Commun. Math. Phys. 104, 271–282 (1986)

Communications in
Mathematical
Physics
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Stability of Coulomb Systems with Magnetic Fields

II. The Many-Electron Atom and the One-Electron Molecule

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Abstract. The analysis of the ground state energy of Coulomb systems interacting with magnetic fields, begun in Part I, is extended here to two cases. Case A: The many electron atom; Case B: One electron with arbitrarily many nuclei. As in Part I we prove that stability occurs if $z\alpha^{12/7} < \text{const}$ (in case A) and $z\alpha^2 < \text{const}$ (in case B), ($z|e| =$ nuclear charge, $\alpha =$ fine structure constant), but a new feature enters in case B. There one *also* requires $\alpha < \text{const}$, regardless of the value of z.

I. Introduction

In the first paper in this series [1] the question of the stability of atoms and molecules in the presence of magnetic fields was raised, and it was answered in the case of the one-electron atom of arbitrary nuclear charge $z|e|$. In the present paper the stability question will be answered in two other cases:

(A) The many electron atom,

(B) The one-electron molecule.

Unfortunately, the stability of the many-electron, many-nucleus system is still an open question.

The reader is referred to the introduction in [1] for the motivation and physical interpretation of this problem. The mathematical essence of the problem is that we want to decide whether or not the energy functional

$$\mathscr{E}(\psi, A, \underline{R}, \underline{z}) \equiv \sum_{j=1}^{N} \int |\sigma_j \cdot (p_j - A(x_j))\psi|^2 \, dx + \varepsilon \int B(x)^2 \, dx + (\psi, V(X, \underline{R}, \underline{z})\psi) \tag{1.1}$$

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* Work partially supported by U.S. National Science Foundation grant PHY-8116101-A03

** Work partially supported by U.S. and Swiss National Science Foundation Cooperative Science Program INT-8503858.

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is bounded below by a suitable constant. The three terms in (1.1) are the electronic kinetic energy, the magnetic field energy and the Coulomb energies respectively. The notation is the following:

The energy unit is 4 Rydbergs $=2mc^2\alpha^2$ and $1/\varepsilon=8\pi\alpha^2$, with $\alpha=e^2/\hbar c=1/137$ being the fine structure constant. The charge unit is $|e|$.

$\psi=\psi(x_1,\dots,x_N,s_1,\dots,s_N)$ is an arbitrary N particle, antisymmetric (electron) wave function. The particle spatial and spin coordinates are x,s with $s=\pm 1$. X denotes the collection $(x_1,\dots,x_N)$. The σ_i^j, $j=1,2,3$ denote the Pauli spin matrices. ψ is assumed to be normalized

$$1=\|\psi\|_2^2=(\psi,\psi)=\sum_{s_1\dots s_N}\int d^{3N}X|\psi(X,s_1,\dots,s_N)|^2\,. \tag{1.2}$$

$A(x)$ is a vector potential and $B=\operatorname{curl}A$ is the magnetic field which is assumed to be in $L^2(\mathbb{R}^3)$. As explained in [1], for any $B\in L^2$, A exists and is uniquely specified by

$$\operatorname{curl}A=B,\ \operatorname{div}A=0,\ A\in L^6(\mathbb{R}^3)\,. \tag{1.3}$$

The first term in (1.1) is the electron kinetic energy. For particle j it is

$$\|\sigma_j\cdot(p_j-A)\psi\|_2^2=\|(p_j-A)\psi\|_2^2-(\psi,\sigma_j\cdot B\psi)\,. \tag{1.4}$$

The Coulomb term is

$$\begin{aligned}V(X,\underline{R},\underline{z})=&\sum_{1\leq i<j\leq N}|x_i-x_j|^{-1}+\sum_{1\leq i<j\leq K}z^iz^j|R_i-R_j|^{-1}\\&-\sum_{i=1}^{N}\sum_{j=1}^{K}z^j|x_i-R_j|^{-1}\,.\end{aligned} \tag{1.5}$$

Here we assume that there are K fixed nuclei of charges $z^j|e|$ and distinct locations $R_j\in\mathbb{R}^3$, $j=1,\dots,K$. The z's and R's will be denoted collectively by $\underline{z}$ and $\underline{R}$. The first term in (1.5) is the electronic repulsion, the second is the nuclear repulsion and the third is the electron-nuclear attraction.

