M P E J

Mathematical Physics Electronic Journal

ISSN 1086-6655
Volume 5, 1999

Paper 6
Received: Sep 21, 1999, Accepted: Dec 7, 1999
Editor: R. de la Llave

STABILITY OF THE BROWN-RAVENHALL OPERATOR

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Abstract. The Brown-Ravenhall Hamiltonian is a model for the behavior of N electrons in a field of K fixed nuclei having the atomic numbers $\mathbf{Z} = (Z_1, \ldots, Z_K)$, which is written, in appropriate units, as

$$B = \Lambda_{+,N}\left(\sum_{n=1}^{N} D_0^{(n)} + \alpha V_c\right)\Lambda_{+,N}$$

acting on the N-fold antisymmetric tensor product $\mathfrak{H}_N$ of $\Lambda_+(L^2(\mathbb{R}^3)\otimes\mathbb{C}^4)$, where $D_0^{(n)}$ denotes the free Dirac operator D_0 acting on the n-th particle, Λ_+ denotes the projection onto the positive spectral subspace of D_0, $\Lambda_{+,N}$ the projection onto $\mathfrak{H}_N$ and the potential V_c is the usual Coulomb interaction of the particles, coupled by the constant α. It is proved in the massless case that for any $\gamma < 2/(2/\pi + \pi/2)$ there exists an α_0 such that for all $\alpha < \alpha_0$ and $\alpha Z_k \leq \gamma$ $(k = 1, \ldots K)$ we have stability, i.e., $B \geq 0$. Using numerical calculations we get stability for the physical value $\alpha \approx 1/137$ up to $Z_k \leq 88$ $(k = 1, \ldots K)$.

1. Introduction

A basic requirement of thermodynamics is the extensivity of the energy. To be able to show this property, it is essential that on a microscopic level the energy per particle is bounded from below independently of the size of the considered system. This property, also referred to as stability of matter, as been proven in the literature for a wide class of models starting from the pioneering work of Dyson and Lenard [6, 7] in the non-relativistic case and of Conlon [3] and Fefferman and de la Llave [9] in the relativistic case. (See [10, 12, 14, 16] for an overview and more references.) A particular interesting work for our purposes is the work of Lieb and Yau [15] who consider the stability of matter of a relativistic system of N (spinless) electrons in a field of K fixed nuclei having atomic numbers $\mathbf{Z} = (Z_1, \ldots, Z_K)$ and positions

Key words and phrases. Dirac operator, stability of relativistic matter.

$\mathbf{R} = (R_1, \dots, R_K)$. Hence the relevant Coulomb potential is

$$V_{(R_1,\dots,R_K;Z_1,\dots,Z_K)}(x_1,\dots,x_N) := \sum_{\substack{n,m=1\\ n<m}}^N \frac{1}{|x_n - x_m|} - \sum_{n=1}^N\sum_{k=1}^K \frac{Z_k}{|x_n - R_k|} + \sum_{\substack{k,l=1\\ k<l}}^K \frac{Z_k Z_l}{|R_k - R_l|}. \tag{1}$$

As an expression for the kinetic energy they use $\sum_{n=1}^N |p|^{(n)}$, where $|p| = \sqrt{-\Delta}$ and $|p|^{(n)}$ acts on the n-th particle, i.e., they examine the Hamiltonian

$$H_{N,K,\mathbf{R},\mathbf{Z}} = \sum_{n=1}^N |p|^{(n)} + \alpha V_{\mathbf{R};\mathbf{Z}},$$

where α is a coupling constant. The physical value of α, the Sommerfeld fine structure constant, is approximately $1/137.037$.

The goal is to prove stability, i.e., the existence of a constant c such that for all K and N

$$H_{N,K,\mathbf{R},\mathbf{Z}} \geq -c(N+K).$$

Due to scaling properties this is equivalent to $H_{N,K,\mathbf{R},\mathbf{Z}} \geq 0$. In [15] stability is proved if $Z\alpha \leq 2/\pi$ and $\alpha < 1/47q$, where $Z := \max\{Z_1,\dots,Z_K\}$ and q is the number of spin states. The bound $2/\pi$ is sharp for this kind of kinetic energy.

The above model has the problem that it does not really account for the spin of the electrons and becomes instable if one of the atomic numbers exceeds $2\alpha/\pi$ (which is about 87.2 for the physical value of α). A model that does not have the problem on the one-particle level for any physical atomic number has been proposed by Brown and Ravenhall [2]. This has been shown on the one-particle level by Evans et al [8] and improved by Tix [17, 18]. Instead of expectations of $|p|$ expectations of the Dirac operator are considered. A collapse to the negative spectral subspace is prevented by restricting to positive energy states only which is a particular way of implementing Dirac's idea of filling the sea of negative states. The precise definition of the Brown-Ravenhall operator is as follows:

Let D_0 denote the free (massless) Dirac operator acting on $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$, Λ_+ the orthogonal projection onto the positive spectral subspace of D_0 and $\mathfrak{H} := \Lambda_+(L^2(\mathbb{R}^3)\otimes\mathbb{C}^4)$. Let $\mathfrak{H}_N := \bigwedge_{n=1}^N \mathfrak{H}$ be the N-fold antisymmetric tensor product of $\mathfrak{H}$ and $\Lambda_{+,N}$ the orthogonal projection from $\bigotimes_{n=1}^N (L^2(\mathbb{R}^3)\otimes\mathbb{C}^4)$ onto $\mathfrak{H}_N$. We consider the operator

$$B_{N,K,\mathbf{R},\mathbf{Z}} = \Lambda_{+,N}\left(\sum_{n=1}^N D_0^{(n)} + \alpha V_{\mathbf{R};\mathbf{Z}}\right)\Lambda_{+,N} \tag{2}$$

on $\mathfrak{H}_N$, where $D_0^{(n)}$ denotes the free Dirac operator D_0 acting on the n-th particle. (The $\Lambda_{+,N}$ on the very right in (2) is superfluous but we write it here and in the following to stress the reduction to the positive subspace.)

