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On the Ionization of Crystals

J.-P. Eckmann* and L.E. Thomas**

Département de Physique Théorique, Université de Genève, Genève, Switzerland

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Abstract. We provide a lower bound for the energy required to ionize an "electron" from a finite crystal of low density and we show that the bound is independent of the crystal size. The electrons interact with each other and with the fixed positive charges by short range interactions from a suitable class of potentials.

I. Introduction

In this article, we prove the following assertion; let $H_M(N, a, m)$ be the Schrödinger operator for M spinless "electrons" of mass m in the presence of N fixed "protons" regularly arranged in a finite lattice with lattice constant a. Assume that the electrons are either Bosons or Fermions and assume that they interact with one another by a positive, short range continuously differentiable potential $v_R(\boldsymbol{x}_i - \boldsymbol{x}_j)$ and interact with the protons by $-v_A(\boldsymbol{x}_i - \boldsymbol{y}_j)$. Here, $\boldsymbol{x}_i$ is the position of the i-th electron and $\boldsymbol{y}_j$ is the position of the j-th proton. Then $H_M(N, a, m)$ has a ground state eigenvalue λ_{MN} uniformly isolated from the continuous spectrum for all N and $M \leqq N$ if a and m are sufficiently large. Hence there is a $g > 0$ such that for all N and $M \leqq N$, $\operatorname{dist}(\lambda_{MN}, \sigma_{MN}) \geqq g$ where σ_{MN} is the continuous spectrum of $H_M(N, a, m)$.

The quantity g is a lower bound for the work function familiar from the photoelectric effect, i.e. the amount of energy required to ionize an electron from the crystal. The fact that the work function is non-vanishing insures that the electrons do not spontaneously escape from the crystal, regardless of the crystal size. Thus the result is related to the more general problem concerning the stability of solids.

Let us now outline the strategy of the proof. By Hunziker's theorem [1, 2], the infimum of the essential spectrum for $H_M(N, a, m)$ lies at $\inf_{M' < M}$ {inf spectrum $H_{M'}(N, a, m)$}. We make the inductive hypothesis that this infimum is actually $\lambda_{M-1,N}$ i.e. the ground state for the Hamiltonian with one less electron. It is therefore natural to consider the tensor product of the corresponding ground state eigenfunction $\psi_{M-1,N}$ (not necessarily unique) with a one particle trial function ϕ and to try to show that the energy expectation value for the tensor product is bounded above by $\lambda_{M-1,N} - g$. This would establish the existence of discrete spectrum for $H_M(N, a, m)$ below $\lambda_{M-1,N} - g$ and therefore the existence of a ground state eigenfunction ψ_{MN} corresponding to $\lambda_{MN} = \inf$ spectrum $H_M(N, a, m)$. The induction then proceeds to $M \leqq N$. However, there are two modifications to this strategy.

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* Supported by the Fonds National Suisse.

** Present address: Dept. of Mathematics, University of Virginia, Charlottesville, Va., USA

The first modification comes about in considering the tensor product of $\psi_{M-1,N}$ and the one particle trial function ϕ. In the case of the electrons obeying Fermi statistics, the tensor product should be antisymmetrized. In order to avoid difficulties arising from matrix elements complicated by the antisymmetrization, we first multiply $\psi_{M-1,N}$ by a symmetric factor $\eta(\boldsymbol{x}_1 \ldots \boldsymbol{x}_{M-1})$ so that the resulting function vanishes whenever any of its variables lies in the support of ϕ. η is constructed so that the norm of $\eta\psi_{M-1,N}$ is near one.

The function $\eta\psi_{M-1,N}$ is further modified by a unitary operation which shifts the variables of $\eta\psi_{M-1,N}$ a small amount in a lattice site where the one particle density $\varrho(\boldsymbol{x}) = \int d\boldsymbol{x}_2 \ldots d\boldsymbol{x}_{M-1} |\psi_{M-1,N}(\boldsymbol{x}, \boldsymbol{x}_2, \ldots \boldsymbol{x}_{M-1})|^2$ is small. The reason for such a shift is seen by the following heuristic argument: In the limit as $a, m \to \infty$ we expect $\varrho(\boldsymbol{x})$ to become highly concentrated about each proton position with weight about equal to $1/N$. If M is approximately equal to N, the potential seen by an additional electron situated at $\boldsymbol{x}$ near one of these positions (say $\boldsymbol{y}_i$) is

$$\begin{aligned} -v_A(\boldsymbol{x}-\boldsymbol{y}_i) + (M-1)\int v_R(\boldsymbol{x}-\boldsymbol{x}')\varrho(\boldsymbol{x}')d\boldsymbol{x}' &\approx -v_A(\boldsymbol{x}-\boldsymbol{y}_i) \\ &+ \frac{(M-1)}{N} v_R(\boldsymbol{x}-\boldsymbol{y}_i) \end{aligned}$$

which may be insufficient to bind this additional electron for $M \approx N \to \infty$ (i.e. the attraction is cancelled by the repulsion). We find however that if $\psi_{M-1,N}$, and hence ϱ, are shifted slightly in the site of the additional electron, it will bind with an overall decrease in energy by g or more. This local shift approximates the polarization of the $M-1$ electrons due to the introduction of an additional electron.

In Section 2 we give the precise statement of the theorem along with its proof, which we discuss in Section 3. An Appendix is included giving simple criteria under which the hypotheses of the theorem are satisfied.

II. The Main Theorem and Its Proof

The class $\mathscr{V}$ of admissible two body potentials is the set of pairs $v = (v_A, v_R)$ of continuously differentiable functions on $[0, \infty)$ such that

$\mathscr{V}_1$: $v_A(r), v_R(r) > 0$ and monotonically decreasing to 0 in r.

$\mathscr{V}_2$: At infinity, $v_A(r)$, $v_R(r) < Cr^{-3-\delta}$ for some $C, \delta > 0$.

$\mathscr{V}_3$: $\lim_{r\to\infty} \frac{d}{dr} \ln v_R(r) = 0.$

$\mathscr{V}_4$: There exist numbers $r_0 > \varepsilon_0 > 0$ such that

$$\sup_{\boldsymbol{x}\in\mathbb{R}^3} \left| v_A(|\boldsymbol{x}|) - v_A(|\boldsymbol{x} + r_0\boldsymbol{e}_1|) + v_R(|\boldsymbol{x} + (r_0+\varepsilon_0)\boldsymbol{e}_1|)\right| - v_A(\varepsilon_0) < -g < 0,$$

where $\boldsymbol{e}_1$ is a unit vector. We also identify

$$v_R(\boldsymbol{x}) = v_R(|\boldsymbol{x}|), \quad v_A(\boldsymbol{x}) = v_A(|\boldsymbol{x}|).$$

We show in the Appendix how to construct functions which are in $\mathscr{V}$.

Our Hamiltonian $H_M(N, a, m)$ depends on $v \in \mathscr{V}$ and on the parameters
N, the number of charges "+1",
M, the number of charges "−1",
a, the lattice constant,
m, the bare mass.

