Stability of Matter for the Hartree-Fock Functional of the Relativistic Electron-Positron Field [1]

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Abstract. We investigate stability of matter of the Hartree-Fock functional of the relativistic electron-positron field – in suitable second quantization – interacting via a second quantized Coulomb field and a classical magnetic field. We are able to show that stability holds for a range of nuclear charges $Z_1, .., Z_K \leq Z$ and fine structure constants α that include the physical value of α and elements up to holmium ($Z = 67$).

Keywords and Phrases: Dirac operator, stability of matter, QED, generalized Hartree-Fock states

1 Introduction

Electrons and positrons can be described just interacting with themselves and the electromagnetic field. However, in many interesting applications these particles do not exist separated from the rest of the world but interact with nuclei, in fact very often with many nuclei. It is therefore of interest, to investigate the stability of quantum electrodynamics, the basic theory describing relativistic electrons and positrons, when coupled to many nuclei. A standard model to incorporate nuclei is to assume them as external sources of the electric field and minimize the energy over all possible pairwise distinct nuclear positions. This is known as the Born-Oppenheimer approximation.

Stability in the context of field theory means, that the energy is bounded from below by a multiple of the number operator of the electron-positron field plus a constant times the number of nuclei involved. In fact, we would like to show positivity of the energy.

The purpose of this paper is to make a step towards this direction. Based on paper of Chaix et al. [4] we showed [2] that the Hartree-Fock functional of the vacuum

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and of atoms with sufficiently small nuclear charge is nonnegative (with or without self-generated magnetic field) provided the Sommerfeld fine structure constant $\alpha = e^2$ is also small where e is the elementary charge unit. These results included the physical value $\alpha \approx 1/137$ and atoms with atomic number up to 67 (holmium). Here we show that positivity even holds when the number of nuclei is no longer restricted, in fact without any essential loss: it holds again up to holmium for the physical value of α.

Our paper is organized as follows: For the readers convenience we fix some notations in Section 2 and Appendix B. Some inequalities used in the proof are collected in Appendix A. Section 3 contains our positivity result for the Hartree-Fock functional disregarding the magnetic field. Section 4 extends this to the case when the self-generated magnetic field of the particle is taken into account on a classical level.

2 DEFINITION OF THE PROBLEM

Before stating our problem precisely, we fix our notations following [2]. (See also Appendix B for additional notations.)

DIRAC OPERATOR The operator for a particle of charge $-e$, in magnetic field $\nabla \times \mathbf{A}$, and interacting with K nuclei of same charge is

$$D^{\mathbf{A},V} := \boldsymbol{\alpha} \cdot (\frac{1}{i}\nabla + e\mathbf{A}) + m\beta + e^2 V,$$

acting in the four components vector space $\mathfrak{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$. The 4×4 matrices $\boldsymbol{\alpha}$ and β are the Dirac matrices in the standard representation [14]. The vector potential $\mathbf{A}$ is assumed to be such that the magnetic induction $\mathbf{B} = \nabla \times \mathbf{A}$ is square integrable. The multiplication operator $-eV$ is the electric potential of K nuclei with charge eZ located at $\mathbf{R}_1, \dots, \mathbf{R}_K$, i.e.,

$$V(\mathbf{x}) := -\sum_{k=1}^{K} \frac{Z}{|\mathbf{x} - \mathbf{R}_k|}. \tag{1}$$

Note that $D^{\mathbf{A},V}$ is self-adjoint with form domain $H^{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^4$ under the assumption on e and Z stated in Theorems 1 and 2.

ENERGY OF A STATE We define $\mathfrak{D}$ to be the set of all states ρ with finite kinetic energy, i.e., $\sum_{i,j \in \mathbb{Z}} (D^{\mathbf{0},0})_{i,j}\, \rho(:\Psi_i^* \Psi_j:)$ converges absolutely where colons denote normal ordering where we fixed an orthonormal basis such that all basis vectors e_i are in $H^{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^4$. We denote by $(D^{\mathbf{A},V})_{i,j} = (e_i, D^{\mathbf{A},V} e_j)$, and by $W_{i,j;k,l}$, the matrix elements of the two-body Coulomb potential $W(\mathbf{x},\mathbf{y}) = 1/|\mathbf{x}-\mathbf{y}|$, i.e.,