With the results of [15] one gets stability also for this model if $Z\alpha \leq 2/\pi$. But it is guessed that $B_{N,K,\mathbf{R},\mathbf{Z}} \geq 0$ if $\alpha Z \leq \gamma_c := \frac{2}{2/\pi+\pi/2}$ perhaps under some restrictions on α. Indeed in [8] this is proved for the special case $N = K = 1$ for the massless case and in [17, 18] in the massive case. In [8] it is also shown that γ_c is optimal: If $\alpha Z > \gamma_c$ then we have instability, i.e., $B_{1,1,R,Z}$ is unbounded from below. The one-electron molecule ($N = 1$, K arbitrary) was treated by Balinsky and Evans [1]; they prove stability for $\alpha Z \leq \gamma_c$ under a constraint on α, which is satisfied by the physical value. We consider the general case (N, K arbitrary):

Theorem 1. *Let $\gamma < \frac{2}{2/\pi+\pi/2}$. Then there exists an α_0 such that for all $\alpha < \alpha_0$ and $Z_1,\dots,Z_K$ with $\alpha Z_k \leq \gamma$ $(k = 1,\dots K)$ we have $B_{N,K,\mathbf{R},\mathbf{Z}} \geq 0$.*

Remark. For the physical value 1/137.037 of α we get stability up to $Z_k \leq 88$ $(k = 1, \dots, K)$. This exceeds the maximal atomic number one would get with the mentioned methods of [15]

It remains as a challenge to improve this to get stability in our model for the physical value of α up to the largest possible atomic number $Z = \gamma_c \alpha^{-1} \approx 124$.

The paper is organized as follows: In Section 2 we introduce some notations and summarize known results, that we will use, so that the rest of the paper should be self-contained. The third section treats a commutator estimate, that will be a crucial ingredient in the proof of our Theorem. This main proof is done in Section 4. The last section contains the numerical results that give the mentioned stability up to $Z = 88$ for the physical value of α.

2. Preliminaries

Here we introduce the notations we will use below and summarize some known results.

Fix $K \geq 2$ nuclei located at distinct points $\mathbf{R} = (R_1, \dots, R_K) \in \mathbb{R}^{3K}$ all with the same atomic number Z. Decompose $\mathbb{R}^3$ in K Voronoi cells Γ_k, which are the nearest neighborhoods to the nuclei:

$$\Gamma_k := \{x : |x - R_k| \leq |x - R_l|, l = 1, \dots, K\}.$$

Let B_k denote the biggest open ball with center R_k in Γ_k and let D_k be its radius:

$$D_k := \mathrm{dist}(R_k, \partial\Gamma_k) = \frac{1}{2} \min\{|R_k - R_l| : l \neq k\}, \quad B_k := \{x : |x - R_k| < D_k\}.$$

Further, for $\sigma \in (0,1)$ let

$$B_k^{(\sigma)} := \{x : |x - R_k| \leq (1-\sigma)D_k\}.$$

We identify sets with their characteristic functions.

Now consider N electrons and let $V_Z := V_{(R_1,\dots,R_K;Z,\dots,Z)}(x_1, \dots, x_N)$ be the Coulomb potential induced by the nuclei with all the same atomic number Z and the electrons as defined in (1).

Proposition 1 ([15], Theorem 6)**.** *For any* $0 < \lambda < 1$

$$V_Z \geq -\sum_{n=1}^{N} W_\lambda(x_n) + \frac{1}{8} Z^2 \sum_{k=1}^{K} \frac{1}{D_k},$$

where, for $x \in \Gamma_k$*,* $W_\lambda(x) := W_{\lambda,k}(x) := \frac{Z}{|x-R_k|} + F_{\lambda,k}(x)$ *with*

$$F_{\lambda,k} := \begin{cases} \frac{1}{2D_k(1 - \frac{1}{{D_k}^2}|x-R_k|^2)} & \text{for} \quad |x - R_k| \leq \lambda D_k, \\ (\sqrt{2Z} + \frac{1}{2})\frac{1}{|x-R_k|} & \text{for} \quad |x - R_k| > \lambda D_k. \end{cases}$$

We will localize the kinetic energy to control the Coulomb singularities. More exactly we shall consider $\mathrm{tr}\gamma|p|$, where γ is a density matrix, i.e., a positive definite trace class operator, on $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$ or on $L^2(\mathbb{R}^3)$.

Proposition 2 ([15],Theorem 10)**.** *Let* $0 < \sigma < 1$ *and* χ_0*,* χ_1 *be Lipschitz continuous nonnegative functions with* ${\chi_0}^2 + {\chi_1}^2 = 1$ *and* χ_1 *supported in* $B_1^{(\sigma)}$*. Define*

$$L(x,y) := \frac{1}{\pi^2} \frac{1 - \chi_0(x)\chi_0(y) - \chi_1(x)\chi_1(y)}{|x-y|^4},$$

$$L_1(x,y) := \begin{cases} L(x,y) & \text{for } \big||x| - |y|\big| \leq \sigma D_1, \ x, y \in B_1, \\ 0 & \text{otherwise}, \end{cases}$$

and $L_0 := L - L_1$. *For any positive function* h *on* B_1 *and for arbitrary* $\varepsilon > 0$ *let*

$$U_1(x) := \begin{cases} \frac{\varepsilon}{D_1} B_1^{(\sigma)}(x) + \frac{1}{h(x)} \int_{B_1} dy\, L_1(x,y)h(y) & \text{for } x \in B_1, \\ 0 & \text{otherwise.} \end{cases}$$

Then, for any density matrix γ *acting on* $L^2(\mathbb{R}^3)$,

$$\mathrm{tr}\gamma|p| \geq \mathrm{tr}\chi_1\gamma\chi_1(|p| - U_1(x)) + \mathrm{tr}\chi_0\gamma\chi_0(|p| - U_1(x)) - \frac{\|\gamma\|}{\varepsilon D_1}\Omega,$$

where $\Omega = \frac{1}{2}{D_1}^2 \int\int dxdy\, L_0(x,y)^2$.

