] :

$$3.4 \quad \forall \delta > 0 \; ; \; \exists C, D > 0 \; ; \; C e^{-(1+\delta)\mathcal{E}^{1/2}|x_1|} \leq u(x_1) \leq D e^{-(1-\delta)\mathcal{E}^{1/2}|x_1|}$$

For fixed a, $1 > a > 0$, we split the integral :

$$3.5 \quad \int dy^{3(N-1)} \frac{\rho_0^N \rho_0^{N-1}}{|x_1 - x_j|} = \int_{|x_j| \leq a|x_1|} dy^{3(N-1)} \frac{\rho_0^N \rho_0^{N-1}}{|x_1 - x_j|} + \int_{|x_j| > |x_1|} dy^{3(N-1)} \frac{\rho_0^N \cdot \rho_0^{N-1}}{|x_1 - x_j|}$$

The first part is bounded by :

$$3.6 \quad \int_{|x_j| \leq a|x_1|} dy^{3(N-1)} \cdot \frac{\rho_0^N \cdot \rho_0^{N-1}}{|x_1 - x_j|} \leq \frac{1}{|1-a|} \cdot \frac{u(x_1)}{|x_1|}$$

By using the explicit bounds on ρ_0^N , ρ_0^{N-1} (see 1.2) respectively we now get :

3.7 $$\int_{|x_j|>a|x_1|} d^{3(N-1)}_y \frac{\rho_0^N \cdot \rho_0^{N-1}}{|x_1 - x_j|} \leq C_\gamma^{-(1-\gamma)\varepsilon^{1/2}|x_1|} \int_{|x_j|>a|x_1|} d^{3(N-1)}_y \frac{e^{-\beta|y|}}{|x_j - x_1|}$$

for $c > 0$ and some $\beta > 0$
and with (3.4), 3.6 gives

3.8 $$\int_{|x_j|>a|x_1|} d^{3(N-1)}_y \frac{\rho_0^N \cdot \rho_0^{N-1}}{|x_1 - x_j|} \leq C_\gamma e^{2\gamma|x_1|} u(x_1) \int_{|x_j|>a|x_1|} d^{3(N-1)}_y \frac{e^{-\beta|y|}}{|x_j - x_1|}$$

Now the integration of the last integral and the choice of suitable γ 3.7 lead to

3.9 $$\int_{|x_j|>a|x_1|} d^{3(N-1)}_y \frac{\rho_0^N \cdot \rho_0^{N-1}}{|x_1 - x_j|} < Cte\left(|x_1| + \frac{1}{|x_1|} + 1\right) e^{-\alpha|x_1|} \cdot u(x_1)$$

for some $\alpha > 0$.

Finally, by lumping together 3.5 and 3.8 we obtain 3.3.

<u>Remark 3.1</u>

In fact, we expect the following more precise result:

3.10 $$V_e(|x_1|) = \frac{N-1}{|x_1|} + O\left(\frac{1}{|x_1|^\beta}\right) \quad \text{for some } \beta > 1$$

This estimate is more difficult to obtain, but not necessary for our purpose.

We can state now the main result of this section:

<u>Theorem 3.1</u>

3.11 $$\lim_{|x_1| \to \infty} \left(\frac{\nabla u}{u}\right) = -\varepsilon^{1/2} \frac{x_1}{|x_1|}$$

<u>Proof</u>:

By using the following transformation $f = -\frac{1}{|x_1|} + \frac{u'}{u}$ in 3.1, one gets :

3.12 $$f' - f^2 + \varepsilon + W_e = 0$$

where

3.13 $W_e(|x_1|) = \frac{-2}{|x_1|} + V_e(|x_1|)$

3.12 is a Riccati-equation which we can analyse as follows : first we assume that $W_e \equiv 0$,then the solutions of 3.12 are :

3.14 $\rho = \varepsilon^{1/2} + 2\varepsilon^{1/2}\left[C e^{-2\varepsilon^{1/2}|x_1|} - 1\right]^{-1}$; $\forall C \geq 0$

3.14 shows the existence of only one solution of 3.12 such that $\rho \to -\varepsilon^{1/2}$ as $|x_1| \to \infty$, otherwise $(C \neq 0)$ $\rho \to +\varepsilon^{1/2}$ as $|x_1| \to \infty$. We are going to show that this asymptotic behaviour is stable under the perturbation W_e given by 3.13.

