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LETTER TO THE EDITOR

On the stability of relativistic one-electron molecules

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Abstract. In appropriate units, the no-pair Hamiltonian for a system of one-electron relativistic molecules with K fixed nuclei, having charge and position $Z_k, \boldsymbol{R}_k$, $k = 1, 2, \ldots, K$, is of the form $\boldsymbol{B}_{1,K} = \Lambda_+(D_0 + \alpha V_c)\Lambda_+$, where Λ_+ is the projection onto the positive spectral subspace of the free Dirac operator D_0 and $V_c = -\sum_{k=1}^{K} \frac{\alpha Z_k}{|x-\boldsymbol{R}_k|} + \sum_{k<l,k,l=1}^{K} \frac{\alpha Z_k Z_l}{|\boldsymbol{R}_k-\boldsymbol{R}_l|}$, with α Sommerfeld's fine structure constant. We discuss the background and significance of our result that for $\alpha Z_k \leqslant \alpha Z_c = \frac{2}{\pi/2+2/\pi}$, $k = 1, 2, \ldots, K$, and $\alpha \leqslant \frac{2\pi}{(\pi^2+4)(2+\sqrt{1+\pi/2})}$, $\boldsymbol{B}_{1,K} \geqslant \text{const} \cdot K$, and give an outline of the main features of our proof.

A system of N electrons and K static nuclei is known to be stable when governed by non-relativistic quantum mechanics. This means that the ground state energy E_0 associated with the Hamiltonian, which, in appropriate units, is of the form

$$\boldsymbol{H}_{N,K} = \sum_{j=1}^{N}(-\Delta_j) + \alpha V_c \tag{1}$$

satisfies

$$E_0 \geqslant \text{const} \cdot (N + K); \tag{2}$$

in (1), α is Sommerfeld's fine structure constant and V_c is the Coulomb potential of the electrons and nuclei, namely

$$V_c(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) = -\sum_{j=1}^{N}\sum_{k=1}^{K} \frac{Z_k}{|\boldsymbol{x}_j - \boldsymbol{R}_k|} + \sum_{1\leqslant j<l\leqslant N} \frac{1}{|\boldsymbol{x}_j - \boldsymbol{x}_l|} + \sum_{1\leqslant j<k\leqslant K} \frac{Z_j Z_k}{|\boldsymbol{R}_j - \boldsymbol{R}_k|} \tag{3}$$

where the $\boldsymbol{x}_j$, $\boldsymbol{R}_k$ denote the coordinates of the jth electron and kth nucleus respectively, and Z_k the charge of the kth nucleus. The result (2) was originally established by Dyson and Lenard in the seminal paper [7]. Subsequently, Lieb and Thirring [13] gave a different and considerably easier proof, and obtained a much improved constant in (2). The latter paper has also had a profound effect on the subject, and has generated a substantial amount of work in this area of research.

If relativistic considerations are introduced, there is an immediate problem if the Laplacian $-\Delta$ in (1) is replaced by the free Dirac operator $D_0 = \frac{1}{i}\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta$ (where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$, and α_j, β are 4×4 Dirac matrices) on account of continuum dissolution; the many-body Hamiltonian ceases to have a spectral gap and hence there are no bound states. To overcome this problem, various approximation have been tried. In [5] Conlon investigated

$$\boldsymbol{H}^{rel}_{N,K} = \sum_{j=1}^{N}\{(-\Delta_j + 1)^{\frac{1}{2}}\} + \alpha V_c \tag{4}$$

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and proved stability for $Z_k = 1$, $k = 1, 2, \ldots, K$, as long as $\alpha < 10^{-200}$; Fefferman and de la Llave [9] improved Conlon's result to a computer-assisted range for α of $\alpha \leqslant 1/2.06\pi$, or $\alpha \leqslant \frac{1}{5}\pi$ otherwise. The single-particle operator

$$\boldsymbol{H}_{1,1}^{rel} = (-\Delta + 1)^{\frac{1}{2}} - \frac{\alpha Z}{|\boldsymbol{x}|} \tag{5}$$

was shown by Herbst in [11] (see also Weder [17]) to be bounded below (and in fact positive) in $L^2(\boldsymbol{R}^3)$ if and only if $\alpha Z \leqslant 2/\pi$, with an absolutely continuous spectrum in $[1, \infty)$ for $\alpha Z < 2/\pi$ and an infinity of positive energy levels accumulating at 1. For the optimal range $\alpha Z_k \leqslant 2/\pi$, $k = 1, 2, \ldots, K$ in (4), Lieb and Yau proved in [14] that there is stability if and only if α is less than some critical value $\alpha_c > \frac{1}{94}$; this paper also contains a comprehensive description of the problem and a survey of the progress that had been made up to that time.