It is useful to have the following notation

$$\tau(\psi,A)\equiv\sum_{j=1}^{N}\|\sigma_j\cdot(p_j-A)\psi\|_2^2+\varepsilon\|B\|_2^2\,, \tag{1.6}$$

$$T(\psi,A)\equiv\sum_{j=1}^{N}\|(p_j-A)\psi\|_2^2\,, \tag{1.7}$$

$$W(\psi,\underline{R},\underline{z})\equiv-(\psi,V(X,\underline{R},\underline{z})\psi)\,. \tag{1.8}$$

We assume $B\in L^2$ and that (1.2) is satisfied. Then, as proved in [1] (with a slight modification to handle the N-coordinate case), in order to make sense of τ and W it is necessary and sufficient to have $\psi\in H^1(\mathbb{R}^{3N})$, i.e. ψ and all its first derivatives are in L^2. The class of all pairs (ψ,A) satisfying the above [and also with ψ normalized as in (1.2)] is denoted by $\mathscr{C}$.

The energy of our system is defined to be

$$E\equiv\inf\{\mathscr{E}(\psi,A,\underline{R},\underline{z})\,|\,(\psi,A)\in\mathscr{C},\ \text{all}\ \underline{R}\}\,. \tag{1.9}$$

This infimum includes an infimum over $\underline{R}$.

From [1] we know that if any single z^j satisfies $z^j > z_c$ (which is evaluated in [1] and which is proportional to α^{-2}), then $E = -\infty$, simply by moving $N-1$ electrons and the other $K-1$ nuclei to infinity. Therefore z_c for the full problem (1.1) is finite. (When $K > 1$, z_c is defined to be the largest z such that E is finite whenever all the $z^j < z$.) Our goal here is to show that z_c is not too small for (1.1). Three cases have to be distinguished.

(A) One nucleus (with $R_1 = 0$ and $z^1 \equiv z$) and an arbitrary number, N, of electrons. In Sect. II we find some $\tilde{z}_c$, which is *independent of* N, such that E is finite when $z < \tilde{z}_c$. We also find some $z_c^L < \tilde{z}_c$ for which we can give a lower bound to E (called E^L) when $z < z_c^L$. Both z_c^L and E^L are *independent of* N. The bound on z_c is

$$z_c > z_c^L \geqq -\tfrac{1}{4} + (0.158)\alpha^{-12/7}. \tag{1.10}$$

Note the exponent 12/7. Is it possible that this can be replaced by 2, as in the one-electron case? We do not know. While our bound on $\tilde{z}_c$ utilizes the electronic Coulomb repulsion in (1.5), we conjecture that the repulsion is not really necessary. This is an interesting open problem.

(B) One electron and an arbitrary number, K, of nuclei. In Sect. III we find, as in case (A), $z_c^L < \tilde{z}_c < z_c$ (with z_c^L and $\tilde{z}_c$ independent of K and proportional to α^{-2}) such that E is finite for $z < z_c$. We also derive a lower bound $E^L < E$ when $z < z_c^L$. However, an important new feature enters here: These results also require that

$$\alpha < \alpha_c \tag{1.11}$$

for some α_c (which is shown to satisfy $0.32 < \alpha_c < 6.7$). In other words, two conditions are required for stability,

$$z^j\alpha^2 \text{ small (all } j) \text{ and } \alpha \text{ small}. \tag{1.12}$$

This situation is reminiscent of the relativistic stability problem [2–4], except that there the requirement is $z^j\alpha$ small and α small. It is interesting to note that there are other indications [5, 6] that the stability of field theory requires a bound on the coupling constant (apart from a bound on z). We shall also prove that the requirement (1.11) for stability is real; it is not an artifact of our proof.

(C) Many electrons and many nuclei. We are unable to solve this problem, but the goal would be to prove that E is finite provided $z^j\alpha^2$ is small (all j) and α is small, and that E is then bounded below by -(const)$(N+K)$.

II. Basic Strategy

The following sections are full of technical details, but the common strategy (similar to that used in [1]) is simple. Let us outline it here. Note that the following steps can be carried out even for the full problem, (C), to give an N and K dependent bound on z_c. It is only in cases A and B that we can eliminate this dependence.