Let $\boldsymbol{y}_1, \ldots \boldsymbol{y}_N$ be N different points on the unit lattice $\mathbb{Z}^3 \subset \mathbb{R}^3$. The "electron-proton" attraction is defined to be

$$V_{\mathrm{ep}}(M, N, a) = -\sum_{j=1}^{N} \sum_{k=1}^{M} v_A(\boldsymbol{x}_k - a\boldsymbol{y}_j). \tag{1}$$

Here, the $\boldsymbol{x}_k$ are the coordinates of the quantum mechanical "electrons", and the $a\boldsymbol{y}_j$ are the fixed positions of the "protons" for lattice constant a. The "electron-electron" repulsion is

$$V_{\mathrm{ee}}(M) = +\sum_{M \geqq j > k \geqq 1} v_R(\boldsymbol{x}_j - \boldsymbol{x}_k), \tag{2}$$

and the total Hamiltonian is

$$H_M = H_M(N, a, m) = -\sum_{j=1}^{M} \frac{\Delta_{x_j}}{2m} + V_{\mathrm{ep}}(M, N, a) + V_{\mathrm{ee}}(M) \tag{3}$$

acting on $\mathscr{H}_M = P(L_2(\mathbb{R}^3)^{\otimes M})$, where P projects on the symmetric subspace if the "electrons" are Bosons and on the antisymmetric subspace if they are Fermions. We may omit the proton-proton repulsion since it is only a function of N and not of M. Our main result is the following theorem.

Theorem 1. *Given $v \in \mathscr{V}$ there are constants a_v, m_v and N_v such that for all lattice constants $a \geqq a_v$, masses $m \geqq m_v$, integers $N \geqq N_v$, and $M \leqq N$ one has* inf spectrum $H_M(N, a, m) \leqq$ inf continuous spectrum $H_M(N, a, m) - q_v$ *for some* $q_v > 0$.

Remark. Our best estimate for q_v in the limit as $a, m \to \infty$ is a g of condition $\mathscr{V}_4$. Note also that for $v \in \mathscr{V}$ the continuous spectrum coincides with the essential spectrum.

Proof. Throughout the proof we let $\psi_{M,N} = \psi_M$ be a ground state eigenfunction for $H_M(N, a, m)$ (no confusion will arise by suppressing sometimes the N, a, m dependence), and let λ_{MN} be its corresponding eigenvalue. The proof starts by reducing the assertion to an induction argument in M. As was remarked in the introduction,

$$\operatorname{inf\,cont\,spec} H_{M+1}(N, a, m) = \inf_{M' \leqq M} \{\operatorname{inf\,spec} H_{M'}(N, a, m)\},$$

by Hunziker's theorem [1, 2]. We make the inductive hypothesis on M that

$$\operatorname{inf\,cont\,spec} H_{M+1}(N, a, m) = \lambda_{M,N} \leqq 0,$$

($\lambda_{0,N}$ is defined to be zero), and that the theorem holds for $M' \leqq M$. It follows that we must show

$$\operatorname{inf\,spec} H_{M+1}(N, a, m) \leqq \lambda_{M,N} - q_v, \tag{4}$$

for some $q_v > 0$, independent of N, a, m, $M < N$ for sufficiently large N, a, m.

In the case $M=0$ let $\phi(\boldsymbol{x})$ be a normalized function with support concentrated around one of the N protons. Then the expectation value $(\phi, H_1(N,a,m)\phi)$ is strictly less than zero uniformly in N,a,m for m sufficiently large. Thus there are eigenvalues $\lambda_{1,N}$ uniformly less than zero and the induction starts. We now proceed to the proof of inequality (4).

We start the proof of Theorem 1 with a geometrical lemma. Given $\boldsymbol{y}_1, \ldots \boldsymbol{y}_N \in \mathbb{Z}^3$ and a, define Λ_N to be the union of the N lattice cubes of side a with centers $a\boldsymbol{y}_1, \ldots a\boldsymbol{y}_N$, and let $S_1, \ldots S_N$ be the cells of Λ_N. Let $\varrho_0, \ldots \varrho_K$ be positive densities on $\mathbb{R}^3$ with $\int_{\mathbb{R}^3} d\boldsymbol{x}\, \varrho_j \leqq 1$. Let $\varrho_{jk} = \int_{S_k} d\boldsymbol{x}\, \varrho_j$.

Lemma 2. *Given $\varepsilon > 0$, there is, for each N sufficiently large, a cube $S_{i_0} \subset \Lambda_N$ such that*

$$\varrho_{0\,i_0} \leqq \frac{1+\varepsilon}{N},$$

$$\varrho_{j i_0} \leqq 2^j \frac{1+\varepsilon}{\varepsilon N}, \qquad j = 1, 2, \ldots K.$$

Proof. Let $\alpha > 1$ be given and define $n_N(\alpha, j)$ to be the number of cells in Λ_N for which $\varrho_{jk} < \alpha/N$. Then $n_N(\alpha, j) \geqq N(\alpha - 1)/\alpha$. If not, then $n_N < N(\alpha - 1)/\alpha$ and the remaining $N - n_N$ cells with $\varrho_{jk} \geqq \alpha/N$ would have total weight at least

$$(N - n_N)\frac{\alpha}{N} > (N - N(\alpha-1)/\alpha)\frac{\alpha}{N} = 1,$$

which is impossible. In particular

$$n_N(1+\varepsilon, 0) \geqq N\frac{\varepsilon}{1+\varepsilon},$$

$$n_N\left(2^j \frac{1+\varepsilon}{\varepsilon}, j\right) \geqq N\frac{2^j(1+\varepsilon) - \varepsilon}{2^j(1+\varepsilon)}, \qquad j = 1, \ldots K.$$

To complete the proof we make the inductive hypothesis that the number of cells m_{N_j} satisfying the first $j+1$ inequalities of the lemma simultaneously is

$$m_{Nj} \geqq \frac{N\varepsilon}{2^j(1+\varepsilon)},$$

which is the case for $j=0$, by inspection. Then

$$\begin{aligned} m_{Nj+1} &\geqq m_{Nj} + n_N\left(2^{j+1}\frac{1+\varepsilon}{\varepsilon}, j\right) - N \\ &\geqq \frac{N\varepsilon}{2^j(1+\varepsilon)} + N\frac{2^{j+1}(1+\varepsilon) - \varepsilon}{2^{j+1}(1+\varepsilon)} - N = \frac{N\varepsilon}{2^{j+1}(1+\varepsilon)}. \end{aligned}$$

In particular, $m_{NK} \geqq \dfrac{N\varepsilon}{2^{K+1}(1+\varepsilon)}$ which is greater than 1 for N sufficiently large, so there is at least one cell with the asserted properties. q.e.d.

By $\mathscr{V}_4$, there is an $\varepsilon > 0$ and an integer k such that

$$(1+\varepsilon)\frac{k}{(k-1-\varepsilon)} \sup_{\boldsymbol{x}\in\mathbb{R}^3} |v_A(\boldsymbol{x}) - v_A(\boldsymbol{x}+r_0\boldsymbol{e}_1) + v_R(\boldsymbol{x}+(r_0+\varepsilon_0)\boldsymbol{e}_1)| \\ - v_A(\varepsilon_0) < -g < 0\,, \tag{5}$$

and we fix now ε and k to such values. We also fix $M \leqq N$ and we omit the subscript N whenever possible. Let ψ_M be a normalized eigenfunction of $H_M(N, a, m)$ with eigenvalue inf spec $H_M(N, a, m)$. We define the following four normalized densities on $\mathbb{R}^3$:

$$\varrho_M(\boldsymbol{x}) = \int |\psi_M(\boldsymbol{x}, \boldsymbol{x}_2, \dots \boldsymbol{x}_M)|^2 d\boldsymbol{x}_2 \dots d\boldsymbol{x}_M\,, \tag{6}$$