(Note the typing error in [15, (3.12)].)

To control the remaining potentials we will use Daubechies' inequality:

Proposition 3 (Daubechies [4], see also [15], Theorem 8)**.** *For any density matrix* γ *on* $L^2(\mathbb{R}^3)$, *any positive function* $U \in L^4(\mathbb{R}^3)$ *and any* $\mu > 0$ *we have*

$$\mathrm{tr}\gamma(\mu|p| - U) \leq -0.0258 \cdot \|\gamma\|\mu^{-3} \int dx\, U(x)^4.$$

We want to apply the above two propositions to the reduced density matrix $\hat{\gamma}$ (without spin) of a density matrix $\Lambda_+\gamma\Lambda_+$ acting on $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$ (using the kernels and indicating the space-spin variables by $(x,s) \in \mathbb{R}^3 \times \{1,\ldots,4\}$ it is $\hat{\gamma}(x,y) := \sum_{s=1}^4 (\Lambda_+\gamma\Lambda_+)((x,s),(y,s))$). If one had no restriction (i.e., without the Λ_+) one could only conclude that $\|\hat{\gamma}\| \leq 4 \cdot \|\gamma\|$. But due to the projection onto the positive spectral subspace we have:

Proposition 4 ([14], Appendix B)**.** *Let* $\hat{\gamma}$ *be the reduced density matrix of* $\Lambda_+\gamma\Lambda_+$ *as above. Then* $\|\hat{\gamma}\| \leq 2 \cdot \|\gamma\|$.

The key estimate we will use is the positivity of the one particle operator ($N = K = 1$ in (2)). Using the notations of the introduction we have:

Proposition 5 ([8], Theorem 1)**.**

$$B_{1,1,R,Z} \geq 0 \quad \text{if} \quad \alpha Z \leq \gamma_c = \frac{2}{\frac{2}{\pi} + \frac{\pi}{2}}.$$

3. A Useful Commutator Estimate

Here we prove a proposition which will be essential in the proof of our main Theorem in Section 4.

Proposition 6. *Let* $0 < \sigma < 1$ *and* χ *be a Lipschitz continuous radial real function with* $\chi(x) = 0$ *if* $|x| \geq 1 - \sigma$, *so that* $\chi_k(x) := \chi(\frac{x - R_k}{D_k})$ *is supported in* $B_k^{(\sigma)}$. *Let* $\Lambda_- := 1 - \Lambda_+$ *and*

$$K := [\chi_k, \Lambda_-]\frac{1}{|x - R_k|}\chi_k - \chi_k\frac{1}{|x - R_k|}[\chi_k, \Lambda_-].$$

Then, for all density matrices γ *acting on* $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$ *and arbitrary* $\delta > 0$,

$$\mathrm{tr}\Lambda_+\gamma\Lambda_+ K \leq \mathrm{tr}\Lambda_+\gamma\Lambda_+ \frac{\delta}{D_k} B_k^{(\sigma)} + \frac{\|\gamma\|}{\delta D_k} C,$$

where (writing $\chi(x) = \chi(|x|)$*)*

$$C = \frac{8}{\pi^2} \int_0^{1-\sigma} dr \int_r^\infty ds\, \frac{|\chi(r) - \chi(s)|^2 |r\chi(s) - s\chi(r)|^2 (r^2 + s^2)}{(r^2 - s^2)^4}$$

Proof. Without loss of generality we can take $R_k = 0$. Because of $\Lambda_- = \frac{1}{2}(1 - \frac{\boldsymbol{\alpha}\cdot p}{|p|})$ with the Dirac matrices $\boldsymbol{\alpha}$ (see [8]) we have

$$[\chi_k, \Lambda_-] = \chi_k \Lambda_- - \Lambda_- \chi_k = \frac{1}{2}\left((\boldsymbol{\alpha}\cdot p)\frac{1}{|p|}\chi_k - \chi_k(\boldsymbol{\alpha}\cdot p)\frac{1}{|p|}\right).$$

Since $\frac{1}{|p|}$ has the integral kernel $\frac{1}{2\pi^2|x-y|^2}$ we could get as an integral kernel of $[\chi_k, \Lambda_-]$ by differentiating

$$\begin{aligned} &\frac{1}{2}\left(\frac{-2\boldsymbol{\alpha}\cdot(x-y)}{2\pi^2 i|x-y|^4}\chi_k(y) - \chi_k(x)\frac{-2\boldsymbol{\alpha}\cdot(x-y)}{2\pi^2 i|x-y|^4}\right) \\ = \; &\frac{1}{2\pi^2 i}\frac{\boldsymbol{\alpha}\cdot(x-y)}{|x-y|^4}(\chi_k(x) - \chi_k(y)). \end{aligned} \tag{3}$$

To justify this in spite of the non-integrable singularity in the first line (notice that due to the Lipschitz continuity of χ the appearing singularity in the second line is integrable) one can argue as follows:

First we regularize $\frac{1}{|p|}$ by considering $\frac{e^{-\varepsilon|p|}}{|p|}$ for $\varepsilon > 0$. By an easy calculation one gets $\frac{1}{2\pi^2|x-y|^2+\varepsilon^2}$ as the integral kernel of $\frac{e^{-\varepsilon|p|}}{|p|}$. Differentiation yields $-\frac{1}{\pi^2 i}\frac{\boldsymbol{\alpha}\cdot(x-y)}{(|x-y|^2+\varepsilon^2)^2}$ as the integral kernel of $\frac{\boldsymbol{\alpha}\cdot p}{|p|}e^{-\varepsilon|p|}$ and for $f \in L^2(\mathbb{R}^2) \otimes \mathbb{C}^4$ we have

$$\frac{\boldsymbol{\alpha}\cdot p}{|p|}e^{-\varepsilon|p|}\chi_k f - \chi_k\frac{\boldsymbol{\alpha}\cdot p}{|p|}e^{-\varepsilon|p|}f = \int dy \frac{1}{\pi^2 i}\frac{\boldsymbol{\alpha}\cdot(x-y)}{(|x-y|^2+\varepsilon^2)^2}(\chi_k(x) - \chi_k(y))f(y).$$

Tending ε to zero we get $e^{-\varepsilon|p|}f \to f$ and $e^{-\varepsilon|p|}\chi_k f \to \chi_k f$ in L^2 and hence – by dominated convergence – (3) as the integral kernel of $[\chi_k, \Lambda_-]$.

So, K has the kernel

$$K(x,y) := \frac{1}{2\pi^2 i}\frac{\boldsymbol{\alpha}\cdot(x-y)}{|x-y|^4}(\chi_k(x) - \chi_k(y))(\frac{\chi_k(y)}{|y|} - \frac{\chi_k(x)}{|x|}). \tag{4}$$

We now proceed as in Section VI of [15], but in contrast to [15] we have to treat variables with spin. Let $\underline{x} := (x,s) \in \mathbb{R}^3 \times \{1,\dots,4\}$ be a space-spin variable and let $\int d\underline{x}$ indicate the integration over $x \in \mathbb{R}^3$ (if not stated otherwise) and summation over $s \in \{1,\dots,4\}$. Let $\gamma_1 := \Lambda_+\gamma\Lambda_+$ and $\gamma_1^{\frac{1}{2}}$ denote the operator square root of γ_1. We identify the operators with their kernels. Since $\gamma_1(\underline{x},\underline{y}) = \overline{\gamma_1(\underline{y},\underline{x})}$ and $K(\underline{x},\underline{y}) = \overline{K(\underline{y},\underline{x})}$ we get

$$\begin{aligned} \mathrm{tr}\gamma_1 K &= \int d\underline{x}\int d\underline{y}\,\gamma_1(\underline{x},\underline{y})K(\underline{y},\underline{x}) \\ &= 2\Re\int d\underline{x}\int_{y:|y|>|x|} d\underline{y}\,\gamma_1(\underline{x},\underline{y})K(\underline{y},\underline{x}) \\ &= 2\Re\int d\underline{x}\int_{y:|y|>|x|} d\underline{y}\int d\underline{z}\,\gamma_1^{\frac{1}{2}}(\underline{x},\underline{z})\gamma_1^{\frac{1}{2}}(\underline{z},\underline{y})K(\underline{y},\underline{x}). \end{aligned}$$

If $(1-\sigma)D_k < |x|$ and $|x| < |y|$ then $\chi_k(x) = \chi_k(y) = 0$, hence $K(\underline{x},\underline{y}) = 0$. Therefore we can add a factor $B_k^{(\sigma)}(x)$ in the integrand. By applying Minkowski's inequality we get

$$\begin{aligned}
&\mathrm{tr}\gamma_1 K\\
=\ & 2\Re\int d\underline{x}\int d\underline{z}\left(\gamma_1^{\frac12}(\underline{x},\underline{z})B_k^{(\sigma)}(x)\right)\cdot\left(B_k^{(\sigma)}(x)\int_{|y|>|x|}d\underline{y}\,\gamma_1^{\frac12}(\underline{z},\underline{y})K(\underline{y},\underline{x})\right)\\
\le\ & \varepsilon\int d\underline{x}\int d\underline{z}\,|\gamma_1^{\frac12}(\underline{x},\underline{z})B_k^{(\sigma)}(x)|^2\\
& +\frac{1}{\varepsilon}\int d\underline{x}\int d\underline{z}\left|B_k^{(\sigma)}(x)\int_{|y|>|x|}d\underline{y}\,\gamma_1^{\frac12}(\underline{z},\underline{y})K(\underline{y},\underline{x})\right|^2\\
=\ & \varepsilon\int d\underline{x}\int d\underline{z}\,\gamma_1^{\frac12}(\underline{x},\underline{z})\gamma_1^{\frac12}(\underline{z},\underline{x})B_k^{(\sigma)}(x)\\
& +\frac{1}{\varepsilon}\int d\underline{y}\int d\underline{y}'\int_{\substack{|x|<\\ \min\{|y|,|y'|\}}}d\underline{x}\int d\underline{z}\,B_k^{(\sigma)}(x)\gamma_1^{\frac12}(\underline{z},\underline{y})K(\underline{y},\underline{x})\overline{\gamma_1^{\frac12}(\underline{z},\underline{y}')K(\underline{y}',\underline{x})}\\
=\ & \varepsilon\int d\underline{x}\,\gamma_1(\underline{x},\underline{x})B_k^{(\sigma)}(x)\\
& +\frac{1}{\varepsilon}\int d\underline{y}\int d\underline{y}'\left(\int d\underline{z}\,\gamma_1^{\frac12}(\underline{y}',\underline{z})\gamma_1^{\frac12}(\underline{z},\underline{y})\right)\cdot\left(\int_M d\underline{x}\,K(\underline{y},\underline{x})K(\underline{x},\underline{y}')\right)\\
=\ & \varepsilon\mathrm{tr}\gamma_1 B_k^{(\sigma)}+\frac{1}{\varepsilon}\int d\underline{y}\int d\underline{y}'\gamma_1(\underline{y}',\underline{y})\left(\int_M d\underline{x}\,K(\underline{y},\underline{x})K(\underline{x},\underline{y}')\right),
\end{aligned}$$