$$W_{i,j;k,l} = (e_i \otimes e_j, W e_k \otimes e_l) = \int_G dx \int_G dy\, \frac{\overline{e_i(x) e_j(y)} e_k(x) e_l(y)}{|\mathbf{x}-\mathbf{y}|}$$

where dx denotes the product measure (Lebesgue measure in the first factor and counting measure in the second factor) of $G := \mathbb{R}^3 \times \{1,2,3,4\}$. The energy of a state $\rho \in \mathfrak{D}$ is thus

$$\begin{aligned}\mathcal{E}_{\mathbf{A},V,\alpha}(\rho) &= \sum_{i,j\in\mathbb{Z}} (D^{\mathbf{A},V})_{i,j}\, \rho(:\Psi_i^*\Psi_j:) + \alpha U \\ &+ \frac{\alpha}{2} \sum_{i,j,k,l\in\mathbb{Z}} W_{i,j;k,l}\, \rho(:\Psi_i^*\Psi_j^*\Psi_l\Psi_k:) + \frac{1}{8\pi}\int_{\mathbb{R}^3} \mathbf{B}^2, \qquad (2)\end{aligned}$$

with $U := \sum_{1\le\kappa<k\le K} Z^2/|\mathbf{R}_\kappa - \mathbf{R}_k|$ describing the energy of the nuclei.

ENERGY OF GENERALIZED HARTREE-FOCK STATES Following the proof of Theorem 1 in [2], we can show that for all generalized Hartree-Fock states $\rho \in \mathfrak{D}_{HF}$ (see Appendix B), the energy (2) can be rewritten as a functional of Γ_ρ, the 1-pdm of ρ:

$$\begin{aligned}\mathcal{E}_{\mathbf{A},V,\alpha}(\rho) = \mathcal{E}^{HF}_{\mathbf{A},V,\alpha}(\Gamma_\rho) := \operatorname{tr}(D^{\mathbf{A},V}\gamma) + \alpha U + \frac{\alpha}{2}\int dxdy \frac{|\upsilon(x,y)|^2}{|\mathbf{x}-\mathbf{y}|} + \alpha D(\rho_\gamma,\rho_\gamma) \\ - \frac{\alpha}{2}\int dxdy\frac{|\gamma(x,y)|^2}{|\mathbf{x}-\mathbf{y}|} + \frac{1}{8\pi}\int_{\mathbb{R}^3}\mathbf{B}^2, \qquad (3)\end{aligned}$$

where $D(f,g) := (1/2)\int_{\mathbb{R}^6} d\mathbf{x}d\mathbf{y}\overline{f(\mathbf{x})}g(\mathbf{y})|\mathbf{x}-\mathbf{y}|^{-1}$ is the Coulomb scalar product, $\upsilon(x,y) := \sum_{i,j\in\mathbb{Z}}(e_i,\upsilon e_j)e_i(x)e_j(y)$, $\gamma(x,y) := \sum_{i,j\in\mathbb{Z}}(e_i,\gamma e_j)e_i(x)\overline{e_j(y)}$ (note the difference to υ), and $\rho_\gamma(\mathbf{x}) := \sum_{\sigma=1}^4 \gamma(x,x)$. (We use the notation $x := (\mathbf{x},\sigma) \in \mathbb{R}^3 \times \{1,\ldots,4\}$.) We also remind the reader that $\alpha = e^2$.

The main goal of this paper is to show positivity of $\mathcal{E}_{\mathbf{A},V,\alpha}(\rho)$ for quasi-free states.

More notations can be found in Appendix B.

3 STABILITY OF RELATIVISTIC MATTER WITHOUT MAGNETIC FIELD

We prove here, in the case $\mathbf{A} = \mathbf{0}$, that the energy functional $\mathcal{E}_{\mathbf{A},V,\alpha}$ defined in (2) is positive on generalized Hartree-Fock states for suitable choice of the electron subspace and α and Z small enough. More precisely, $\mathfrak{H}_+ := [\chi_{[0,\infty)}(D^{\mathbf{0},V_{\text{eff}}})](\mathfrak{H})$ is the positive spectral subspace associated to $D^{\mathbf{0},0} + \alpha V_{\text{eff}}$, where

$$V_{\text{eff}} := -Z\sum_{k=1}^K \frac{\chi_{\Upsilon_k}(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_k|}. \qquad (4)$$