$$\tau_M(\boldsymbol{x}) = \int \frac{|\mathrm{grad}_x \psi_M(\boldsymbol{x}, \boldsymbol{x}_2, \dots \boldsymbol{x}_M)|^2 d\boldsymbol{x}_2 \dots d\boldsymbol{x}_M}{\|\mathrm{grad}_x \psi_M\|_{L^2}^2}\,, \tag{7}$$

$$v_M(\boldsymbol{x}) = \frac{\int v_R(\boldsymbol{x}-\boldsymbol{x}_2)\,|\psi_M(\boldsymbol{x}, \boldsymbol{x}_2, \dots \boldsymbol{x}_M)|^2 d\boldsymbol{x}_2 \dots d\boldsymbol{x}_M}{\int v(\boldsymbol{x}_1-\boldsymbol{x}_2)\,|\psi_M(\boldsymbol{x}_1, \boldsymbol{x}_2, \dots \boldsymbol{x}_M)|^2 d\boldsymbol{x}_1 \dots d\boldsymbol{x}_M}\,, \tag{8}$$

$$v_{Ma}(\boldsymbol{x}) = \frac{\int v_{Ra}(\boldsymbol{x}-\boldsymbol{x}_1)\,|\psi_M(\boldsymbol{x}_1, \dots \boldsymbol{x}_M)|^2 d\boldsymbol{x}_1 \dots d\boldsymbol{x}_M}{\int v_{Ra}(\boldsymbol{x}-\boldsymbol{x}_1)\,|\psi_M(\boldsymbol{x}_1, \dots \boldsymbol{x}_M)|^2 d\boldsymbol{x}\, d\boldsymbol{x}_1 \dots d\boldsymbol{x}_M}\,, \tag{9}$$

where

$$\begin{aligned} v_{Ra}(r) &= 0 \quad \text{if} \quad r < a/4\,, \\ v_{Ra}(r) &= v_R(r) \quad \text{if} \quad r \geqq a/4\,. \end{aligned} \tag{10}$$

By Lemma 2, there exists an $S_{i_0} \subset \Lambda_N$, provided N is sufficiently large, such that

$$\varrho_{M i_0} \leqq \frac{1+\varepsilon}{N}\,, \tag{11}$$

$$\tau_{M i_0} \leqq \frac{2(1+\varepsilon)}{\varepsilon N}\,, \tag{12}$$

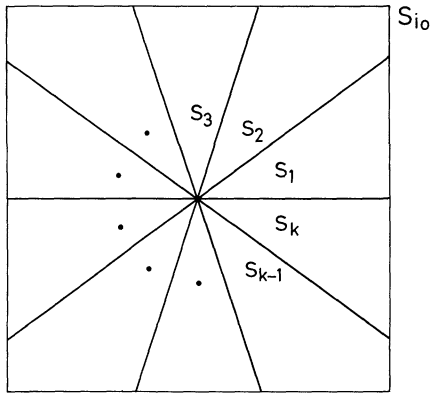
$$v_{M i_0} \leqq \frac{4(1+\varepsilon)}{\varepsilon N}\,, \tag{13}$$

$$v_{M a i_0} \leqq \frac{8(1+\varepsilon)}{\varepsilon N}\,. \tag{14}$$

Refer now to Fig. 1. We divide the region S_{i_0} into k subregions or wedges $s_1, \dots s_k$ with wedge axis passing through the center of S_{i_0} and pointing in the $\boldsymbol{x}^{(3)}$-direction. The wedges have opening angle $2\pi/k$. It is evident that for one of these subregions, say s_{j_0} we will have the inequality

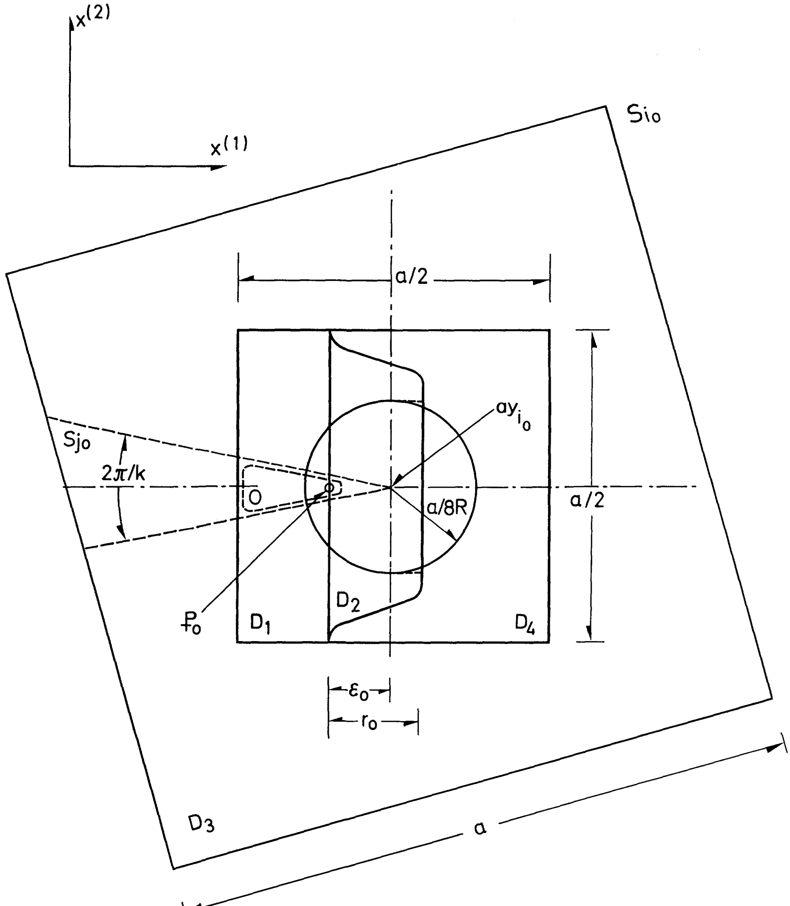
$$\int_{s_{j_0} \subset S_{i_0}} d\boldsymbol{x}\, \varrho(\boldsymbol{x}) \leqq \frac{1+\varepsilon}{kN}\,. \tag{15}$$

Refer now to Fig. 2.



S_{i_0}
S_3
S_2
S_1
S_k
S_{k-1}

Fig. 1



$x^{(2)}$
$x^{(1)}$
S_{i_0}
$a/2$
ay_{i_0}
S_{j_0}
$2\pi/k$
O
$a/8R$
$a/2$
P_0
D_1
D_2
D_4
ε_0
r_0
D_3
a

Fig. 2

Assume that new coordinates are chosen as shown, so that the wedge opening is symmetrical with respect to the $x^{(2)}=0$ plane and with edge running along the $x^{(3)}$-axis. Let $\eta_0(x)$ be a piecewise continuously differentiable function on $\mathbb{R}^3$ with the properties

$$\eta_0(x)=1 \quad \text{on} \quad \mathbb{R}^3-(s_{j_0}\cap(D_1\cup D_2)), \tag{16}$$

$$\eta_0(x)=0 \quad \text{in the open set} \quad \mathcal{O}\subset(s_{j_0}\cap(D_1\cup D_2)) \text{ containing } p_0 \tag{17}$$

and η_0 interpolates linearly otherwise. The maximal derivative of η_0 is independent of the lattice constant a for a large enough.