From general theorems on the stability of asymptotic behaviour for non linear differentials equations [9] , there exists some solution ρ_0 of 3.12 such that:

3.15 $\lim_{|x_1| \to \infty} \rho_0 = \varepsilon^{1/2}$

Let be ρ_0 a solution of 3.12 satisfying 3.15, the linearisation method for the Riccati-equation gives the general solution of 3.12:

3.16 $\rho = \rho_0 + \Psi^{-2}\left[C - \int_{|x_1|}^{\infty} dt\, \Psi^{-2}(t)\right]^{-1}$; $\forall C \geq 0$

with

3.17 $\Psi(|x_1|) = \exp\left[\int_b^{|x_1|} \rho_0(t)\, dt\right]$ for some $b > 0$

According to the fact that $\rho_0' / \rho_0^2 \to 0$ as $|x_1| \to \infty$, the integration by parts leads to:

3.18 $\rho = \rho_0 + \Psi^{-2}\left[C - \left[(1 + K(|x_1|)).2\rho_0\right]^{-1}.\Psi^{-2}\right]^{-1}$

where K is a function such that: $K(|x_1|) \to 0$ as $|x_1| \to \infty$

This last expression shows that there exists only one solution such that $\rho \to -\varepsilon^{1/2}$ as $|x_1| \to \infty$ corresponding to C=0 whereas for $C \neq 0$ the limit is $+\varepsilon^{1/2}$

Now, since $u(|x_1|)$ is non increasing function, $\frac{u'}{u} \to -\varepsilon^{1}$ as $|x_1| \to \infty$.

We close this section, with remarks about the regularity of function u .

Remark 3.2

i) Let S_θ the domain: $S_\theta = \{ z \in \mathbb{C} \setminus |\mathrm{Arg}\, z| < \pi/2 \}$ φ_θ^N , φ_θ^{N-1} being analytic vectors for the group of dilatation in S_θ . u has an analytic continuation in S_θ [10] , [11] .

ii) By using the explicit Kernel of $(-\Delta_r + 1)^{-1}$, where Δ_r is the radial Laplacian operator, one can show that u has bounded first radial derivative [12] .

Remark 3.3(Conditions (*))

From remark 3.2i), and theorem 3.1, one has :

i) $\frac{\nabla u}{u} = \frac{u'}{u} \frac{x_1}{|x_1|}$ is bounded on $\mathbb{R}^3$

In the other hand, it is not difficult to show from the equation 3.1 and theorem 3.1 that :

ii) $\nabla\left(\frac{\nabla u}{u}\right) \in L^2_{loc}(\mathbb{R}^3) + L^\infty_\varepsilon(\mathbb{R}^3)$

IV - SPECTRAL ANALYSIS OF THE OPERATORS FAMILY

This analysis is an extension of the geometrical method used in the proof of HVZ theorem [2] , [17] to non self adjoint operators with N-body interaction.

Let us start with some definitions. In the following the fixed nucleus will be the particle labelled by "o". Let $D = \{(C_1, C_2)\}$ be the set of two-cluster decompositions ; for each D we define the operator :

$$4.1 \quad H_D(\alpha) = H^N(\alpha) + \delta P - V_D$$

where V_D is the intercluster potential and P is considered as an interaction between particles "0,2...N" ; so P is *included in* V_D *unless* $D = \{(C_1, C_2)\}$ with $C_1 = \{1\}$, $C_2 = \{0, 2 \ldots N\}$
The Simon partition of unity [2] , is a collection of functions $J_D \in C^\infty$ homogeneous of degree zero for $|x_i| > 1$,such that

$$4.2 \quad \begin{cases} (i) \displaystyle\sum_{D=(C_1,C_2)} J_D^2 = 1 \\ (ii) \ \mathrm{Support}(J_D) \subseteq \{ x \in \mathbb{R}^{3N} / |x_i - x_j| \geq d|x| \text{ for } i \in C_1, j \in C_2 \text{ and some } d > 0 \} \end{cases}$$