Here $\Upsilon_\kappa := \{\mathbf{x}\in\mathbb{R}^3 \ :\ |\mathbf{x}-\mathbf{R}_\kappa| \le |\mathbf{x}-\mathbf{R}_k|, \forall k = 1,\ldots,K\}$ denotes the κ-th Voronoi cell and χ_M is the characteristic function of the set M. Our first result is

THEOREM 1. *Pick $\mathfrak{H}_+ := [\chi_{[0,\infty)}(D^{\mathbf{0},V_{\text{eff}}})](\mathfrak{H})$ as electron subspace. Let $L_{1/2,3}$ be the constant in the Lieb-Thirring inequality[2] for moments of order $1/2$. If $\epsilon \in (0,1)$, $\alpha \in [0,4/\pi]$ and $Z \in [0,\infty)$ are such that*

$$1 - \epsilon - \pi^2\alpha^2/16 - 4(1/\epsilon - 1)\alpha^2 Z^2 > 0,$$

[2]See Appendix A.

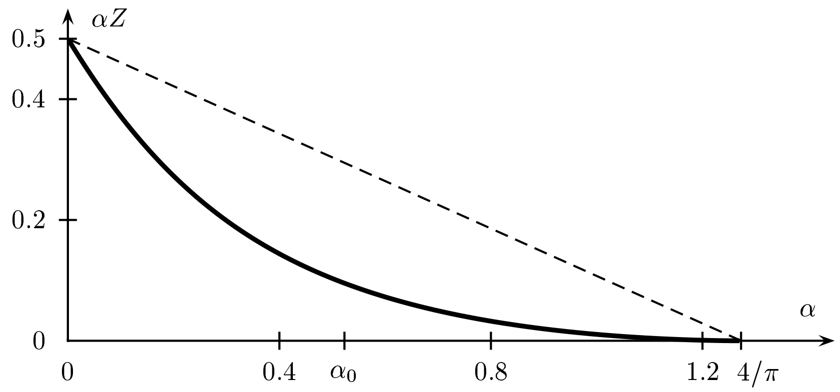

Figure 1: The plain curve gives an estimate from below of the critical value of the pair $(\alpha, \alpha Z)$, for which the energy $\mathcal{E}_{\mathbf{0},V,\alpha}$ is positive. For the physical value $\alpha \approx 1/137.0359895$ we obtain $\alpha Z \approx 0.489576$, i.e., $Z \approx 67.089649$. The dashed curve is the one obtained in [2] in the case of a single nucleus of atomic number Z

and

$$\frac{26296\pi L_{1/2,3}(1/\epsilon - 1)^2}{105(1 - \epsilon - \pi^2\alpha^2/16 - 4(1/\epsilon - 1)\alpha^2 Z^2)^{3/2}}\alpha^3 Z^2 \leq 1,$$

then $\mathcal{E}_{\mathbf{0},V,\alpha}$ *is nonnegative on* $\mathfrak{D}_{HF}$.

Remark that we do not assume that 0 is not in the spectrum of $D^{\mathbf{0},V_{\text{eff}}}$. This means in particular that $\mathfrak{H}_+$ includes the null space of $D^{\mathbf{0},V_{\text{eff}}}$. Note also that ϵ is a free parameter that we can use to optimize the value of α and Z. Instead of giving a cumbersome analytic formula, Figure 1 gives the result when picking ϵ suitably.

The proof of the theorem consists of five steps:

- Replace the Dirac operator $D^{\mathbf{0},V}$ by $D^{\mathbf{0},V_{\text{eff}}}$ which is done by reducing the Coulomb potential V in each Voronoi cell to a one-nucleus/electron Coulomb potential V_{eff}.
- Dominate the exchange energy W_X by the kinetic energy.
- Control the difference of the kinetic energy and the energy of the modified Dirac operator $D^{\mathbf{0},V_{\text{eff}}}$ by applying the Birman-Koplienko-Solomyak inequality [3] to obtain a Schrödinger like operator.
- Estimate the resulting expression by a localized Hardy inequality of Lieb and Yau [12] going back to Dyson and Lenard [5].
- Apply the Lieb-Thirring inequality [10] for moment 1/2 to estimate the trace.