with $M:=\{\underline{x}:x\in B_k^{(\sigma)},|x|\le\min\{|y|,|y'|\}\}$. The last summand is equal to $\frac{1}{\varepsilon}\mathrm{tr}\gamma_1\tilde K^*\tilde K$, where $\tilde K$ has the kernel

$$\tilde K(x,y):=K(x,y)\cdot 1_{\{(x,y):x\in B_k^{(\sigma)},|x|\le|y|\}}(x,y) \tag{5}$$

with the characteristic function 1_A of the set A. Since $\mathrm{tr}\gamma_1\tilde K^*\tilde K=\mathrm{tr}\gamma\Lambda_+\tilde K^*\tilde K\Lambda_+$ we get, using $|\mathrm{tr}AB|\le\|A\|\mathrm{tr}B$ if B is positive and taking $\varepsilon=\frac{\delta}{D_k}$ above,

$$\mathrm{tr}\gamma_1 K\le\frac{\delta}{D_k}\mathrm{tr}\gamma_1 B_k^{(\sigma)}+\frac{D_k}{\delta}\|\gamma\|\mathrm{tr}\Lambda_+\tilde K^*\tilde K\Lambda_+. \tag{6}$$

Similar to [14], Appendix B, we claim

$$\mathrm{tr}\Lambda_+\tilde K^*\tilde K\Lambda_+=\frac12\mathrm{tr}\tilde K^*\tilde K. \tag{7}$$

Because of

$$\mathrm{tr}\tilde K^*\tilde K=\mathrm{tr}(\Lambda_+^2+\Lambda_-^2)\tilde K^*\tilde K=\mathrm{tr}\Lambda_+\tilde K^*\tilde K\Lambda_++\mathrm{tr}\Lambda_-\tilde K^*\tilde K\Lambda_-$$

it is enough to prove $\mathrm{tr}\Lambda_+\tilde K^*\tilde K\Lambda_+=\mathrm{tr}\Lambda_-\tilde K^*\tilde K\Lambda_-$.

Let $U:=\begin{pmatrix}0&1\\-1&0\end{pmatrix}$ where 1 indicates the 2×2 unit matrix. Then it is easy to verify that $\Lambda_-=U^*\Lambda_+U$, hence

$$\mathrm{tr}\Lambda_-\tilde K^*\tilde K\Lambda_-=\mathrm{tr}U^*\Lambda_+U\tilde K^*\tilde K U^*\Lambda_+U=\mathrm{tr}\Lambda_+U\tilde K^*U^*U\tilde K U^*\Lambda_+.$$

Now, U commutes with scalar multiplications. Hence, having (5) and (4) in mind, the fact

$$U^*(\boldsymbol{\alpha}\cdot(x-y))U=U(\boldsymbol{\alpha}\cdot(x-y))U^*=-\boldsymbol{\alpha}\cdot(x-y)$$

yields $U\tilde K U^*=-\tilde K$ and $U\tilde K^*U^*=-\tilde K^*$. Thus

$$\mathrm{tr}\Lambda_-\tilde K^*\tilde K\Lambda_-=\mathrm{tr}\Lambda_+\tilde K^*\tilde K\Lambda_+$$

and we get (7).

Now, continuing (6), we have

$$\mathrm{tr}\gamma_1 K\le\frac{\delta}{D_k}\mathrm{tr}\gamma_1 B_k^{(\sigma)}+\frac{D_k}{\delta}\|\gamma\|\cdot\frac12\mathrm{tr}\tilde K^*\tilde K$$

and it remains to calculate the last trace. Using (4) and the fact that $(\boldsymbol{\alpha}\cdot(x-y))^2 = (x-y)^2$, elementary calculations give

$$\begin{aligned} \frac{1}{2}\mathrm{tr}\tilde{K}^*\tilde{K} &= \frac{1}{2}\int d\underline{y}\int_{\substack{x\in B_k^{(\sigma)};\\ |x|\leq|y|}} d\underline{x}\,|K(x,y)|^2 \\ &= \frac{1}{{D_k}^2}\frac{8}{\pi^2}\int_0^{1-\sigma}dr\int_r^\infty ds\,\frac{|\chi(r)-\chi(s)|^2|r\chi(s)-s\chi(r)|^2(r^2+s^2)}{(r^2-s^2)^4}, \end{aligned}$$

and we are done. □

4. Proof of the Theorem

We want to prove

$$B_{N,K,\mathbf{R},\mathbf{Z}} = \Lambda_{+,N}\left(\sum_{n=1}^N D_0^{(n)} + \alpha V_{\mathbf{R};\mathbf{Z}}\right)\Lambda_{+,N} \geq 0$$

for $\mathbf{Z} = (Z_1,\ldots,Z_K)$. Using the same convexity arguments as in [5, p. 507] it is enough to prove $B_{N,K,\mathbf{R},\mathbf{Z_c}} \geq 0$ with $\mathbf{Z_c} = (Z,\ldots,Z)$, $Z \geq \max\{Z_1,\ldots,Z_K\}$. Applying Proposition 1 and the fact that $\Lambda_+ D_0\Lambda_+ = \Lambda_+|p|\Lambda_+$ we get