According to these properties of J_D , one can easily show that

$|\nabla \mathcal{J}_D|$ and $\mathcal{J}_D/|x_i - x_j|$ for i, j belonging to different clusters of D are H_0^N -compact (in fact, by using the definitions of $\mathcal{J}_D$, it is easy to see that these functions decay as $|x|^{-1}$).

With the partition given by the $\mathcal{J}_D$'s we can write a localisation formula for the resolvent operators [14] :

$$4.3 \quad (H^N(\alpha) + \delta P - z)^{-1}(1 + K(z)) = \sum_D \mathcal{J}_D (H_D(\alpha) - z)^{-1} \mathcal{J}_D$$

with

$$4.4 \quad K(z) = \sum_D \left[(H^N(\alpha) + \delta P)\mathcal{J}_D - \mathcal{J}_D H_D \right] (H_D(\alpha) - z)^{-1} \mathcal{J}_D$$

Actually, K(Z) is a sum of compact operators. For the coulombic potentials and the terms $[H_0^N, \mathcal{J}_D]$ this comes from the properties of $\mathcal{J}_D$ stated above. We also have to consider the term $[P, \mathcal{J}_D]$ when $D = (C_1, C_2)$ with $C_1 = \{1\}$ and $C_2 = \{0, 2 \ldots N\}$. One has

$$4.5 \quad [P, \mathcal{J}_D] = P(\mathcal{J}_D - 1) + (\mathcal{J}_D - 1)P$$

and

$$4.6 \quad P(\mathcal{J}_D - 1)(H_0^N + 1)^{-1} = P\left(1 + \sum_{j=2}^N |x_j|\right)(1 - \mathcal{J}_D)\left(1 + \sum_{j=2}^N |x_j|\right)^{-1}(H_0^N + 1)^{-1}$$

$(1 - \mathcal{J}_D)(1 + \sum_j |x_j|)^{-1} (H_0^N + 1)^{-1}$ is compact because on the support of $(1 - \mathcal{J}_D)$. There is at least $j \neq 1$ such that $|x_j| > d|x|$. The exponential decay of φ_0^N implies that $P(1 + \sum |x_j|)$ is bounded so that $P(\mathcal{J}_D - 1)(H_0^N + 1)^{-1}$ is a compact operator. By standard arguments the same is true for $(\mathcal{J}_D - 1)P(H_0^N + 1)^{-1}$

Note that an H_0^N -compact operator is also $H_D(\alpha)$ -compact since $H_D(\alpha)$ is obtained from H_0^N by adding relatively bounded perturbations with arbitrarily small bound.

Now the sectoriality of $H_D(\alpha)$, $\forall D$ implies there exists some Z such that $(1 + K(z))$ has a bounded inverse ; hence by the analytic Fredholm theorem [15] , $(1 + K(z))^{-1}$ is a meromorphic family in $\mathbb{C}$. By (4.3) $(H^N(\alpha) + \delta P - z)^{-1}$ also is meromorphic if $z \in \bigcap_D \rho(H_D(\alpha))$ (where $\rho(A)$ is the resolvent set for A). Therefore one has

$$4.7 \quad \sigma_{ess}(H^N(\alpha) + \delta P) \subset \bigcup_D \sigma(H_D(\alpha))$$

<u>Remark 4.1</u>
The poles of $(H^N(\alpha)+\delta P - z)^{-1}$ are the discrete eigenvalues of $H^N(\alpha)+\delta P$