Another way to proceed in the relativistic case is to follow the lead of Brown and Ravenhall in [3] and work with the Hamiltonian

$$\boldsymbol{B}_{N,K} = \Lambda_+ \left(\sum_{j=1}^{N} D_0^{(j)} + \alpha V_c \right) \Lambda_+ \tag{6}$$

where Λ_+ is the projection onto the electronic Hilbert space of antisymmetric spinors

$$\mathcal{H}_{(N)} = \bigwedge_{j=1}^{N} \mathcal{H}_+^{(j)}$$

where $\mathcal{H}_+^{(j)}$ is the positive spectral subspace of the Dirac operator $D_0^{(j)}$ acting in the space of the jth electron. In the case of one electron ($N = 1$) the explicit form of the projection is

$$\Lambda_+ = \frac{1}{2} \left\{ \mathbf{1}_4 + \frac{\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta}{e(\boldsymbol{p})} \right\} \tag{7}$$

where $e(\boldsymbol{p}) = \sqrt{\boldsymbol{p}^2 + 1}$, and $\mathbf{1}_4$ is the unit 4×4 matrix. Some interesting properties of the one-electron operator

$$\boldsymbol{B}_{1,1} = \Lambda_+ \left[D_0 - \frac{\alpha Z}{|\boldsymbol{x}|} \right] \Lambda_+ \tag{8}$$

in $\mathcal{H} \equiv \mathrm{L}^2(\boldsymbol{R}^3) \otimes \boldsymbol{C}^4$ have been uncovered in recent years. For instance, we have the following:

- In [8], $\boldsymbol{B}_{1,1}$ is shown to be bounded below if and only if $\alpha Z \leqslant \alpha Z_c =: \gamma_c = 2/(\frac{\pi}{2} + \frac{2}{\pi})$, thus confirming a prediction of Hardekopf and Sucher in [10] based on numerical considerations. The critical charge Z_c is approximately 124 on taking $\alpha = \frac{1}{137}$, and hence all known elements are included in the range. In [4, 15] it was proved that $\boldsymbol{B}_{1,1}$ is in fact positive for $Z \leqslant Z_c$.
- When $\alpha Z \leqslant \gamma_c$, the essential spectrum of $\boldsymbol{B}_{1,1}$ coincides with $[1, \infty)$, the singular continuous spectrum being empty if $\alpha Z < \gamma_c$.
- The upper bound $\max(1, 2\alpha Z - \frac{1}{2})$ for eigenvalues was obtained in [1] using a virial theorem, and this implies that the spectrum of $\boldsymbol{B}_{1,1}$ is absolutely continuous in $[1, \infty)$ if $\alpha Z \leqslant \frac{3}{4}$. The number $\frac{3}{4}$ features in other interesting ways for $\boldsymbol{B}_{1,1}$ (see [16]).

As a first step in a projected investigation of the relativistic stability problem using the Hamiltonian $\boldsymbol{B}_{N,K}$ as model, the single-electron case $N = 1$ is considered in [2], the objective being to establish stability for the optimal range $\alpha Z_k \leqslant \gamma_c$, $k = 1, 2, \ldots, K$, and a range $\alpha \leqslant \alpha_c$ which includes the physical value $\approx \frac{1}{137}$. The strategy is based on that of Daubechies and Lieb in [6] who considered the analogous problem for the Hamiltonian $\boldsymbol{H}_{1,K}^{rel}$. The main result is as follows.

Theorem (Stability of one-electron molecules in the Brown–Ravenhall model). *Let* $\alpha Z_k \leqslant \gamma_c = 2/(\frac{\pi}{2} + \frac{2}{\pi})$, $k = 1, 2, \ldots, K$ *and* $\alpha \leqslant \frac{2\pi}{(\pi^2+4)(2+\sqrt{1+\pi/2})}$. *Then* $\boldsymbol{B}_{1,K}$ *exhibits stability, i.e.* $\boldsymbol{B}_{1,K} \geqslant \text{const} \cdot K$ *in* $\mathcal{H}$.

To achieve this, substantial modifications to the elegant proof of Daubechies and Lieb are necessary, in the absence of inequalities for symmetric decreasing rearrangements of functions which play a prominent role in [7], and the presence of an indefinite integral kernel. The first step is the reduction of the problem for the single-particle operator $\boldsymbol{B}_{1,1}$ to that for an operator $b_{1,1}$ acting on Pauli spinors in $\mathcal{H}_2 \equiv \mathrm{L}^2(\boldsymbol{R}^3) \otimes \boldsymbol{C}^2$, using the observation that any $\psi \in \Lambda_+\mathcal{H}$ has Fourier transform of the form

$$\hat{\psi}(\boldsymbol{p}) = \frac{1}{n(\boldsymbol{p})} \begin{pmatrix} [e(\boldsymbol{p}) + 1]u(\boldsymbol{p}) \\ (\boldsymbol{p} \cdot \boldsymbol{\sigma})u(\boldsymbol{p}) \end{pmatrix}$$

where $n(\boldsymbol{p}) = [2e(\boldsymbol{p})(e(\boldsymbol{p}) + 1)]^{1/2}$ and $u \in \mathcal{H}_2$. The operator $b_{1,1}$ is bounded below if and only if the (massless) homogeneous operator