The quantities $\tau(\psi, A)$ and $T(\psi, A)$ were defined in (1.6), (1.7); the following quantity Q is also needed. Let $\varrho(x)$ be the one-particle density associated with ψ:

$$\varrho_\psi(x) = \sum_{j=1}^{N} \sum_{s_1,\ldots,s_N} \int |\psi(X, s_1, \ldots, s_N)|^2 \, d^{3N-3}X^j. \tag{2.1}$$

(X^j means all N variables *except* x_j.) Of course, for fermions we do not have to sum on j. Merely take $j=1$ and then multiply by N. The general expression (2.1) is used because much of the following holds for any statistics (i.e. without symmetry). Then define Q by

$$Q(\psi)=(1/4\varepsilon)\int \varrho_\psi(x)^2\,dx=(1/4\varepsilon)\,\|\varrho_\psi\|_2^2\,. \tag{2.2}$$

Another important quantity is the quantum ground state energy when the $\sigma\cdot B$ and the $\varepsilon\int B^2$ terms are eliminated:

$$E^q(\underline{z})=\inf\{T(\psi,A)-W(\psi,\underline{R},\underline{z})\,|\,(\psi,A)\in\mathscr{C},\ \text{all }\ \underline{R}\}\,. \tag{2.3}$$

Of course $E^q<0$. It is well known that E^q is always finite and that the Lieb-Thirring [7] proof of stability carries through for this case [8].

Given ψ, A, and $\underline{R}$, consider the following scaling (with $\lambda>0$):

$$\begin{aligned}\psi(X,\underline{s})&\to\lambda^{3N/2}\,\psi(\lambda X,\underline{s})\,,\\ A(x)&\to\lambda A(\lambda X)\,,\\ B(x)&\to\lambda^2 B(\lambda x)\,,\\ \underline{R}&\to(1/\lambda)\underline{R}\,.\end{aligned} \tag{2.4}$$

The various quantities scale as

$$\begin{aligned}&W(\psi,\underline{R},\underline{z})\to\lambda W(\psi,\underline{R},\underline{z})\,,\\ &T(\psi,A)\to\lambda^2T(\psi,A),\ \tau(\psi,A)\to\lambda^2\tau(\psi,A)\,,\\ &Q(\psi)\to\lambda^3Q(\psi)\,.\end{aligned} \tag{2.5}$$

If we define

$$W(\psi,\underline{z})=\sup_{\underline{R}}W(\psi,\underline{R},\underline{z})\,, \tag{2.6}$$

then W scales as

$$W(\psi,\underline{z})\to\lambda W(\psi,\underline{z})\,. \tag{2.7}$$

Note that

$$\begin{aligned}E^q(\underline{z})&=\inf_\psi T(\psi,A)-W(\psi,\underline{z})\,,\\ E(\underline{z})&=\inf_\psi \tau(\psi,A)-W(\psi,z)\,.\end{aligned} \tag{2.8}$$

From (2.5)–(2.7) we deduce (as in the case of the one-electron atom) that

$$4|E^q(\underline{z})|\,T(\psi,A)\geqq W(\psi,\underline{z})^2\geqq W(\psi,\underline{R},\underline{z})^2\,. \tag{2.9}$$

The strategy has 7 steps.

Step 1. In [1, Lemma 3.1] a bound for τ in terms T and Q was derived (which trivially extends to N-particles). There are two cases (depending on ψ and A).

Case 1. $T(\psi, A) \geqq 2Q(\psi)$. Then

$$\tau(\psi, A) \geqq T(\psi, A) - Q(\psi). \tag{2.10}$$

Case 2. $T(\psi, A) \leqq 2Q(\psi)$. Then

$$\tau(\psi, A) \geqq \tfrac{1}{4} T(\psi, A)^2 / Q(\psi). \tag{2.11}$$

As will be seen, Case 1 is relevant for determining E^L while Case 2 is relevant for determining $\tilde{z}_c$.

Step 2. (This step is trivial for $K=1$.) Pick some $\underline{z}_0 = (z_0^1, \ldots, z_0^K)$ and consider the rectangle $\underline{z} \prec \underline{z}_0$ (which means $0 \leqq z^j \leqq z_0^j$, all j). For each fixed ψ and $\underline{R}$, the minimum of $W(\psi, \underline{R}, \underline{z})$ in this rectangle occurs at one of the 2^K vertices. This is proved in [2] Lemma 2.3 et. seq. From this it follows that $W(\psi, \underline{z})$, $-E^q(\underline{z})$ and $-E(\underline{z})$ are monotone nondecreasing functions of $\underline{z}$ (with the above order relation). Hence if stability holds for $\underline{\tilde{z}} = (\tilde{z}, \ldots, \tilde{z})$ then it holds when all $z^j \leqq \tilde{z}$.