We next define a diffeomorphism f on $\mathbb{R}^3$ (also depending on a) which approximates the polarization of the charges due to the introduction of another particle at p_0. It has the properties

F1) f is the identity on $(\mathbb{R}^3-S_{i_0})\cup D_3$, (18)

F2) $f^{(j)}(x)=x^{(j)}$ for $j=2,3$,[1] (19)

F3) f maps D_1 onto $D_1\cup D_2$ and it maps no point from the exterior of $\mathcal{O}$ into $\mathcal{O}$, (20)

F4) $\sup_x|f(x)-x|\leqq r_0$ and in the region R, $f(x)=x+e^{(1)}r_0$, where $e^{(1)}$ is the unit vector in the positive $x^{(1)}$-direction, (21)

F5) $\partial^{(i)}\partial^{(j)}f^{(l)}\to 0$ and $\partial^{(i)}f^{(j)}\to\delta_{ij}$ as $a\to\infty$.

By F5), f will satisfy an inequality of the form

$$|f(x)-f(y)-(x-y)|\leqq K_f(a)|x-y|, \tag{22}$$

with $K_f(a)\to 0$ as $a\to\infty$. Property F5) and an inequality like (22) hold for the inverse mapping f^{-1}.

We extend now η_0 and f to operators η and U acting on $L_2(\mathbb{R}^{3M})$. Let $\eta=\bigotimes^M\eta_0$ be the multiplication operator acting on all variables of $L_2(\mathbb{R}^{3M})$ simultaneously and let $U=\bigotimes^M U_0$ be the unitary operator on $L_2(\mathbb{R}^{3M})$ where U_0 acts on $L_2(\mathbb{R}^3)$ by the unitary action

$$U_0\phi(x)=\sqrt{\partial f^{-1}(x)}\,\phi(f^{-1}(x)), \quad \phi\in L_2(\mathbb{R}^3), \tag{23}$$

and where ∂f^{-1} is the Jacobian. Let $\Phi(x)$ be a C^2 function with supp Φ concentrated about p_0 and contained in $\mathcal{O}$ and $\|\Phi\|=1$. Let $\wedge$ denote the antisymmetrical tensor product when the electrons are Fermions, and the symmetric tensor product if they are Bosons.

Lemma 3. $(U\eta\psi_M)(x_1,\dots x_M)=0$ *if any argument lies in* $\mathcal{O}$. *Also*

$$\begin{aligned}\|\Phi\wedge U\eta\psi_M\|^2_{L_2(\mathbb{R}^{3(M+1)})}&=\|U\eta\psi_M\|^2_{L^2(\mathbb{R}^{3M})}\\&=\|\eta\psi_M\|^2_{L_2(\mathbb{R}^{3M})}\geqq\frac{k-1-\varepsilon}{k}.\end{aligned}\tag{24}$$

[1] $f^{(j)}$ is the j-th component of f.

Proof. The first assertion follows by inspection from the definition of η_0 and U_0. The equality of norms is then a consequence of the normalization of Φ and of the fact that U is unitary. Finally

$$\|\eta\psi_M\|^2 \geqq \|\psi_M\|^2 - M \int_{S_{j_0} \times \mathbb{R}^{3(M-1)}} dx_1 \dots dx_M \, |\psi_M(x_1, \dots x_M)|^2$$
$$\geqq 1 - \frac{M(1+\varepsilon)}{kN} \geqq \frac{k-1-\varepsilon}{k},$$

by the inequalities (11) and (15), which proves the lemma.

We now estimate the energy expectation value for the trial function $\Phi \wedge U\eta\psi_M$. Using Lemma 3, we find

$$\begin{aligned} &\frac{(\Phi \wedge U\eta\psi_M, H_{M+1}(N, a, m)\, \Phi \wedge U\eta\psi_M)}{\|\Phi \wedge U\eta\psi_M\|^2} \\ &= \frac{(U\eta\psi_M, H_M(N, a, m)\, U\eta\psi_M)}{\|\eta\psi_M\|^2} + (\Phi, H_1(N, a, m)\Phi) \\ &+ \frac{M}{\|\eta\psi_M\|^2} \int dx_1 \dots dx_{M+1} \, |\Phi(x_1) U\eta\psi_M(x_2, \dots x_{M+1})|^2 \, v_R(x_1 - x_2)\,. \end{aligned} \tag{25}$$

The idea is to undo the effect of the U transformation in the first term on the r.h.s. of Eq. (25), which we consider now.

Lemma 4. *One has*

$$\begin{aligned} &(U\eta\psi_M, H_M(N, a, m) U\eta\psi_M) \\ &= \lambda_{MN} \|\eta\psi_M\|^2 - M(\eta\psi_M, \{v_A(f(x_1) - a y_{i_0}) - v_A(x_1 - a y_{i_0})\}\eta\psi_M) + \gamma_0(a, m)\,, \end{aligned} \tag{26}$$

where $\gamma_0(a, m) \to 0$ *as* $a, m \to \infty$, *uniformly in* $N, M \leqq N$.

Proof of Lemma 4. We begin with the kinetic energy part of the l.h.s. of Eq. (26). With the notation $\partial_1 = \mathrm{grad}_{x_1}$, it is

$$\frac{M}{m} \|\partial_1 U\eta\psi_M\|^2 = \frac{M}{m} \|\partial_1 U_0 \eta\psi_M\|^2\,, \tag{27}$$

where U_0 acts just on the first variable. A simple calculation yields

$$\begin{aligned} &U_0^{-1} \partial^{(k)} U_0 \\ &= U_0^{-1} \frac{(\partial^{(k)} \sqrt{\partial f^{-1}})}{\sqrt{\partial f^{-1}}} U_0 + \sum_{j=1}^{3} U_0^{-1}((\partial^{(k)} f^{-1(j)}) - \delta_{kj}) U_0 \partial^{(j)} + \partial^{(k)}\,. \\ &= G_{1k} + \sum_j G_{2jk} \partial^{(j)} + \partial^{(k)}\,. \end{aligned} \tag{28}$$

Here, G_{1k} and G_{2jk} are just functions with support in S_{i_0}. Let $\gamma_1(a)$ and $\gamma_2(a)$ be bounds for G_{1k} and G_{2jk}, $j, k = 1, \dots 3$, respectively. By Condition F5) on f, $\gamma_1(a)$ and $\gamma_2(a)$ become arbitrarily small as $a \to \infty$. By Eq. (28),

$$\|\partial_1 U_0 \eta\psi_M\|^2 = \|U_0^{-1} \partial_1 U_0 \eta\psi_M\|^2 = \|\partial_1 \eta\psi_M\|^2 + \gamma_k(a)\,, \tag{29}$$

with

$$\begin{aligned} |\gamma_k(a)| \leqq\, &3\gamma_1^2 \|P_0 \eta\psi_M\|^2 + 6\gamma_1\gamma_2 \|P_0 \eta\psi_M\| \, \|P_0 \partial_1 \eta\psi_M\| \\ &+ 6\gamma_1 \|P_0 \eta\psi_M\| \, \|P_0 \partial_1 \eta\psi_M\| + 3\gamma_2^2 \|P_0 \partial_1 \eta\psi_M\|^2 + 6\gamma_2 \|P_0 \partial_1 \eta\psi_M\|^2\,, \end{aligned} \tag{30}$$