Proof. Set d_k to be half the distance of the k-th nucleus to its nearest neighbor, then the electrostatic inequality of Lieb and Yau [12], p. 196, Formula (4.4), implies with

$d\nu(x) := \rho(\mathbf{x})d\mathbf{x}$

$$\begin{aligned}\mathcal{E}_{\mathbf{0},V,\alpha} &\geq \operatorname{tr}(D^{\mathbf{0},V}\gamma) + \alpha U + \alpha D(\rho_\gamma,\rho_\gamma) - \frac{\alpha}{2}\int dxdy \frac{|\gamma(x,y)|^2}{|\mathbf{x}-\mathbf{y}|} \\ &\geq \operatorname{tr}(D^{\mathbf{0},V_{\text{eff}}}\gamma) + \frac{\alpha Z^2}{8}\sum_{k=1}^K d_k^{-1} - \frac{\alpha}{2}\int dxdy\frac{|\gamma(x,y)|^2}{|\mathbf{x}-\mathbf{y}|}. \end{aligned} \tag{5}$$

Using Kato's inequality (see Appendix A) and then Inequalities (22) and (23) we get

$$\begin{aligned}\frac{2}{\pi}\sum_{s,t=1}^4 \int \frac{|\gamma(x,y)|^2}{|\mathbf{x}-\mathbf{y}|}dxdy &\leq \operatorname{tr}[(|\nabla|\otimes \mathbf{1})\gamma^2] \leq \operatorname{tr}(|D^{\mathbf{0},0}|\gamma^2) \\ &\leq \operatorname{tr}(|D^{\mathbf{0},0}|(\gamma_{++}-\gamma_{--})). \end{aligned}\tag{6}$$

So far we have not used the choice of the subspaces $\mathfrak{H}_+$ and $\mathfrak{H}_-$ specified in the hypothesis. In order to control the trace in (6) with the trace on the right hand side of (5), we now use that $\mathfrak{H}_+$ is the positive spectral subspace of $D^{\mathbf{0},V_{\text{eff}}}$, i.e., $\mathfrak{H}_+ := \left[\chi_{[0,\infty)}(D^{\mathbf{0},V_{\text{eff}}})\right](\mathfrak{H})$. This implies $\operatorname{tr}(D^{\mathbf{0},V_{\text{eff}}}\gamma) = \operatorname{tr}(|D^{\mathbf{0},V_{\text{eff}}}|(\gamma_{++}-\gamma_{--}))$, and thus

$$\mathcal{E}_{\mathbf{0},V,\alpha} \geq \operatorname{tr}\left[\left(|D^{\mathbf{0},V_{\text{eff}}}| - \frac{\pi\alpha}{4}|D^{\mathbf{0},0}|\right)(\gamma_{++}-\gamma_{--})\right] + \frac{\alpha Z^2}{8}\sum_{k=1}^K d_k^{-1}. \tag{7}$$

If we bound below the trace on the right hand side of (7) by using the Birman-Koplienko-Solomyak inequality [3] (see also Appendix A), and noting that $0 \leq \gamma_{++} - \gamma_{--} \leq 1$, we obtain

$$\begin{aligned}\operatorname{tr}\left[\left(|D^{\mathbf{0},V_{\text{eff}}}| - \alpha\pi|D^{\mathbf{0},0}/4|\right)(\gamma_{++}-\gamma_{--})\right] &\geq -\operatorname{tr}\left(|D^{\mathbf{0},V_{\text{eff}}}| - \alpha\pi|D^{\mathbf{0},0}|/4\right)_- \\ &\geq -\operatorname{tr}\left\{\left[(D^{\mathbf{0},V_{\text{eff}}})^2 - \pi^2\alpha^2(D^{\mathbf{0},0})^2/16\right]_-^{1/2}\right\} \\ &\geq -\operatorname{tr}\left\{\left[(1-\epsilon-\pi^2\alpha^2/16)(D^{\mathbf{0},0})^2 - (1/\epsilon-1)\alpha^2V_{\text{eff}}^2\right]_-^{1/2}\right\} \end{aligned}\tag{8}$$

where the subscript minus denotes the negative part $(|A|-A)/2$ of the operator A. To bound the trace on the right hand side of (8) from below, we use the localized Hardy inequality of Lieb and Yau [12, Formula (5.2)] (see also Appendix A), K times with $k = 1,\ldots,K$ and $B_k := B_{d_k}(\mathbf{R}_k)$, we have

$$\int_{\mathbb{R}^3}|\nabla f(\mathbf{x})|^2 d\mathbf{x} \geq \sum_{k=1}^K\left(\int_{B_k}\left(\frac{1}{4|\mathbf{x}-\mathbf{R}_k|^2} - \frac{1}{d_k^2}\left(1+\frac{|\mathbf{x}-\mathbf{R}_k|^2}{4d_k^2}\right)\right)|f(\mathbf{x})|^2 d\mathbf{x}\right). \tag{9}$$