Step 3 (Definition of $\tilde{z}_c$). Define

$$\delta(\psi, A, \underline{z}) = \tfrac{1}{4} T(\psi, A)^2 / Q(\psi) - W(\psi, \underline{z}). \tag{2.12}$$

The two terms of (2.12) scale the same way [see (2.5) and (2.7)], so that the infimum of $\delta(\psi, A, \underline{z})$ (over ψ and A) is either zero or $-\infty$. We define [with $\underline{\tilde{z}} \equiv (\tilde{z}, \ldots, \tilde{z})$]

$$\tilde{z}_c = \sup\{\tilde{z} \,|\, \delta(\psi, A, \underline{\tilde{z}}) \geqq 0 \text{ for all } (\psi, A) \in \mathscr{C}\}. \tag{2.13}$$

Step 4. Suppose that $z^j < \tilde{z}_c$ for all j and let $(\psi, A) \in \mathscr{C}$ be given. If case 1, (2.10), holds then

$$\mathscr{E}(\psi, A, \underline{R}, \underline{z}) \geqq \tfrac{1}{2} T(\psi, A) - W(\psi, \underline{R}, \underline{z}) \geqq 2E^q(\underline{z}), \tag{2.14}$$

by scaling. If case 2 holds then $\delta(\psi, A, \underline{z}) \geqq 0$. In either case $E(\underline{z})$ is finite and thus

$$\tilde{z}_c \leqq z_c. \tag{2.15}$$

Step 5. We want to find a lower bound (which we call z_c^L) to $\tilde{z}_c$. A lower bound on $T(\psi, A)$ is needed and this is provided by the Lieb-Thirring estimate [9]

$$T(\psi, A)^{3/2} \geqq GQ(\psi)/\alpha^2, \tag{2.16}$$

for a universal constant $G = 1.28$, explicated in (3.8). This leads to the bound

$$\delta(\psi, A, \underline{z}) \geqq \tfrac{1}{4}(G\alpha^{-2})\, T(\psi, A)^{1/2} - W(\psi, \underline{z}). \tag{2.17}$$

Combining this with the bound (2.9) [and the trivial fact that we need only consider $W(\psi, \underline{z}) \geqq 0$] we see that $\delta(\psi, A, \underline{z}) \geqq 0$ if

$$|E^q(\underline{z})| \leqq (G/8\alpha^2)^2. \tag{2.18}$$

By (2.13)

$$\tilde{z}_c \geqq z_c^L \equiv \sup\{z \,|\, |E^q(\underline{z})| \leqq (G/8\alpha^2)^2\}, \tag{2.19}$$

[$\underline{z}$ means $(z, \ldots, z)$]. The monotonicity given in Step 2 has been used.

Step 6 (Bound on the energy). Suppose that $z^j \leqq z_c^L$ for all j. Let $(\psi, A) \in \mathscr{C}$ be given. Case 2 is irrelevant since $\delta(\psi, A, \underline{z}) \geqq 0$ by definition. Therefore a lower bound, $E^L(\underline{z})$, to $E(\underline{z})$ can be obtained by the following minimization problem:

$$E^L(\underline{z}) = \min(T - Q - W), \tag{2.20}$$

under the conditions

$$T \geqq 2Q, \; T \geqq (GQ/\alpha^2)^{2/3}, \; T \geqq W^2/4|E^q(\underline{z})|. \tag{2.21}$$

This algebraic problem is solved in Appendix B of [1] and the result is

$$E(\underline{z}) \geqq E^L(\underline{z}) = E^q(\underline{z}) f(\gamma), \tag{2.22}$$

$$f(\gamma) \equiv \tfrac{4}{3}\gamma^{-2}\{3\gamma - 2 + 2(1-\gamma)^{3/2}\}, \tag{2.23}$$

$$\gamma \equiv 6|E^q(\underline{z})|^{1/2}\alpha^2/G. \tag{2.24}$$

Equation (2.22) gives E^L as the exact E^q times a correction factor, f, which depends on γ, where γ is proportional to $|E^q|^{1/2}$. Two things should be noted: By the definition (2.19),

$$\gamma \leqq 3/4, \tag{2.25}$$

when $z^j < z_c^L$ (all j). Second, the function f is monotone increasing in γ on $[0, 1]$.