where P_0 is the characteristic function in the first variable for S_{i_0}. Now

$$\begin{aligned}\|P_0\partial_1\eta\psi_M\| &\leqq \|P_0(\partial_1\eta)\psi_M\| + \|P_0\eta\partial_1\psi_M\| \\ &\leqq \|\partial_1\eta\|_\infty\left(\frac{1+\varepsilon}{N}\right)^{1/2} + \left(\frac{2+2\varepsilon}{\varepsilon N}\right)^{1/2}\|\partial_1\psi_M\|,\end{aligned} \tag{31}$$

by the inequalities (11) and (12). We now use

$$\begin{aligned}\frac{1}{m}\|\partial_1\psi_M\|^2 &= \frac{1}{M}\{(\psi_M, H_M\psi_M) - (\psi_M, V_{\mathrm{ep}}(M)\psi_M) - (\psi_M, V_{\mathrm{ee}}(M)\psi_M)\} \\ &\leqq \frac{1}{M}\left\{\lambda_{MN} + M\sup_{\boldsymbol{x}}\sum_{j=1}^{N} v_A(\boldsymbol{x}-a\boldsymbol{y}_j)\right\} \leqq \sup_{\boldsymbol{x}}\sum_{j=1}^{N} v_A(\boldsymbol{x}-a\boldsymbol{y}_j).\end{aligned} \tag{32}$$

We have used the induction hypothesis $\lambda_{MN} \leqq 0$, and $\mathscr{V}_1$. The r.h.s. of (32) is uniformly bounded as $a \to \infty$, by $\mathscr{V}_2$. Inserting (32) into (31) and applying (11) and (31) to (30) and (29), we obtain the estimate

Est. 1. $\dfrac{M}{m}\|\partial_1 U\eta\psi_M\|^2 = \dfrac{M}{m}\|\partial_1\eta\psi_M\|^2 + \gamma_{\mathrm{k}}(a,m)$ *where* $\gamma_{\mathrm{k}}(a,m) \to 0$ *as* $a, m \to \infty$, *uniformly in* N *and* $M \leqq N$.

We next consider the V_{ep} matrix element contained in $(U\eta\psi_M, H_M U\eta\psi_M)$. We have

$$\begin{aligned}&(U\eta\psi_M, V_{\mathrm{ep}}(M)U\eta\psi_M) \\ &= (\eta\psi_M, V_{\mathrm{ep}}(M)\eta\psi_M) + (\eta\psi_M, \{U^{-1}V_{\mathrm{ep}}(M)U - V_{\mathrm{ep}}(M)\}\eta\psi_M) \\ &= (\eta\psi_M, V_{\mathrm{ep}}(M)\eta\psi_M) - M(\eta\psi_M, \{U_0^{-1}v_A(\boldsymbol{x}_1 - a\boldsymbol{y}_{i_0})U_0 - v_A(\boldsymbol{x}_1 - a\boldsymbol{y}_{i_0})\}\eta\psi_M) \\ &\quad - M\sum_{i \neq i_0}(\eta\psi_M, \{U_0^{-1}v_A(\boldsymbol{x}_1 - a\boldsymbol{y}_i)U - v_A(\boldsymbol{x}_1 - a\boldsymbol{y}_i)\}\eta\psi_M).\end{aligned} \tag{33}$$

The last term on the r.h.s. of Eq. (33) is bounded in absolute value by

$$\frac{2M(1+\varepsilon)}{N}\sup_{\boldsymbol{x}\in S_{i_0}}\sum_{i \neq i_0} v_A(\boldsymbol{x}-a\boldsymbol{y}_i) \leqq \mathrm{const}/a^\delta,$$

using inequality (11), assumption $\mathscr{V}_2$ and the fact that $U_0^{-1}v_A(\boldsymbol{x}_1 - a\boldsymbol{y}_i)U_0 - v_A(\boldsymbol{x}_1 - a\boldsymbol{y}_i)$, $i \neq i_0$ is zero unless $\boldsymbol{x}_1 \in S_{i_0}$. Hence this term can be made arbitrarily small for $a \to \infty$. Thus

Est. 2.

$$\begin{aligned}&(U\eta\psi_M, V_{\mathrm{ep}}(M)U\eta\psi_M) = (\eta\psi_M, V_{\mathrm{ep}}(M)\eta\psi_M) \\ &\quad - M(\eta\psi_M, \{v_A(\boldsymbol{f}(\boldsymbol{x}_1) - a\boldsymbol{y}_{i_0}) - v_A(\boldsymbol{x}_1 - a\boldsymbol{y}_{i_0})\}\eta\psi_M) + \gamma_{\mathrm{ep}}(a),\end{aligned}$$

where $\gamma_{\mathrm{ep}}(a) \to 0$ *as* $a \to \infty$.

The V_{ee} repulsion matrix element of $(U\eta\psi_M, H_M U\eta\psi_M)$ is equal to

$$\begin{aligned}&(U\eta\psi_M, V_{\mathrm{ee}}(M)U\eta\psi_M) = (\eta\psi_M, V_{\mathrm{ee}}(M)\eta\psi_M) \\ &+ \frac{M(M-1)}{2}\int d\boldsymbol{x}_1 \ldots d\boldsymbol{x}_M\,|\eta\psi_M(\boldsymbol{x}_1, \ldots \boldsymbol{x}_M)|^2\big(v_R(\boldsymbol{f}(\boldsymbol{x}_1) - \boldsymbol{f}(\boldsymbol{x}_2)) - v_R(\boldsymbol{x}_1 - \boldsymbol{x}_2)\big).\end{aligned} \tag{34}$$

We will establish the following lemma.

Lemma 5.

$$|v_R(f(x_1)-f(x_2))-v_R(x_1-x_2)| \leqq c(a)\, v_R(x_1-x_2) \tag{35}$$

where $c(a)\to 0$ *as* $a\to\infty$.

Postponing the proof of the lemma for the moment, we apply it to the second term on the r.h.s. of Eq. (34), whose absolute value is therefore bounded by

$$c(a)M(M-1)\int_{S_{i_0}\times\mathbb{R}^{3(M-1)}} dx_1\dots dx_M\,|\eta\psi_M(x_1,\dots x_M)|^2 v_R(x_1-x_2)$$

$$\leqq c(a)M(M-1)\frac{4(1+\varepsilon)}{\varepsilon N}\int dx_1\dots dx_M\,|\eta\psi_M(x_1,\dots x_M)|^2 v_R(x_1-x_2)$$

$$\leqq c(a)\frac{8(1+\varepsilon)}{\varepsilon N}(\psi_M, v_R(x_1-x_2)\psi_M) \leqq c(a)\frac{8(1+\varepsilon)}{\varepsilon N} M \sup_x \sum_{i=1}^{N} v_A(x-ay_i)$$

which tends to zero as $a\to\infty$. We have used inequality (13) and the fact that the expectation value for V_{ee} is less than the expectation value for V_{ep}, because $\lambda_{MN}\leqq 0$ and $-\Delta\geqq 0$. Therefore we have shown

Est. 3. $(U\eta\psi_M, V_{\mathrm{ee}}(M)U\eta\psi_M)=(\eta\psi_M, V_{\mathrm{ee}}(M)\eta\psi_M)+\gamma_{\mathrm{ee}}(a)$, *where* $\gamma_{\mathrm{ee}}(a)\to 0$ *as* $a\to 0$. (36)