Inequality (9) together with (8) gives

$$\begin{aligned}\mathcal{E}_{\mathbf{0},V,\alpha} \geq -\operatorname{tr}\Bigg\{\Bigg[&\left(1-\epsilon-\alpha^2\pi^2/16 - 4(1/\epsilon-1)\alpha^2Z^2\right)(D^{\mathbf{0},0})^2 \\ -(1/\epsilon-1)\alpha^2Z^2\sum_{k=1}^K&\left(\frac{\chi_{\Upsilon_k\setminus B_k}(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_k|^2} - \frac{4}{d_k^2}\left(1+\frac{|\mathbf{x}-\mathbf{R}_k|^2}{4d_k^2}\right)\chi_{B_k(\mathbf{x})}\right)\Bigg]_-^{\frac{1}{2}}\Bigg\} + \frac{\alpha Z^2}{8}\sum_{k=1}^K d_k^{-1}. \end{aligned}\tag{10}$$

Using the Lieb-Thirring inequality (see Appendix A) for the exponent 1/2 in (10) implies

$$\begin{aligned}\mathcal{E}_{\mathbf{0},V,\alpha} \geq\ & \frac{-L_{1/2,3}(\frac{1}{\epsilon}-1)^2\alpha^4 Z^4}{(1-\epsilon-\pi^2\alpha^2/16-4(1/\epsilon-1)\alpha^2Z^2)^{3/2}}\left\{\sum_{k=1}^K\int_{\Upsilon_k\setminus B_k}\frac{1}{|\mathbf{x}-\mathbf{R}_k|^4}d\mathbf{x}\right.\\ & \left.+16\sum_{k=1}^K\int_{B_k}\frac{1}{d_k^4}\left(1+\frac{|\mathbf{x}-\mathbf{R}_k|^2}{4d_k^2}\right)^2 d\mathbf{x}\right\}+\frac{\alpha Z^2}{8}\sum_{k=1}^K d_k^{-1} \qquad (11)\\ \geq\ & \left(\frac{\alpha Z^2}{8}-\frac{\pi(3+64(1/3+1/10+1/112)L_{1/2,3}(1/\epsilon-1)^2\alpha^4Z^4}{\left(1-\epsilon-\frac{\pi^2\alpha^2}{16}-4(1/\epsilon-1)\alpha^2Z^2\right)^{\frac{3}{2}}}\right)\sum_{k=1}^K d_k^{-1}.\end{aligned}$$

Note that the numerical value of the Lieb-Thirring constant $L_{1/2,3}$ does not exceed 0.06003. In (11), we have estimated the first term in the parenthesis with Inequality (4.6) in [8]. □

4 Inclusion of the Magnetic Field

We now consider the whole energy functional $\mathcal{E}_{\mathbf{A},V,\alpha}$ given in (3), i.e., we include also magnetic fields $\mathbf{B} := \nabla \times \mathbf{A}$ of finite field energy.

Theorem 2. *Take* $\mathfrak{H}_+ := [\chi_{[0,\infty)}(D^{\mathbf{A},V_{\text{eff}}})](\mathfrak{H})$. *If* $\epsilon \in (0,1)$, $\epsilon' \in (0,\infty)$, $\alpha \in [0,4/\pi]$ *and* $Z \in [0,\infty)$ *verify*

$$1-\epsilon-\pi^2\alpha^2/16-4(1/\epsilon-1)\alpha^2Z^2 > 0, \qquad (12)$$

$$\frac{26296\pi L_{1/2,3}(1/\epsilon-1)^2(1+\epsilon')}{105(1-\epsilon-\pi^2\alpha^2/16-4(1/\epsilon-1)\alpha^2Z^2)^{3/2}}\alpha^3Z^2 \leq 1, \qquad (13)$$

and

$$\frac{8\pi L_{1/2,3}(1-\epsilon)^2(1+1/\epsilon')}{(1-\epsilon-\pi^2\alpha^2/16-4(1/\epsilon-1)\alpha^2Z^2)^{3/2}}\alpha \leq 1 \qquad (14)$$

then $\mathcal{E}_{\mathbf{A},V,\alpha}$ *is nonnegative on* $\mathfrak{D}_{HF}$.