Step 7. To utilize (2.19) and (2.22) we require a bound on $E^q(\underline{z})$. Let

$$E_L^q(\underline{z}) \leqq E^q(\underline{z}) < 0, \tag{2.26}$$

be any lower bound to E^q. Inserting $E_L^q(\underline{z})$ in (2.19) will give a lower bound to $z_c^L \leqq z_c$. Inserting $E_L^q(\underline{z})$ in (2.24) and then inserting this γ in (2.23) and (2.22) will (assuming that $\gamma \leqq 1$) give a lower bound to E^L. In cases A and B we can get an effective $E_L^q(\underline{z})$ which is independent of N and K. The former uses the Lieb-Thirring technique [7] together with a novel bound on the Coulomb energy. This is done in Sect. III. Case B is controlled by relating it to a relativistic problem solved in [2]; this is done in Sect. IV.

Remark. In case B we deal with only one electron. Given this restriction on N, (2.16) holds with a larger value of G, namely $G = 3.83$. This larger G can be used in Steps 5–7.

III. The Many-Electron Atom

Our first task is to prove the kinetic energy estimate (2.16). Consider the single-particle Schrödinger operator $h = (p - A)^2 - V(x)$, where $V(x) \geqq 0$ and consider also the N-particle operator $H = \sum_j h_j$. The q spin state fermionic ground state energy of H, E, satisfies $E \geqq q \sum_i e_i$, where the e_i are the negative eigenvalues of h. ($q = 2$ in our case.) We have that

$$\sum_i e_i \geqq -|e_1|^{1/2} \sum_i |e_i|^{1/2}, \tag{3.1}$$

where e_1 is the ground state energy. In [1, (3.19)] we quoted a result of [9] that

$$|e_1|^{1/2} \leqq L^1_{\frac{1}{2},3} \|V\|_2^2, \tag{3.2}$$

where $L^1_{1/2,3} = 0.0135$ to three significant figures.

In [9] it is also shown that

$$\sum_i |e_i|^{1/2} \leqq L_{\frac{1}{2},3} \|V\|_2^2. \tag{3.3}$$

Strictly speaking, (3.3) was shown only for $A=0$ in [9] and it is not known whether the (unknown) *sharp* constant L in (3.3) occurs for $A=0$. However, as pointed out in [8, 11], the L actually obtained in [9] holds for all A. The L obtained by using the method of [12] also holds for all A (see [11] for a discussion of the Ito-Nelson integral). The latter method gives a better value for L and the numerical computation is most clearly explained in [10, Eqs. (46)–(51)]. In the notation of [10], we take $a=0.61$ exactly and $b=3.6807$. Then (3.3) holds with

$$L_{\frac{1}{2},3} = b(4\pi)^{-3/2}\Gamma(\tfrac{3}{2})\tfrac{1}{2}a^{-1} = 0.060021, \tag{3.4}$$

to 5 figures. Thus,

$$\sum_i |e_i| \leqq L^1_{\frac{1}{2},3} L_{\frac{1}{2},3} \|V\|_2^4 \leqq (0.000810)\, \|V\|_2^4. \tag{3.5}$$

Now take $V(x) = c\varrho_\psi(x)$, where ϱ_ψ is given by (2.1). Then

$$T(\psi, A) - c\int \varrho_\psi^2 = (\psi, H\psi) \geqq -q\sum_i |e_i|. \tag{3.6}$$

Using (3.5) and (3.6), with $c^{-3} = 4qL^1_{\frac{1}{2},3} L_{\frac{1}{2},3} \int \varrho_\psi^2$, we obtain

$$T(\psi, A) \geqq \tfrac{3}{4}(4qL^1_{\frac{1}{2},3} L_{\frac{1}{2},3})^{-1/3} \{\textstyle\int \varrho_\psi^2\}^{2/3} \geqq (4.02)\{\textstyle\int \varrho_\psi^2\}^{2/3}, \tag{3.7}$$

for $q=2$. Thus, (2.16) holds [recalling (2.2)] with

$$G = 8.07/2\pi = 1.28. \tag{3.8}$$

Our second task is to find a lower bound for $E^q(\underline{z})$, given by (2.3). Again we use an inequality derived in [7, 9], but with a better constant derived in [10, Eq. (52)]:

$$T(\psi, A) \geqq (2.7709) \int \varrho_\psi(x)^{5/3}\, dx. \tag{3.9}$$

The second term in V, (1.5), is absent since there is only one nucleus, located at $R=0$. The third term contributes the following to W:

$$W_3(\psi, z) = z \int \varrho_\psi(x)\, |x|^{-1}\, dx. \tag{3.10}$$

The first term in V (call its contribution W_1) requires some elaboration. For $x, y \in \mathbb{R}^3$ and $R > 0$,

$$|x-y|^{-1} \geqq \{|x| + |y|\}^{-1} \geqq \tfrac{1}{2} R f(x) f(y), \tag{3.11}$$

$$\begin{aligned} f(x) &= 1/|x| \quad \text{if} \quad |x| \geqq R, \\ &= 0 \qquad\ \ \text{if} \quad |x| < R. \end{aligned} \tag{3.12}$$