For the purpose of the inductive proof of theorem 4.1 below, we need to consider separatly the transformed family of P - electrons operators :

$$4.8 \quad H(\alpha) = (i\nabla_1 + \alpha \frac{\nabla u}{u})^2 - \sum_{i=2}^{P} \Delta_i + \sum_{i\neq j}^{P} \frac{1}{|x_i - x_j|}$$

It corresponds to a cluster hamiltonian $H_0(\alpha)$, for N=P and $D=(C_1, C_2)$ with $C_1 = \{0\}$ and $C_2 = \{1,2 \ldots N\}$. The essential spectrum of $H(\alpha)$ is given by the following:

<u>Lemma 4.1</u> : $\sigma_{ess}(H(\alpha)) \subset \{ z \in \mathbb{C} \setminus \mathrm{Re}\, z \geq -(\mathrm{Im}\,\alpha)^2 \mathcal{E} \}$
where $\mathcal{E} = E_0^{N-1} - E_0^N$

<u>Proof</u> :

One has

$$4.9 \quad H(\alpha) = (i\nabla_1 + \alpha \mathcal{E}^{1/2} . \frac{x_1}{|x_1|})^2 - \sum_{i=2}^{P} \Delta_i + \sum_{i\neq j}^{P} \frac{1}{|x_i - x_j|} + V_{01}$$

with

$$4.10 \quad V_{01} = (i\nabla_1 + \alpha \frac{\nabla u}{u})^2 - (i\nabla_1 + \alpha \mathcal{E}^{1/2} \frac{x_1}{|x_1|})^2$$

V_{01} is an interaction between $\{1\}$ and fictitions fixed source which is labelled by "O" ; by theorem 3.1 V_{01} is Δ_1 - compact. Then :

$$4.11 \quad \sigma_{ess}(H(\alpha)) \subset \{ z \in \mathbb{C} \setminus \mathrm{Re}\, z \geq -(\mathrm{Im}\,\alpha)^2 \mathcal{E} \}$$

We prove this inclusion by an H.V.Z. analysis of $\sigma_{ess}(H(\alpha))$ along the lines given above. Let us consider for example the hamiltonian $\tilde{H}_0(\alpha)$ with $D=(C_1, C_2)$, $C_1 = \{0\}$ and $C_2 = \{1,2 \ldots P\}$. We have for the corresponding cluster hamiltonian:

$$4.12 \quad \tilde{H}_0(\alpha) = (i\nabla_1 + \alpha \mathcal{E}^{1/2} \frac{x_1}{|x_1|})^2 - \sum_{i=2}^{P} \Delta_i + \sum_{i\neq j}^{P} \frac{1}{|x_i - x_j|}$$

By Sigal's theorem [17] one gets :

4.13 $$\inf(\mathrm{Re}\,\sigma_{ess}(\tilde{H}_0(\alpha))) \geq \inf \sigma_{ess}\left(-\sum_{i=1}^{p}\Delta_i + \sum_{i>j}^{p}\frac{1}{|x_i-x_j|} - (\mathrm{Im}\,\alpha)^2\varepsilon\right) \geq -(\mathrm{Im}\,\alpha)^2\varepsilon$$

Therefore

4.14 $$\sigma_{ess}(\tilde{H}_0(\alpha)) \subset \{ z \in \mathbb{C} \setminus \mathrm{Re}\, z \geq -(\mathrm{Im}\,\alpha)^2 \varepsilon \}$$

Finally by standard arguments [10], $\tilde{H}_0(\alpha)$ has no eigenvalues so that $\sigma(\tilde{H}_0(\alpha)) = \sigma_{ess}(\tilde{H}_0(\alpha))$.

The other cases follow from this one by induction.

Now we are ready to state the main result of this section namely $\sigma_{ess}(H^N(\alpha) + \delta P)$ is included in the half plane : $\mathrm{Re}\, z \geq \Sigma - (\mathrm{Im}\,\alpha)^2 \varepsilon$ where Σ is the smallest threshold of the system.