Proof of Lemma 5. We shall show: For every $c>0$ there exists an $a<\infty$ for which the assertion holds with $c(a)=c$. Let $c>0$ be given. By condition $\mathscr{V}_3$ on v_R, there exists a $x_0\geqq 2r_0$ so large that

$$|v_R'(x)/v_R(x)|\leqq\alpha \tag{37}$$

for $x\geqq x_0-2r_0$ where $\alpha>0$ is a fixed number satisfying

$$2\alpha r_0\exp(2\alpha r_0)\leqq c\,. \tag{38}$$

Then on integrating (37) we obtain

$$v_R(x\pm 2r_0)/v_R(x)\leqq\exp(2\alpha r_0)\quad\text{for}\quad x\geqq x_0\,, \tag{39}$$

and so

$$\begin{aligned}|v_R(x\pm 2r_0)-v_R(x)| &\leqq \left|\int_x^{x\pm 2r_0} dy\, v_R'(y)\right| \leqq \alpha\left|\int_x^{x\pm 2r_0} dy\, v_R(y)\right|\\ &\leqq 2\alpha r_0\exp(2\alpha r_0)\,v_R(x)\leqq c v_R(x)\quad\text{for}\quad x\geqq x_0\,.\end{aligned} \tag{40}$$

Thus, for $|x-y|\geqq x$,

$$\begin{aligned}&|v_R(f(x)-f(y))-v_R(x-y)|\\ &=|v_R(f(x)-x-f(y)+y+x-y)-v_R(x-y)|\\ &\leqq \big|v_R(|x-y|\pm 2r_0)-v_R(x-y)\big|\leqq c\,v_R(x-y)\,,\end{aligned} \tag{41}$$

where the first inequality holds by $\mathscr{V}_1$ and by F_4. The plus or minus sign is selected according to whichever makes the bound larger. This proves the assertion (35) for $|x-y|\geqq x_0=x_0(c)$.

Now suppose $|x-y|<x_0$. Since v_R is differentiable,

$$|v_R'(x)/v_R(x)|\leqq\alpha_0\quad\text{for all}\quad x\,. \tag{42}$$

Choose now a so large that $K_f(a) \leqq 1$ and

$$\alpha_0 K_f(a) x_0 \exp(\alpha_0 K_f(a) x_0) < c\,, \tag{43}$$

cf. Eq. (22). Then by an argument similar to that for $|\boldsymbol{x}-\boldsymbol{y}| \geqq x_0$ we have for $|\boldsymbol{x}-\boldsymbol{y}| < x_0$,

$$\begin{aligned}
&|v_R(\boldsymbol{f}(\boldsymbol{x})-\boldsymbol{f}(\boldsymbol{y})) - v_R(\boldsymbol{x}-\boldsymbol{y})| = |v_R(\boldsymbol{f}(\boldsymbol{x})-\boldsymbol{f}(\boldsymbol{y})-\boldsymbol{x}+\boldsymbol{y}+\boldsymbol{x}-\boldsymbol{y}) - v_R(\boldsymbol{x}-\boldsymbol{y})| \\
&\leqq |v_R(|\boldsymbol{x}-\boldsymbol{y}| \pm K_f(a)|\boldsymbol{x}-\boldsymbol{y}|) - v_R(\boldsymbol{x}-\boldsymbol{y})| \\
&\leqq \alpha_0 K_f(a) x_0 \exp(\alpha_0 K_f(a) x_0)\, v_R(\boldsymbol{x}-\boldsymbol{y}) < c\, v_R(\boldsymbol{x}-\boldsymbol{y})
\end{aligned}$$

and this proves Lemma 5 (all cases).[2]

We return to the proof of Lemma 4. From Est. 1–3 it follows that

$$\begin{aligned}
&(U\eta\psi_M, H_M U\eta\psi_M) \\
&= (\eta\psi_M, H_M \eta\psi_M) - M(\eta\psi_M, \{v_A(\boldsymbol{f}(\boldsymbol{x}_1) - a\boldsymbol{y}_{i_0}) - v_A(\boldsymbol{x}_1 - a\boldsymbol{y}_{i_0})\}\eta\psi_M) + \gamma_3(a,m)
\end{aligned} \tag{44}$$

with $\gamma_3(a,m) \to 0$ as $a, m \to \infty$. Since ψ_M is an eigenfunction for H_M (by the induction hypothesis), we have that [3, p. 458]

$$\begin{aligned}
(\eta\psi_M, H_M \eta\psi_M) &= \lambda_{MN} \|\eta\psi_M\|^2 + \frac{M}{m} \|(\partial_1 \eta)\psi_M\|^2 \\
&\leqq \lambda_{MN} \|\eta\psi_M\|^2 + \frac{M}{m} \frac{(1+\varepsilon)}{N} \|\partial_1 \eta\|_\infty^2\,,
\end{aligned} \tag{45}$$

by inequality (11). The assertion of Lemma 4 follows now by inserting (45) into (44).

We now continue the analysis of Eq. (25) and we pass to the term $(\Phi, H_1(N,a,m)\Phi)$. It clearly approaches $-v_A(\boldsymbol{p}_0 - a\boldsymbol{y}_{i_0})$ as $a, m \to \infty$ when the support of Φ is chosen highly concentrated about $\boldsymbol{p}_0$, i.e. we have the estimate

Est. 4.

$$(\Phi, H_1(N,a,m)\Phi) = -v_A(\varepsilon_0) + \gamma_1(a,m) \tag{46}$$

where $\gamma_1(a,m) \to 0$ as $a, m \to \infty$.

Finally, we analyze the last term on the r.h.s. of Eq. (25). The numerator can be estimated by

$$\begin{aligned}
&M \int d\boldsymbol{x}\, d\boldsymbol{x}_1 \ldots d\boldsymbol{x}_M |\Phi(\boldsymbol{x}) U\eta\psi_M(\boldsymbol{x}_1, \ldots \boldsymbol{x}_M)|^2 v_R(\boldsymbol{x}-\boldsymbol{x}_1) \\
&= M \int_{\boldsymbol{x}_1 \in S_{i_0}} \ldots + M \int_{\boldsymbol{x}_1 \in \mathbb{R}^3 \setminus S_{i_0}} \\
&\leqq M \int_{\boldsymbol{x}_1 \in S_{i_0}} d\boldsymbol{x}_1 \ldots d\boldsymbol{x}_M |\eta\psi_M(\boldsymbol{x}_1, \ldots \boldsymbol{x}_M)|^2 v_R(\boldsymbol{f}(\boldsymbol{x}_1) - \boldsymbol{p}_0) \\
&\quad + M \sup_{\boldsymbol{x} \in \operatorname{supp}\Phi} \int d\boldsymbol{x}_1 \ldots d\boldsymbol{x}_M |\eta\psi_M(\boldsymbol{x}_1, \ldots \boldsymbol{x}_M)|^2 |v_R(\boldsymbol{f}(\boldsymbol{x}_1) - \boldsymbol{x}) - v_R(\boldsymbol{f}(\boldsymbol{x}_1) - \boldsymbol{p}_0)| \\
&\quad + M \int_{\boldsymbol{x}_2 \in \mathbb{R}^3 \setminus S_{i_0}} d\boldsymbol{x}_1 \ldots d\boldsymbol{x}_M |\Phi(\boldsymbol{x}_1) U\eta\psi_M(\boldsymbol{x}_2, \ldots \boldsymbol{x}_{M+1})|^2 v_R(\boldsymbol{x}_1 - \boldsymbol{x}_2)\,.
\end{aligned} \tag{47}$$

[2] An inspection of the proof of Lemma 5 and of Theorem 1 shows that a uniform gap exists also if $\mathscr{V}_3$ is replaced by $\mathscr{V}_3'$: $\lim_{r\to\infty} \frac{d}{dr} \ln v_R(r) = \alpha_1$, with $2\alpha_1 r_0 \exp(2\alpha_1 r_0) < (g/v_A(0))\,(\varepsilon/8(1+\varepsilon))$.