Using (3.11) and the positivity of $|\psi|^2$ and $|x_i - x_j|^{-1}$, we have, for any $0 \leqq \sigma \leqq 1$,

$$\begin{aligned} W_1(\psi, z) &\leqq -\tfrac{1}{4} R\sigma \left(\psi, \left\{ \left[\sum_{i=1}^{N} f(x_i) \right]^2 - \sum_{i=1}^{N} f(x_i)^2 \right\} \psi \right) \\ &\leqq -\tfrac{1}{4} R\sigma \{ [\int \varrho_\psi f]^2 - \int \varrho_\psi f^2 \}, \end{aligned} \tag{3.13}$$

since $\langle (\sum f)^2 \rangle \geqq \langle \sum f \rangle^2$.

Combining (3.9), (3.10), (3.13),

$$\begin{aligned} T(\psi, A) - W(\psi, z) \equiv \mathscr{E}^q(\psi, A) &\geqq \mathscr{E}_{R,\sigma}(\varrho_\psi, z) \\ &\equiv (2.7709) \int \varrho_\psi^{5/3} - z \int \varrho_\psi |x|^{-1} + \tfrac{1}{4} R\sigma [\int \varrho_\psi f]^2 \\ &\quad - \tfrac{1}{4} R\sigma \int \varrho_\psi f^2 . \end{aligned} \tag{3.14}$$

Therefore,

$$E^q(z) \geqq \sup_{0 \leqq \sigma \leqq 1} \sup_{R > 0} \inf_{\varrho} \mathscr{E}_{R,\sigma}(\varrho, z) . \tag{3.15}$$

We could, of course, impose the extra condition $\int \varrho = N$ in (3.15) but, as we desire an N-independent bound for E^q, we forego this.

First minimize (3.14) with respect to $\varrho(x)$ for $|x| \leqq R$. Only the first two terms are relevant in this region. Define $\Gamma = (5/3)(2.7709)$. Then $\Gamma \varrho^{2/3}(x) = z/|x|$. The first two terms contribute (for $|x| < R$)

$$-z^{5/2} \Gamma^{-3/2} (16\pi/5) R^{1/2} . \tag{3.16}$$

Next we consider the contributions for $|x| > R$. Here we merely omit the $\varrho^{5/3}$ term and we use $R|x|^{-2} \leqq |x|^{-1}$ in the last term. Let $Y \equiv \int_{|x|>R} \varrho(x) |x|^{-1} dx$. Then the sum of the last three terms is not less than the minimum (with respect to Y) of $-(z + \frac{1}{4}\sigma) Y + \frac{1}{4} R\sigma Y^2$. This minimum is

$$-(z + \tfrac{1}{4}\sigma)^2 / R\sigma . \tag{3.17}$$

The maximum of this with respect to $\sigma \in [0, 1]$ is

$$-M(z)/R , \tag{3.18}$$

$$\begin{aligned} M(z) &= z && \text{if} \quad z \leqq 1/4 , \\ &= (z + \tfrac{1}{4})^2 && \text{if} \quad z \geqq 1/4 . \end{aligned} \tag{3.19}$$

Adding (3.16) and (3.18) and then maximizing with respect to $R > 0$ gives

$$\begin{aligned} E^q(z) &\geqq -3 z^{5/3} \Gamma^{-1} (8\pi/5)^{2/3} M(z)^{1/3} \\ &= -(1.9062) z^{5/3} M(z)^{1/3} . \end{aligned} \tag{3.20}$$

As we shall be primarily interested in $z > 1/4$, the little exercise with σ is academic; it was done merely to demonstrate a z^2 (instead of $z^{5/3}$) bound when $z \leqq 1/4$.

With these results we can now bound z_c, see (2.19) and E^L, see (2.22). Since z_c will be large, let us use the bound $z^{5/3} M(z)^{1/3} \leqq (z + \frac{1}{4})^{7/3}$ for all $z > 0$. Then, from (2.19)

$$z_c \geqq \tilde{z}_c \geqq z_c^L \geqq -\tfrac{1}{4} + (0.158) \alpha^{-12/7} \geqq 720 . \tag{3.21}$$

This bound (720) is about 25 times smaller than the z_c^L obtained in [1] for the one-electron atom. It is about 290 times less than the *upper* bound on z_c obtained in [13], see also [1, (3.24)]. This upper bound ($z_c \leqq 208{,}000$) also holds, of course, for the full problem with K nuclei and N electrons.