<u>Theorem 4.1</u>

4.15 $$\sigma_{ess}(H^N(\alpha) + \delta P) \subset \{ z \in \mathbb{C} \setminus \mathrm{Re}\, z \geq E_0^{N-1} + \delta - (\mathrm{Im}\,\alpha)^2 \varepsilon \}; \text{ for } 0<\delta<E_1^{N-1} - E_0^{N-1}$$

By induction assume that theorem 4.1 holds for all subsystems of less than (N+1) particles. Assumed particle 1 is in C_1. One has for $D = (C_1, C_2)$:

4.16 $$H_D(\alpha) = H_{C_1}(\alpha) \otimes 1 + 1 \otimes H_{C_2}$$

and by Ichinoze lemma [10] :

4.17 $$\sigma(H_D(\alpha)) = \sigma(H_{C_1}(\alpha)) + \sigma(H_{C_2})$$

We have two different types of cluster decomposition. Firstly, the nucleus is in C_1, then if N_{C_1} (N_{C_2}) denotes the number of particles in C_1 (C_2), one has by induction hypothesis :

4.18 $$\sigma_{ess}(H_{C_1}(\alpha)) \subset \{ z \in \mathbb{C} \setminus \mathrm{Re}\, z \geq E_0^{N_{C_1}-1} - (\mathrm{Im}\,\alpha)^2 \varepsilon \}$$

and by some analyticity arguments mentionned above the isolated eigenvalue of $H_{C_1}(\alpha)$ remain independent of α as long as they are not adsorbed in the essential system. H_{C_2} being a positive operator, for such a D one gets :

4.19 $$\sigma(H_D(\alpha)) \subset \{ z \in \mathbb{C} \setminus \mathrm{Re}\, z \geq \min(E_0^{N_{C_1}}, E_0^{N_{C_1}-1} - (\mathrm{Im}\,\alpha)^2 \varepsilon) \}$$

Now, if the nucleus is in C_2, then H_{C_2} is the hamiltonian of an atomic system with N_{C_2} electrons, and its spectrum is given by:

$$4.20 \quad \sigma(H_{C_2}) = [E_0^{N_{C_2}}, E_1^{N_{C_2}}, \ldots\ldots) \cup [E_0^{N_{C_2}-1}, +\infty)$$

By lemma 4.1

$$4.21 \quad \sigma(H_{C_1}(\alpha)) \subset \{ z \in \mathbb{C} \setminus \operatorname{Re} z \geqslant -(\operatorname{Im}\alpha)^2 \varepsilon \}$$

Therefore

$$4.22 \quad \sigma(H_D(\alpha)) \subset \{ z \in \mathbb{C} \setminus \operatorname{Re} z \geqslant E_0^{N_{C_2}} - (\operatorname{Im}\alpha)^2 \varepsilon \}$$

Finally, under the condition on δ , the minimum over D gives 4.15.

Remark 4.2:
A complete characterization of $\sigma_{ess}(H^N(\alpha) + \delta P)$ is given in [12] . It consists of an union of paraboloids centered at various thresholds of the system, but 4.15 is sufficient for our investigations.

V - MAIN RESULTS

Combining the theorems 2.1 and 4.1 we have :

$$5.1 \quad u^{-i\alpha} Q \rho_0^N \in W^{2,2}(\mathbb{R}^{3N}) \quad \text{for } \alpha \in \Omega$$

From this we get the following lemma :

Lemma 5.1

$$5.2 \quad \zeta(|x_1|) = \left\| \frac{Q \rho_0^N}{u} \right\|_{L^2(\mathbb{R}^{3(N-1)})} (|x_1|) \leq \frac{C}{|x_1|}$$

for some $C > 0$ and $|x_1| \geqslant a > 0$

Proof :

Let:

5.3 $\mathcal{B}(|x_1|) = \{ r \in \mathbb{R}^+ \setminus |r - |x_1|| \leq 1 \}$

and $\varphi \in W^{2,1}(\mathcal{B}(|x_1|); dr)$ ($W^{2,1}$ denotes the usual Sobelev space). By Sobelev embedding theorem [16] one gets :

5.4 $|\varphi(|x_1|)| \leq D \, \|\varphi\|_{W^{2,1}(\mathcal{B}(|x_1|))}$ for some $D > 0$

Setting $\varphi(|x_1|) = |x_1| \, \zeta^2(|x_1|)$ one has

5.5 $\left| |x_1| \zeta^2(|x_1|) \right| \leq D \int_{\mathcal{B}(|x_1|)} \left(\left| \frac{d^2}{dr^2} r \zeta^2 \right| + |r \zeta^2| \right) dr$

then

5.6 $\left| |x_1| \zeta^2(|x_1|) \right| \leq \frac{D}{1 + |x_1|} \int_{\mathcal{B}(|x_1|)} \left(|\Delta_r \zeta^2| + |\zeta^2| \right) r^2 \, dr$

Now, by using the definition of ζ^2 , 5.6 leads to

5.7 $|\zeta(|x_1|)| \leq \frac{C}{|x_1|} \left\| \frac{Q \rho_0^N}{u} \right\|_{W^{2,2}(\mathbb{R}^{3N})}$

for some $C > 0$ and $|x_1| \geq a > 0$

<u>Remark 5.1</u>
By integration of $\left\| \frac{Q \rho_0^N}{u} \right\|^2_{L^2(\mathbb{R}^{3(N-1)})}$ one has:

5.8 $\left\| \frac{Q \rho_0^N}{u} \right\|^2 = \left| 1 - \frac{u^2}{\rho} \right|$

5.8 an the lemma 5.1 imply

5.9 $u(|x_1|) = \rho^{1/2}(|x_1|) \left(1 + O\left(\frac{1}{|x_1|^2} \right) \right)$

We can now prove our main result:

Theorem 5.1

$$5.10 \quad \begin{cases} i) \ \left\| \frac{\rho_0^N}{\rho^{1/2}} - \rho_0^{N-1} \right\|_{L^2(\mathbb{R}^{3(N-1)})} = O\left(\frac{1}{|x_1|}\right) \\ ii) \ \left(\frac{\rho_0^N}{\rho^{1/2}}, (H^{N-1} - E_0^{N-1}) \frac{\rho_0^N}{\rho^{1/2}} \right)_{L^2(\mathbb{R}^{3(N-1)})} = O\left(\frac{1}{|x_1|^2}\right) \end{cases}$$

Proof:

One has:

$$5.11 \quad \left\| \frac{\rho_0^N}{\rho^{1/2}} - \rho_0^{N-1} \right\|_{L^2(\mathbb{R}^{3(N-1)})} \leq \left\| \frac{P\rho_0^N}{\rho^{1/2}} - \rho_0^{N-1} \right\|_{L^2(\ )} + \left\| \frac{Q\rho_0^N}{\rho^{1/2}} \right\|_{L^2(\ )}$$

Now $\left\| \frac{Q\rho_0^N}{\rho^{1/2}} \right\|_{L^2(\ )} \leq \left\| \frac{Q\rho_0^N}{u} \right\|_{L^2(\ )}$, and by lemma 5.1:

$$5.12 \quad \left\| \frac{Q\rho_0^N}{\rho^{1/2}} \right\|_{L^2(\mathbb{R}^{3(N-1)})} \leq \frac{C}{|x_1|} \quad \text{for some } C>0$$

For the second term in the rhs of 5.11,one gets:

$$5.13 \quad \left\| \frac{P\rho_0^N}{\rho^{1/2}} - \rho_0^{N-1} \right\|_{L^2(\ )} = \left| 1 - \frac{u}{\rho^{1/2}} \right|$$