The second term on the r.h.s. of (47) is bounded by

$$M\frac{(1+\varepsilon)}{N}\sup_{\boldsymbol{x}\in\operatorname{supp}\Phi}|v_R(\boldsymbol{f}(\boldsymbol{x}_1)-\boldsymbol{x})-v_R(\boldsymbol{f}(\boldsymbol{x}_1)-\boldsymbol{p}_0)|$$

which goes to zero in the limit of the support of Φ becoming highly concentrated about $\boldsymbol{p}_0$. The last term of (47) is bounded by $\sup_{\boldsymbol{x}\in\operatorname{supp}\Phi} I(\boldsymbol{x})$ where $I(\boldsymbol{x})$ is defined by

$$I(\boldsymbol{x})=M\int_{\boldsymbol{x}_1\in\mathbb{R}^3\setminus S_{i_0}} d\boldsymbol{x}_1\ldots d\boldsymbol{x}_M\,|\eta\psi_M(\boldsymbol{x}_1,\ldots\boldsymbol{x}_M)|^2\,v_R(\boldsymbol{x}-\boldsymbol{x}_1)\,. \tag{48}$$

Let D_0 be a cube of fixed side length d independent of N, a, m, M containing supp Φ, and contained in $D_1\cup D_2$. Then for a sufficiently large,

$$\begin{aligned}\int_{D_0} d\boldsymbol{x}\,I(\boldsymbol{x}) &\leqq M\int_{D_0\times\mathbb{R}^{3M}} d\boldsymbol{x}\,d\boldsymbol{x}_1\ldots d\boldsymbol{x}_M\,|\psi_M(\boldsymbol{x}_1,\ldots\boldsymbol{x}_M)|^2\,v_{Ra}(\boldsymbol{x}-\boldsymbol{x}_1)\\ &\leqq M\frac{8(1+\varepsilon)}{\varepsilon N}\int d\boldsymbol{x}\,d\boldsymbol{x}_1\ldots d\boldsymbol{x}_M\,|\psi_M(\boldsymbol{x}_1,\ldots\boldsymbol{x}_M)|^2\,v_{Ra}(\boldsymbol{x}-\boldsymbol{x}_1)\\ &\leqq\frac{8(1+\varepsilon)}{\varepsilon}\int d\boldsymbol{x}\,v_{Ra}(\boldsymbol{x})\,,\end{aligned}$$

by inequality (14). Thus there is a point $\boldsymbol{p}_1\in D_0$ such that

$$I(\boldsymbol{p}_1)<\frac{8(1+\varepsilon)}{\varepsilon d^3}\int_{|\boldsymbol{x}|\geqq a/4} d\boldsymbol{x}\,v_R(\boldsymbol{x})\,. \tag{49}$$

Furthermore, $I(\boldsymbol{x})$ satisfies a differential inequality,

$$\begin{aligned}|\partial I(\boldsymbol{x})| &\leqq M\int d\boldsymbol{x}_1\ldots d\boldsymbol{x}_M\,|\eta\psi_M(\boldsymbol{x}_1,\ldots\boldsymbol{x}_M)|^2\,|\partial v_R(\boldsymbol{x}-\boldsymbol{x}_1)|\\ &\leqq\alpha_0\int d\boldsymbol{x}_1\ldots d\boldsymbol{x}_M\,|\eta\psi_M(\boldsymbol{x}_1,\ldots\boldsymbol{x}_M)|^2\,v_R(\boldsymbol{x}-\boldsymbol{x}_1)\\ &\leqq\alpha_0 I(\boldsymbol{x})\,,\end{aligned}$$

by inequality (42), so that

$$I(\boldsymbol{x})\leqq\exp(\sqrt{3}\,d\alpha_0)\,I(\boldsymbol{p}_1),\quad\text{for}\quad \boldsymbol{x}\in D_0\,. \tag{50}$$

Therefore

$$\begin{aligned}&M\int d\boldsymbol{x}\,d\boldsymbol{x}_1\ldots d\boldsymbol{x}_M\,|\Phi(\boldsymbol{x})\eta\psi_M(x_1,\ldots x_M)|^2\,v_R(x-x_1)\\ &\leqq M\frac{8(1+\varepsilon)}{\varepsilon d^3 N}\exp(\sqrt{3}\,d\alpha_0)\int_{|\boldsymbol{x}|\geqq a/4} d\boldsymbol{x}\,v_R(\boldsymbol{x})\end{aligned} \tag{51}$$

which goes to zero as $a\to\infty$. We thus obtain the estimate

Est. 5.

$$\begin{aligned}&M\int d\boldsymbol{x}\,d\boldsymbol{x}_1\ldots d\boldsymbol{x}_M\,|\Phi(\boldsymbol{x})\eta\psi_M(\boldsymbol{x}_1,\ldots\boldsymbol{x}_M)|^2\,v_R(\boldsymbol{x}-\boldsymbol{x}_1)\\ &=M\int_{\boldsymbol{x}_1\in S_{i_0}} d\boldsymbol{x}_1\ldots d\boldsymbol{x}_M\,|\eta\psi_M(\boldsymbol{x}_1,\ldots\boldsymbol{x}_M)|^2\,v_R(\boldsymbol{f}(\boldsymbol{x}_1)-\boldsymbol{p}_0)+\gamma_2(a,m)\end{aligned}$$

where $\gamma_2(a,m)\to 0$ as $a, m\to\infty$.

We insert the estimates Lemma 4, Est. 4, Est. 5, and Lemma 3 into Eq. (25) and obtain

$$\begin{aligned}
&\frac{(\Phi \wedge U\eta\psi_M, H_{M+1}(N,a,m)\Phi \wedge U\eta\psi_M)}{\|\Phi \wedge U\eta\psi_M\|^2} \\
&\leqq \lambda_{MN} + \frac{M}{\|\eta\psi_M\|^2}(\eta\psi_M, P_0\{v_A(\boldsymbol{x}_1 - a\boldsymbol{y}_{i_0}) - v_A(f(\boldsymbol{x}_1) - a\boldsymbol{y}_{i_0}) + v_R(f(\boldsymbol{x}_1) - \boldsymbol{p}_0)\}\eta\psi_M) \\
&\quad - v_A(\varepsilon_0) + \gamma(a,m) \\
&\leqq \lambda_{MN} + \frac{M(1+\varepsilon)k}{N(k-1-\varepsilon)} \sup_{\boldsymbol{x}} |v_A(\boldsymbol{x}) - v_A(f(\boldsymbol{x})) + v_R(f(\boldsymbol{x}) + \varepsilon_0 \boldsymbol{e}^{(1)})| - v_A(\varepsilon_0) + \gamma(a,m) \\
&= \lambda'.
\end{aligned}$$

Here, P_0 is the projection onto S_{i_0}. By F4), the sup is bounded by

$$\sup_{|\boldsymbol{x}| \leqq \frac{a}{8}} |v_A(\boldsymbol{x}) - v_A(\boldsymbol{x} + r_0 \boldsymbol{e}^{(1)}) + v_R(\boldsymbol{x} + (r_0 + \varepsilon_0)\boldsymbol{e}^{(1)})| + \gamma'(a)$$

where $\gamma'(a) = v_R\left(\frac{a}{8} - r_0\right) + v_A\left(\frac{a}{8} - r_0 - \varepsilon_0\right) \to 0$ as $a \to \infty$.