The lower bound (2.22) on the energy is

$$E^L = E^q(z)\, f(\gamma) \tag{3.22}$$

and, using (3.20),

$$\begin{aligned}\gamma &\leqq 6\alpha^2(1.9062)^{1/2}\,(z+\tfrac{1}{4})^{7/6}/G \\ &\leqq (6.47)\,\alpha^2(z+\tfrac{1}{4})^{7/6} \\ &\leqq (0.000345)\,(z+\tfrac{1}{4})^{7/6}\,.\end{aligned} \tag{3.23}$$

As an illustration, take $z=100$. By (2.23) the fractional change in the energy, $f(\gamma)-1$, is less than 0.013, which is about $1\tfrac{1}{2}\%$.

IV. The One-Electron Molecule

Our first task is to find a lower bound to E^q in (2.3) with

$$V(x, \underset{\sim}{R}, \underset{\sim}{z}) = -\sum_{j=1}^{K} z^j|x-R_j|^{-1} + \sum_{i<j} z^i z^j |R_i - R_j|^{-1}\,. \tag{4.1}$$

Since $N=1$, we can use the diamagnetic inequality (see [1]): $T(\psi, A) \geqq T(|\psi|, 0) \equiv T(\psi) = \|\nabla|\psi|\,\|_2^2$, and hence can assume that ψ is real and positive and $A=0$. Define

$$\bar{V}(x, \underset{\sim}{R}) = -(2/\pi)\sum_{j=1}^{K} |x-R_j|^{-1} + (12/\pi)\sum_{i<j} |R_i - R_j|^{-1}\,. \tag{4.2}$$

It is proved in [2, Proposition 2.2] that for all $\psi \in L^2$, $(-\Delta)^{1/4}\psi \in L^2$ and all $\underset{\sim}{R}$,

$$(\psi, (-\Delta)^{1/2}\psi) \geqq -(\psi, \bar{V}\psi)\,. \tag{4.3}$$

We also have the fact (Schwarz inequality) that

$$\|\nabla\psi\|_2^2 \geqq (\psi, (-\Delta)^{1/2}\psi)^2\,, \tag{4.4}$$

when $\|\psi\|_2 = 1$.

Given $\underset{\sim}{z}$, define

$$Z = \max(z^1, \ldots, z^K) \quad \text{and} \quad \underset{\sim}{Z} = (Z, \ldots, Z)\,. \tag{4.5}$$

As shown in Step 2,

$$E^q(\underset{\sim}{z}) \geqq E^q(\underset{\sim}{Z})\,. \tag{4.6}$$

Suppose that $Z \geqq 6$. Then

$$(\pi Z/2)\,\bar{V}(x, \underset{\sim}{R}) \leqq V(x, \underset{\sim}{R}, \underset{\sim}{Z})\,. \tag{4.7}$$

Combining (4.3), (4.4), (4.7) and with $t=(\psi,(-\Delta)^{1/2}\psi)$

$$E^q(\underline{z}) \geqq \inf_t \{t^2-(\pi Z/2)t\} = -(\pi Z/4)^2 . \tag{4.8}$$

[Note: When $K=1$, the exact result is $-(Z/2)^2$.]

By monotonicity (4.6), when $Z<6$

$$E^q(Z) \geqq E^q(6) \geqq -(3\pi/2)^2 . \tag{4.9}$$

Combining (4.6), (4.8), (4.9) we obtain for *all* $\underline{z}$

$$|E^q(\underline{z})|^{1/2} \leqq (\pi/4) \max\{6, z^1, \ldots, z^K\} . \tag{4.10}$$

Turning now to (2.19) and using (4.10) we have that

$$z_c^L \geqq \sup\left\{ z \,\middle|\, \frac{\pi}{4}\max(6,z) \leqq G/8\alpha^2 \right\} . \tag{4.11}$$

As remarked at the end of Sect. II, since $N=1$ we are entitled to replace $L_{\frac{1}{2},3}$ by $L^1_{\frac{1}{2},3}$ in (3.7), (3.8), and (2.16). Thus,

$$G=3.83 , \tag{4.12}$$

in our case.