$$\begin{aligned} B_{N,K,\mathbf{R},\mathbf{Z_c}} &\geq \Lambda_{+,N}\left(\sum_{n=1}^N D_0^{(n)} - \alpha\sum_{n=1}^N W_\lambda(x_n) + \frac{1}{8}\alpha Z^2\sum_{k=1}^K\frac{1}{D_k}\right)\Lambda_{+,N} \\ &= \Lambda_{+,N}\left(\sum_{n=1}^N h_n\right)\Lambda_{+,N} + D \end{aligned}$$

with $h_n := |p|^{(n)} - \alpha W_\lambda(x_n)$ and $D := \frac{1}{8}\alpha Z^2\sum_{k=1}^K\frac{1}{D_k}$ (note that we are acting on $\mathfrak{H}_N$ and $\Lambda_{+,N}|_{\mathfrak{H}_N} = \mathrm{Id}$). Hence the positivity of $B_{N,K,\mathbf{R},\mathbf{Z}}$ is implied by $\Lambda_{+,N}\left(\sum_{n=1}^N h_n\right)\Lambda_{+,N} \geq -D$. Proving this for all N is equivalent to showing

$$\mathrm{tr}\gamma\Lambda_+ h\Lambda_+ \geq -D = -\frac{1}{8}\alpha Z^2\sum_{k=1}^K\frac{1}{D_k} \tag{8}$$

with $h := |p| - \alpha W_\lambda$ (acting componentwise on $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$) for all density matrices γ on $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ with $0\leq\gamma\leq 1$ (cf. [11] and [15, (2.22)]). This is, what we want to do now.

Fix some Lipschitz continuous nonnegative radial function $0\leq\chi\leq 1$ with $\chi(x) = 1$ if $|x|\leq 1-3\sigma$ and $\chi(x) = 0$ if $|x|\geq 1-\sigma$ and so that $\sqrt{1-\chi^2}$ is also Lipschitz continuous. Define $\chi_k(x) := \chi(\frac{x-R_k}{D_k})$ $(k = 1,\ldots,K)$ as in Proposition 6 and let $\chi_{0,k}$ be nonnegative functions with $\chi_k^2+\chi_{0,k}^2 = 1$. (The Lipschitz continuity of $\sqrt{1-\chi^2}$ implies the same for $\chi_{0,k}$).

We borrow a part $\mu|p|$ $(\mu\in(0,1))$ of the kinetic energy to control the remaining potentials in the end and set $\nu := 1-\mu$. Now we fix a density matrix γ acting on $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ with $0\leq\gamma\leq 1$. First we observe that – for estimating $\mathrm{tr}\Lambda_+\gamma\Lambda_+(\nu|p|-\alpha W_\lambda)$ – it is enough to consider the reduced density matrix $\hat{\gamma}$ without spin (see the definition before Proposition 4) instead of $\Lambda_+\gamma\Lambda_+$. We then can apply Proposition 2 to $\hat{\gamma}$. Using the fact that $\|\hat{\gamma}\|\leq 2$ (Proposition 4) and going back to the full density matrix we get with $\tilde\alpha := \nu^{-1}\alpha$

$$\begin{aligned}
&\mathrm{tr}\Lambda_+\gamma\Lambda_+\Big(\nu|p| - \alpha W_\lambda\Big)\\
\geq\ & \mathrm{tr}\chi_1\Lambda_+\gamma\Lambda_+\chi_1\Big(\nu|p| - \frac{\alpha Z}{|x-R_1|} - \alpha F_{\lambda,1}(x) - \nu U_1(x)\Big)\\
&+\mathrm{tr}\chi_{0,1}\Lambda_+\gamma\Lambda_+\chi_{0,1}\Big(\nu|p| - \alpha W_\lambda(x) - \nu U_1(x)\Big) - \frac{2\nu\Omega}{\varepsilon D_1}\\
=\ & \nu\mathrm{tr}\gamma\Lambda_+\chi_1\Big(|p| - \frac{\tilde\alpha Z}{|x-R_1|}\Big)\chi_1\Lambda_+ \qquad (9)\\
&+\mathrm{tr}\chi_{0,1}\Lambda_+\gamma\Lambda_+\chi_{0,1}\Big(\nu|p| - \alpha W_\lambda(x)\Big) \qquad (10)\\
&-\mathrm{tr}\Lambda_+\gamma\Lambda_+\Big(\alpha{\chi_1}^2F_{\lambda,1} + \nu U_1(x)\Big) - \frac{2\nu\Omega}{\varepsilon D_1}.
\end{aligned}$$

To handle the first summand (9) we want to apply Proposition 5. Using the definition of the operator K in Proposition 6 (with $k=1$) and $\Lambda_+ + \Lambda_- = 1$, $\Lambda_+\Lambda_- = 0$ it is easy to see that

$$\begin{aligned}
-\Lambda_+\chi_1\frac{1}{|x-R_1|}\chi_1\Lambda_+ \;=\;& -\Lambda_+\chi_1\Lambda_+\frac{1}{|x-R_1|}\Lambda_+\chi_1\Lambda_+ - \Lambda_+K\Lambda_+\\
&+\Lambda_+\chi_1\Lambda_-\frac{1}{|x-R_1|}\Lambda_-\chi_1\Lambda_+.
\end{aligned}$$