Therefore,

$$\begin{aligned}
\lambda' &\leqq \lambda_{MN} + \frac{M}{N}\frac{(1+\varepsilon)k}{(k-1-\varepsilon)} \sup_{\boldsymbol{x}} |v_A(\boldsymbol{x}) - v_A(\boldsymbol{x} + r_0\boldsymbol{e}^{(1)}) + v_R(\boldsymbol{x} + (r_0 + \varepsilon_0)\boldsymbol{e}^{(1)})| \\
&\quad - v_A(\varepsilon_0) + \gamma''(a,m) \\
&\leqq \lambda_{M,N} - g + \gamma'''(a,m), \quad \text{by} \quad (5)
\end{aligned}$$

with $\gamma'''(a,m) \to 0$ as $a, m \to \infty$, and this proves inequality (4) and hence the Theorem 1.

III. Discussion

In this section, we add some further remarks to the main result. One might ask why neither the Coulomb case nor the finite range case (i.e. the case of a potential with compact support) are covered in this paper. We feel that the main difficulty in handling these two cases lies in the fact that one needs more specific information about the eigenfunction ψ_M of $H_M(N, a, m)$ than its mere existence (which is all we have used). In particular, we do not know the charge density distribution, which should be concentrated around the proton sites. In the finite range case, for essentially the same reason, we have no control over the increase in repulsion as the charges are moved slightly by the transformation U. To our knowledge, no appropriate rigorous results are known about the shape of ground state wave functions for the Hamiltonians in question, so that without further work on this problem, the geometrical Lemma 2 concerning families of probability distributions seems to be the only available tool.

Finally we note that some local singular behaviour of the potentials can be accomodated: If v_A, v_R satisfy the hypotheses of our theorem and the particle mass and lattice spacing imply that the conclusion of the theorem holds, then there is also a uniform gap under the perturbation $v_A \to v_A + v_A^{\rm sing}$, $v_R \to v_R + v_R^{\rm sing}$ provided the $L^{3/2}(\mathbb{R}^3)$ norms of $v_A^{\rm sing}$, $v_R^{\rm sing}$ are sufficiently small. The proof of this remark is effected by use of a Sobolev inequality with which one estimates the expectation value for a contribution to the potential energy in terms of the kinetic energy expectation value. We do not know of a decomposition of $v_A = v_R =$ Yukawa potential into singular and continuous parts for which a uniform gap can be shown.

Appendix

The set $\mathscr{V}$ contains pairs $v = (v_A, v_R)$ with $v_A = v_R$ $(= V)$.

Lemma. *Let $\omega(r) \geqq 0$ be a monotonically decreasing function, and let*

(i) $\omega(r) = 0$ iff $r \geqq r_1$,

(ii) $\omega(r_2) = \omega(0)/3$,

(iii) $\omega'(0) = 0$,

(iv) $-a < \omega''(r) < -b < 0$ for $r \leqq r_1$ and $2b > a$.

Then there is a constant $g(\omega) > 0$ such that for $r_0 = \dfrac{r_1 - r_2}{3}$ and some small $\varepsilon > 0$,

$$\begin{aligned}\Delta(x, y) := {}& |\omega(\sqrt{x^2+y^2}) - \omega(\sqrt{(x+r_0)^2+y^2}) + \omega(\sqrt{(x+r_0+\varepsilon)^2+y^2})| \\ & - \omega(\varepsilon) < -g(\omega)\,.\end{aligned}$$

Proof. (I) Let $|y| \geqq r_2$. Then

$$\Delta(x, y) \leqq \omega(r_2) + \omega(r_2) - \omega(\varepsilon) = \frac{2\omega(0)}{3} - \omega(\varepsilon) = -a_1 < 0$$

for $\varepsilon > 0$ small enough.

(II) Let $|y| \leqq r_2$, $x \geqq \frac{2}{3}(r_1 - r_2) + \varepsilon$. Then

$$\Delta(x, y) \leqq \omega(\sqrt{x^2+y^2}) - \omega(\varepsilon) \leqq \omega(\tfrac{2}{3}(r_1 - r_2)) - \omega(\varepsilon) \leqq -a_2 < 0$$

for $\varepsilon > 0$ small enough, since $r_1 \neq r_2$.

(III) $|y| \leqq r_2$, $x \leqq -(r_1 - r_2)$. Then

$$\begin{aligned}\Delta(x, y) &\leqq \omega(\sqrt{(x+r_0+\varepsilon)^2+y^2}) - \omega(\varepsilon) \\ &\leqq \omega(\tfrac{2}{3}(r_1 - r_2) - \varepsilon) - \omega(\varepsilon) \leqq a_3 < 0\end{aligned}$$

for $\varepsilon > 0$ small enough.

(IV) $$\left.\begin{array}{l}|y| \leqq r_2 \\ -(r_1 - r_2) \leqq x \leqq \frac{2}{3}(r_1 - r_2) + \varepsilon\end{array}\right\} = R\,.$$

Then $\sqrt{x^2+y^2} \leqq r_1$, and hence in this region for $\varepsilon > 0$ small (iv) holds.

(IVa) $\sup\limits_{y \in R} \Delta(x, y) = \Delta(x, 0)$.

Proof. We show $\dfrac{d}{dy} \Delta(x, y) = 0$ iff $y = 0$. Indeed

$$\frac{d}{dy} \Delta(x, y) = y \left\{ \frac{\omega'(\sqrt{x^2+y^2})}{\sqrt{x^2+y^2}} - \frac{\omega'(\sqrt{(x+r_0)^2+y^2})}{\sqrt{(x+r_0)^2+y^2}} + \frac{\omega'(\sqrt{(x+r_0+\varepsilon)^2+y^2})}{\sqrt{(x+r_0+\varepsilon)^2+y^2}} \right\}.$$

But $-za \leqq \omega'(z) \leqq -zb$ by (iv) for $0 < z < r_1$ so that $\{\ \} \leqq 2b + a < 0$ and (IVa) follows.

(IVb) So we have to show

$$\underset{x \in R}{\Delta} (x, 0) \leqq -a_4 < 0 .$$

But

$$\Delta(x,0) = \int_0^{\varepsilon} d\xi \int_0^{r_0} d\eta\, \omega''(x+\xi+\eta) + \omega(x+\varepsilon) - \omega(\varepsilon) \leqq -\varepsilon \cdot r_0 b + a\frac{\varepsilon^2}{2} < 0$$

for ε small enough, so that $\Delta(x, y) \leqq -g(\omega) < 0$ as asserted.

Corollary. *Let $V(x) = \omega(x) + y(x)$ with $\omega(x)$ satisfying the hypotheses of the Lemma and*

(i) $0 < y(x) \leqq g(\omega)/4$
(ii) $y(x) \leqq \mathcal{O}(1)\,|x|^{-3-\varepsilon}$
(iii) $\lim\limits_{x \to \infty} \ln y(x)' = 0.$

Then $v = (V, V)$ satisfies the hypotheses of the main theorem.

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Communicated by W. Hunziker

J.-P. Eckmann
L. E. Thomas
Département de Physique Théorique
Université de Genève
32 Boulevard d'Yvoy
CH-1211 Genève 4, Switzerland