Suppose that

$$\alpha^2 \leqq \alpha_c^2 \equiv G/(12\pi) = 0.102 . \tag{4.13}$$

Then, from (4.11)

$$z_c^L \geqq G/(2\pi\alpha^2) = 0.609\alpha^{-2} > 11{,}400 . \tag{4.14}$$

(This number, 11,400, compares favorably with 17,900 obtained in [1] for $K=1$.) In the opposite case [(4.13) is violated], the set of z's in (4.13) is empty and our method gives no bound at all on $E(\underline{z})$ for $\underline{z} \neq 0$. Thus, our method requires *two* conditions for stability

(i) $$\alpha^2 z^j \leqq 0.609 \quad \text{for all } j , \tag{4.15}$$

(ii) $$\alpha \leqq \alpha_c = (0.102)^{1/2} = 0.319 . \tag{4.16}$$

One can question whether the condition (4.16) on α is an artifact of our method or whether there really is an α_c (which will, of course, be greater than 0.319 – but finite). The second alternative is correct as we now prove.

Lemma. *Suppose that*

$$\alpha > 6.67 , \tag{4.17}$$

then for every $\underline{z}=(z,\ldots,z)$ with $z>0$ there is a K such that $E(\underline{z})=-\infty$.

Remark. The right side of (4.17) is not the best bound that can be obtained by the following method.

Proof. In [1] we showed that $E=-\infty$ when $K=1$ if

$$z\alpha^2 > \inf\{\textstyle\int B^2\}\,\{8\pi(\psi,|x|^{-1}\psi\}^{-1} \equiv P , \tag{4.18}$$

where (ψ, A) runs over $\mathscr{F} = \{(\psi, A) \in \mathscr{C} | \sigma \cdot (p - A)\psi = 0\}$. $\mathscr{F}$ is not empty [13]. By taking a particular example, one finds $P \leqq 9\pi^2/8 = 11.10$. Therefore, if $\alpha^2 > P$, we can take $K = 1$ and achieve instability for all $z \geqq 1$. Using the above bound, this is also achieved for $z \geqq 1$ if $\alpha > 3.34$.

Next, to investigate $z < 1$, take any $(\psi, A) \in \mathscr{F}$, whence

$$\mathscr{E}(\psi, A, \underline{R}, \underline{z}) = \varepsilon \int B^2 + \int \varrho_\psi(x)\, V(x, \underline{R}, \underline{z})\, dx\,, \tag{4.19}$$

with $\varrho_\psi(x) = \langle \psi, \psi \rangle (x)$. We want to show that for suitable α and K, $\mathscr{E}$ is negative for some $\underline{R}$. [If it is negative then, by the scaling (2.4), $\mathscr{E}$ can be made arbitrarily negative.] To show this, it suffices to average $\mathscr{E}$ with some probability density $F(R^1, \ldots, R^K)$, $\int F d^K R = 1$, and to show that $\langle \mathscr{E} \rangle \equiv \int \mathscr{E} F d^K R < 0$. Take $F = \varrho_\psi(R^1) \ldots \varrho_\psi(R^K)$. The result is

$$\langle \mathscr{E} \rangle = \varepsilon \int B^2 - \tfrac{1}{2} zK[2 - z(K-1)]\, I(\varrho_\psi)\,, \tag{4.20}$$

$$I(\varrho) = \int\int \varrho(x)\, \varrho(y)\, |x-y|^{-1}\, dx\, dy\,. \tag{4.21}$$

Choose K to be the smallest integer closest to $\frac{1}{2} + 1/z$. Then $zK = (z/2) + 1 + \mu$ with $|\mu| \leqq \frac{1}{2} z$ and $zK[2 - z(K-1)] = [1 + (z/2)]^2 - \mu^2 \geqq 1 + z > 1$. Therefore, if

$$\alpha^2 > (4\pi)^{-1} \inf_{\mathscr{F}} \int B^2 / I(\varrho)\,, \tag{4.22}$$

instability occurs for all $0 < z < 1$.

For the particular example in [13] quoted above, one has

$$|B(x)| = 12(1 + |x|^2)^{-2}, \varrho(x) = [\pi(1 + |x|^2)]^{-2}\,,$$

and one computes

$$\int B^2 = 18\pi^2,\ I(\varrho) = 1/\pi\,. \tag{4.23}$$

Therefore, if $\alpha > 3 \cdot 2^{-1/2}\pi = 6.67$, instability also occurs for all $z < 1$. □

Acknowledgements. It is a pleasure to thank J. Fröhlich and H.-T. Yau for helpful discussions.

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Communicated by A. Jaffe

Received October 10, 1985