Neglecting the last term, which is positive, and using $|p| \geq \Lambda_+|p|\Lambda_+$ and Proposition 5 we get, as soon as $\tilde\alpha Z \leq \gamma_c$,

$$\begin{aligned}
&\Lambda_+\chi_1\Big(|p| - \frac{\tilde\alpha Z}{|x-R_1|}\Big)\chi_1\Lambda_+\\
\geq\ & \Lambda_+\chi_1\Big(\Lambda_+|p|\Lambda_+ - \Lambda_+\frac{\tilde\alpha Z}{|x-R_1|}\Lambda_+\Big)\chi_1\Lambda_+ - \tilde\alpha Z\Lambda_+K\Lambda_+\\
\geq\ & -\tilde\alpha Z\Lambda_+K\Lambda_+.
\end{aligned}$$

Thus, Proposition 6 yields

$$(9) \geq -\nu\tilde\alpha Z\mathrm{tr}\Lambda_+\gamma\Lambda_+K \geq -\alpha Z\mathrm{tr}\Lambda_+\gamma\Lambda_+\frac{\delta}{D_1}B_1^{(\sigma)} - \frac{\alpha Z}{\delta D_1}C. \qquad (11)$$

We now repeat the whole strategy treating the second summand (10) and the second nucleus: Applying Proposition 2 to the reduced density matrix (without spin) of $\tilde\gamma := \chi_{0,1}\Lambda_+\gamma\Lambda_+\chi_{0,1}$ we get with the corresponding definition of U_2 (notice that by scaling Ω does only depend on χ and not on D_k)

$$\begin{aligned}
(10)\ \geq\ & \mathrm{tr}\chi_2\tilde\gamma\chi_2\Big(\nu|p| - \frac{\alpha Z}{|x-R_2|} - \alpha F_{\lambda,2}(x) - \nu U_2(x)\Big)\\
&+\mathrm{tr}\chi_{0,2}\tilde\gamma\chi_{0,2}\Big(\nu|p| - \alpha W_\lambda(x) - \nu U_2(x)\Big) - \frac{2\nu\Omega}{\varepsilon D_2}\\
=\ & \nu\mathrm{tr}\gamma\Lambda_+\chi_2\Big(|p| - \frac{\tilde\alpha Z}{|x-R_2|}\Big)\chi_2\Lambda_+\\
&+\mathrm{tr}\chi_{0,2}\chi_{0,1}\Lambda_+\gamma\Lambda_+\chi_{0,1}\chi_{0,2}\Big(\nu|p| - \alpha W_\lambda(x)\Big)\\
&-\mathrm{tr}\Lambda_+\gamma\Lambda_+\Big(\alpha{\chi_2}^2F_{\lambda,2} + \nu U_2(x)\Big) - \frac{2\nu\Omega}{\varepsilon D_2}.
\end{aligned}$$

(For the last equality notice $\chi_2\chi_{0,1} = \chi_2$ and $U_2\chi_{0,1} = U_2$.) We can estimate the first summand similarly to above (cf. (11)). Repeating this procedure for all other nuclei we get

$$\begin{aligned}
&\mathrm{tr}\Lambda_+\gamma\Lambda_+\Big(\nu|p|-\alpha W_\lambda\Big)\\
\geq\quad & -\alpha Z\,\mathrm{tr}\Lambda_+\gamma\Lambda_+\left(\sum_{k=1}^K \frac{\delta}{D_k}B_k^{(\sigma)}\right)-\alpha Z\frac{C}{\delta}\sum_{k=1}^K\frac{1}{D_k}\\
&-\mathrm{tr}\Lambda_+\gamma\Lambda_+\left(\sum_{k=1}^K(\alpha{\chi_k}^2F_{\lambda,k}+\nu U_k)\right)-\frac{2\nu\Omega}{\varepsilon}\sum_{k=1}^K\frac{1}{D_k}\\
&+\mathrm{tr}\chi_{0,K}\dots\chi_{0,1}\Lambda_+\gamma\Lambda_+\chi_{0,1}\dots\chi_{0,K}\Big(\nu|p|-\alpha W_\lambda\Big).
\end{aligned}$$

Introducing a new parameter $\beta\in(0,1)$ we split the potential W_λ in the last summand into two parts. One part is joined with the other potentials. To the other part we can add a factor R, where R is the characteristic function of the complement of $\bigcup_{k=1}^K B_k^{(3\sigma)}$. Together with the remaining $\mu|p|$ and using the abbreviations

$$G_k:=\alpha{\chi_k}^2F_{\lambda,k}+(1-\mu)U_k+\alpha Z\frac{\delta}{D_k}B_k^{(\sigma)},\quad A:=\frac{2(1-\mu)\Omega}{\varepsilon}+\alpha Z\frac{C}{\delta}$$

we get

$$\begin{aligned}
&\mathrm{tr}\Lambda_+\gamma\Lambda_+\Big(|p|-\alpha W_\lambda\Big)\\
\geq\quad & \mathrm{tr}\Lambda_+\gamma\Lambda_+\Big(\mu|p|-(1-\beta)\alpha\chi_{0,1}^2\dots\chi_{0,K}^2W_\lambda-\sum_{k=1}^K G_k\Big)-A\sum_{k=1}^K\frac{1}{D_k}\\
&+\mathrm{tr}\chi_{0,K}\dots\chi_{0,1}\Lambda_+\gamma\Lambda_+\chi_{0,1}\dots\chi_{0,K}\Big((1-\mu)|p|-\beta\alpha W_\lambda R\Big)
\end{aligned}$$