$$\tilde{b}_{1,1} = |\boldsymbol{p}| - \frac{1}{2}\alpha Z \left(\frac{1}{|x|} + \frac{\boldsymbol{p} \cdot \boldsymbol{\sigma}}{|\boldsymbol{p}|} \frac{1}{|x|} \frac{\boldsymbol{p} \cdot \boldsymbol{\sigma}}{|\boldsymbol{p}|} \right)$$

is non-negative, as their difference can be extended to a bounded operator on $\mathcal{H}_2$. The non-negativeness of $\tilde{b}_{1,1}$ for $\alpha Z \leqslant \gamma_c$ is equivalent to the fact that the non-negative operator $\mathcal{K} = \gamma_c \frac{1}{\sqrt{|x|}} P_+ \frac{1}{|\boldsymbol{p}|} P_+ \frac{1}{\sqrt{|x|}}$, where $P_+ = \frac{1}{2}(1 + \frac{\boldsymbol{p} \cdot \boldsymbol{\sigma}}{|\boldsymbol{p}|})$, satisfies $\sup_{\|\psi\|=1}(\psi, \mathcal{K}\psi) = 1$; here $(\cdot, \cdot)$ and $\|\cdot\|$ denote the inner-product and norm respectively in the underlying Hilbert space. A local form of the latter fact has a pivotal role in the proof: for all $\psi \in \mathcal{H}_2$ with support in the ball $B(0, R) = \{\boldsymbol{x} : |\boldsymbol{x}| < R\}$,

$$(\psi, \mathcal{K}\psi) \leqslant \|\psi\|^2 - \frac{1}{(\pi^3 + 4\pi)R^3} \left(\int_{\boldsymbol{R}^3} |\psi(\boldsymbol{x})| \frac{\mathrm{d}\boldsymbol{x}}{\sqrt{|\boldsymbol{x}|}} \right)^2. \tag{9}$$

To prove this a partial wave decomposition of $\mathcal{H}_2$ in terms of spherical spinors is used, and an important role is played by the inequality

$$\frac{\boldsymbol{p} \cdot \boldsymbol{\sigma}}{|\boldsymbol{p}|^2} \leqslant \frac{\boldsymbol{x} \cdot \boldsymbol{\sigma}}{|\boldsymbol{x}|} \frac{1}{|\boldsymbol{p}|} \frac{\boldsymbol{x} \cdot \boldsymbol{\sigma}}{|\boldsymbol{x}|} \tag{10}$$

which relates to the different expressions for $\boldsymbol{B}_{1,1}$ in $\boldsymbol{x}$ and $\boldsymbol{p}$ spaces. Once (9) is available the strategy of Daubechies and Lieb can be followed.

Other obstacles have to be overcome for the many-particle problem for $\boldsymbol{B}_{N,K}$. In the general case when relativity and spin–field interaction are included, the Hamiltonian is

$$\boldsymbol{B}_{N,K}(\boldsymbol{A}) = \Lambda_+(\boldsymbol{A}) \left(\sum_{j=1}^{N} D_{\boldsymbol{A}}^{(j)} + \alpha V_c \right) \Lambda_+(\boldsymbol{A}) + H_{field} \tag{11}$$

where

$$D_{\boldsymbol{A}} = \boldsymbol{\alpha} \cdot \left(\frac{1}{i} \boldsymbol{\nabla} + \boldsymbol{A} \right) + \beta$$

H_{field} is the field energy

$$H_{field} = \frac{1}{8\pi\alpha} \int_{\boldsymbol{R}^3} \boldsymbol{B}(\boldsymbol{x})^2 \, \mathrm{d}\boldsymbol{x}$$

and $\boldsymbol{B} = \operatorname{curl} \boldsymbol{A}$ is the magnetic field. However, the choice of $\Lambda_+(\boldsymbol{A})$ in (11) is critical as demonstrated in [12]. In [12] it is shown that if $\Lambda_+(\boldsymbol{A})$ is chosen to be Λ_+, the projection onto $\mathcal{H}_{(N)}$, then given any positive α and Z_k, there are values of N and K for which

$$\inf(\psi, \boldsymbol{B}_{N,K}(\boldsymbol{A})\psi) = -\infty;$$

here the infimum is taken over all magnetic potentials A in the Coulomb guage, all nuclear positions and all normalized $\psi \in \mathcal{H}_{(N)}$. However, the choice for $\Lambda_+(\boldsymbol{A})$ of the projection onto

$$\mathcal{H}_{N,\boldsymbol{A}} = \bigwedge_{j=1}^{N} \mathcal{H}_+^{(j)}(\boldsymbol{A})$$

where $\mathcal{H}_+^{(j)}(\boldsymbol{A})$ is the positive spectral subspace of $D_{\boldsymbol{A}}^{(j)}$ guarantees stability for small enough values of α and Z_k, e.g. $Z_k \leqslant 56$ for $\alpha = \frac{1}{137}$.

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