The remark 5.1 shows that this term decays like $1/|x_1|^2$. This proves 5.10i). To prove 5.10ii) we proceed analogously :

$$5.14 \quad \left(\frac{\rho_0^N}{\rho^{1/2}}, (H^{N-1} - E_0^{N-1}) \frac{\rho_0^N}{\rho^{1/2}} \right)_{L^2(\ )} \leq \left(\frac{Q\rho_0^N}{u}, (H^{N-1} - E_0^{N-1}) \frac{Q\rho_0^N}{u} \right)_{L^2(\ )}$$

Let us set $\xi(|x_1|) = \left(Q\rho_0^N/u, (H^{N-1} - E_0^{N-1}) Q\rho_0^N/u\right)$; $\xi(|x_1|)$ is spherically symmetric, and by the same arguments as in the proof of lemma 5.1 one has :

$$5.15 \quad \left| |x_1| \, \xi(|x_1|) \right| \leq \frac{D}{1+|x_1|} \int_{\mathbb{R}^3} \left(|\Delta_r \xi| + |\xi| \right) d^3x$$

Now, the Cauchy Shwartz inequality leads to:

5.16 $$\int_{\mathbb{R}^3} d^3x \; |\Delta_r \xi| \leq D \left\{ \| \Delta_1 \, Q \underline{\rho_o^N} \|_{L^2(\mathbb{R}^{3N})} \cdot \| (H^{N-1} - E_o^{N-1}) \, Q \underline{\rho_o^N} \|_{L^2(\mathbb{R}^{3N})} \right.$$
$$\left. + \; \| (H^{N-1} - E_o^{N-1})^{1/2} \nabla_1 \, Q \underline{\rho_o^N} \|_{L^2(\mathbb{R}^{3N})} \right.$$

for some $D > 0$.

Noting that the last term can be estimated by :

5.17 $$\| (H^{N-1} - E_o^{N-1})^{1/2} \cdot \nabla_1 \, Q \underline{\rho_o^N} \|^2 \leq \| (-\Delta_1 + H^{N-1} - E_o^{N-1}) \, Q \underline{\rho_o^N} \|^2$$

We see that the integral in lhs of 5.16 is finite; therefore by 5.15 :

5.18 $$\xi(x_1) \leq C/|x_1|^2 \qquad \text{for some } C > 0 \text{ and } |x_1| \geq a > 0$$

REFERENCES

1 J.M.COMBES, L. THOMAS, CMP 34, 251-270 (1973).

2 B. SIMON, CMP 55, 259-274 (1977).

3 P. DEIFT, W. HUNZIKER, B. SIMON, E. VOCK CMP 64, 1-34 (1978).

4 R. AHLRICHS, M. and T. HOFFMAN-OSTENOF, Phys. Rev. A23, 2106 (1981).

5 S. AGMON, Proc. A. Pleigel Conf., Uppsala (1979).

6 R. CARMONA, B. SIMON, CMP 80, 59-98 (1981).

7 J.M. COMBES, M. and T. HOFFMAn-OSTENOF, J. Math. Phys. 22, 1299 (1981).

8 E.H. LIEB, B. SIMON, Adv. Applied Math., 7,324 (1980).

9 CODDINGTON-LEVINSON :Mc Graw-Hill Book Company (1955).

10 M. REED, B. SIMON, Vol. III-Academic Press (1978).

11 D. BABBITT, E. BALSLEV, J. of Funct.Anal. 18,1-14 (1975).

12 P. BRIET, Thèse 3ème Cycle, Université d'Aix-Marseille II (1983).

13 T. KATO, Springer-Verlag (1966).

14 J.M. COMBES, Wightman, Velo Edits. Plenum Press (1981).

15 M. REED, B. SIMON, Vol. I, Academic Press (1975).

16 R.A. ADAMS, Academic Press (1975).

17 I. SIGAL, CMP 85, 309-354 (1982).

18 P. LOWDIN, Int. Summ. School, Menton (1965).

19 J.M.COMBES, CMP 12, 283-295 (1969).

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