Finally we estimate the first and last summand applying Daubechies' inequality (Proposition 3). As above, we make again use of the fact that only the reduced density matrix without spin is relevant and that its norm does not exceed two (cf. Proposition 4):

$$\begin{aligned}
&\mathrm{tr}\Lambda_+\gamma\Lambda_+h\\
\geq\quad & -0.0258\cdot 2\mu^{-3}\int\Big((1-\beta)\alpha\chi_{0,1}(x)^2\dots\chi_{0,K}(x)^2W_\lambda(x)+\sum_{k=1}^K G_k(x)\Big)^4dx\\
&-0.0258\cdot 2(1-\mu)^{-3}\int\beta^4\alpha^4W_\lambda(x)^4R(x)\,dx-A\sum_{k=1}^K\frac{1}{D_k}.
\end{aligned}$$

To estimate the integrals we consider each Voronoi cell Γ_k separately. Since the support of G_k lies in B_k, outside of B_k we have only to consider W_λ. There

$$W_\lambda(x)=\frac{Z_0}{|x-R_k|}\quad\text{with}\quad Z_0:=Z+\sqrt{2Z}+\frac{1}{2}.$$

If we estimate the integral over $\Gamma_k\setminus B_k$ by integrating over one side of the mid-plane defined by the nearest nucleus (cf. [13, p. 982]) minus B_k we get

$$\int_{\Gamma_k\setminus B_k}dx\,W_\lambda(x)^4\leq {Z_0}^4\frac{3\pi}{D_k}.$$

Since all terms scale in the right way, the integral over B_k gives a factor $\frac{1}{D_k}$ times an integral over normalized functions (with 1 instead of D_k and 0 instead of R_k).

Hence we get, indicating the normalized functions by the symbols without indices

$$\begin{aligned} &\mathrm{tr}\Lambda_+\gamma\Lambda_+ h \\ (12)\quad \geq\ & -\Big\{0.0516\mu^{-3}\Big[3\pi(1-\beta)^4\alpha^4 {Z_0}^4 \\ (13)\quad & \qquad + \int_B dx\Big((1-\beta)\alpha(1-\chi(x)^2)\big(F_\lambda(x)+\frac{Z}{|x|}\big)+G(x)\Big)^4\Big] \\ & +0.0516(1-\mu)^{-3}\beta^4\alpha^4\Big[3\pi {Z_0}^4 + \int_{B\setminus B^{(3\sigma)}} dx\big(F_\lambda(x)+\frac{Z}{|x|}\big)^4\Big] + A\Big\} \\ & \cdot\sum_{k=1}^K \frac{1}{D_k}. \end{aligned}$$

In view of (8) we get stability, if the above expression in braces is smaller than or equal to $\frac{1}{8}\alpha Z^2$ and $\tilde\alpha Z = \alpha Z(1-\mu)^{-1} \leq \gamma_c$.

To get the statement of the Theorem we choose $\gamma < \gamma_c$. We want to consider $\alpha Z_k \leq \gamma$ $(k = 1, \dots, K)$. Due to the convexity argument mentioned in the beginning it is enough to consider $Z := \gamma\alpha^{-1}$. We choose $(1-\mu) = \frac{\gamma}{\gamma_c}$ (thus $\alpha Z \leq (1-\mu)\gamma_c$ is satisfied) and fix all other parameters arbitrarily. With these choices and using $Z_0 \leq 4Z$ for $Z \geq 1$, which is valid for small values of α, all expressions inside the braces above can be estimated by a constant (independent of α). Now, we only have to guarantee that this constant is less than or equal to $\frac{1}{8}\alpha Z^2 = \frac{\gamma^2}{8}\alpha^{-1}$, which is fulfilled for small values of α.

5. Numerical Calculations.

To show the mentioned stability for the physical value $\alpha = 1/137.037$ up to $Z = 88$ we choose as in [15] $\sigma = 0.3$,

$$\chi(r) = \begin{cases} 1 & \text{for } r \leq 0.1, \\ \cos\big((x-0.1)\frac{\pi}{1.2}\big) & \text{for } 0.1 < r \leq 0.7, \\ 0 & \text{for } r > 0.7, \end{cases}$$

and

$$rh(r) = \begin{cases} 1 & \text{for } r \leq 0.1 \text{ and } 0.7 \leq r \leq 1, \\ 2 - \frac{|r-0.4|}{0.3} & \text{for } 0.1 < r < 0.7, \end{cases}$$

so that we can also use the estimate (see [15, Section VIII(B)])

$$U(r) \leq \varepsilon + \begin{cases} 0.5751 & \text{for } r \leq 0.7, \\ \frac{\pi}{64\cdot 0.3^5}(1.6-r)(1-r)^3 & \text{for } 0.7 < r \leq 1. \end{cases}$$

For $Z = 88$ we choose $\mu = 0.291$ (then $\alpha Z \leq (1-\mu)\gamma_c$) and $\lambda = 0.98$, $\varepsilon = 0.159$, $\delta = 0.374$ and $\beta = 0.874$. We do the angular integrations of the integrals analytically (cf. [15, Section VIII(A)]) and the remaining integrations on a computer. (The numerical reliability of our results is enhanced by the fact that all occurring integrands are regular.)

So we get $\Omega < 0.116$, $C < 1.289$, hence $A < 3.248$. For the integrals the result is

$$\int_B dx\Big((1-\beta)\alpha(1-\chi(x)^2)\big(F_\lambda(x)+\frac{Z}{|x|}\big)+G(x)\Big)^4 < 0.861$$

and

$$\int_{B\setminus B^{(3\sigma)}} dx\big(F_\lambda(x)+\frac{Z}{|x|}\big)^4 < 6.864\cdot 10^9.$$

Thus the first summand in the braces of (12) and (13) is smaller than 1.805, the second one smaller than 1.887 and the whole expression is bounded by 6.94 whereas $\frac{1}{8}\alpha Z^2 > 7.06$ yielding the desired estimate.

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