Again, note that ϵ and ϵ' are free parameters that can be picked arbitrarily within the given ranges. However, we refrain to give cumbersome optimal expressions. Instead we – once again – optimize numerically, insert, and show the result in Figure 2.

Proof. By the (relativistic) diamagnetic inequality (see, e.g., the appendix of [8], see also Appendix A)

$$\frac{\alpha}{2}\int dx\int dy|\gamma(x,y)|^2/|\mathbf{x}-\mathbf{y}| \leq \frac{\pi\alpha}{4}\,\mathrm{tr}(\gamma^*|-i\nabla+\sqrt{\alpha}\mathbf{A}|\gamma). \qquad (15)$$

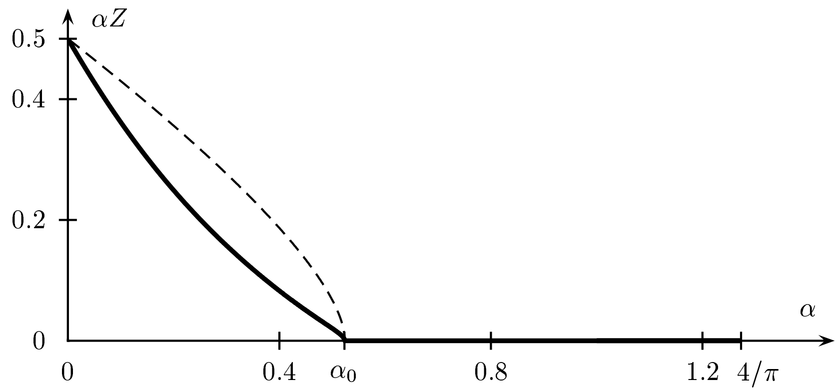

Figure 2: The plain curve gives an estimate from below of the critical value of the pair $(\alpha, \alpha Z)$, for which the energy $\mathcal{E}_{\mathbf{A},V,\alpha}$ is positive. For the physical value $\alpha \approx 1/137.0359895$ we obtain $\alpha Z \approx 0.48899985$, i.e., $Z \approx 67.0105779$. The dashed curve shows the critical curve obtained in [2] in the case of a single nucleus. The numerical value where both curves cut the abscissa is $\alpha_0 \approx 0.5235$.

Now, following the proof of Theorem 1 using (5) to (8) and (15), we obtain for $\mathfrak{H}_+ := [\chi_{[0,\infty)}(D^{\mathbf{A},V_{\mathrm{eff}}})](\mathfrak{H})$ and for any $\epsilon \in (0,1)$

$$\begin{aligned} T &:= \mathrm{tr}((D^{\mathbf{A},0} + \alpha V_{\mathrm{eff}})\gamma) - \frac{\alpha}{2}\int \frac{|\gamma(x,y)|^2}{|\mathbf{x}-\mathbf{y}|} dx dy \\ &\geq -\,\mathrm{tr}\left\{ \left[(1-\epsilon)(D^{\mathbf{A},0})^2 - (\frac{1}{\epsilon}-1)\alpha^2 {V_{\mathrm{eff}}}^2 - \frac{\pi^2\alpha^2}{16}|-i\nabla + \sqrt{\alpha}\mathbf{A}|^2 \right]_-^{\frac{1}{2}} \right\} \\ &\geq -\,\mathrm{tr}\left\{ \left[(1-\epsilon-\frac{\pi^2\alpha^2}{16})|-i\nabla+\sqrt{\alpha}\mathbf{A}|^2 - (\frac{1}{\epsilon}-1)\alpha^2 {V_{\mathrm{eff}}}^2 - (1-\epsilon)\sqrt{\alpha}|\mathbf{B}| \right]_-^{\frac{1}{2}} \right\}. \end{aligned}$$

Combining first (9) with the nonrelativistic diamagnetic inequality for Schrödinger operators (Simon [13], see also Appendix A) gives

$$\begin{aligned} &\int_{\mathbb{R}^3} |(-i\nabla + \sqrt{\alpha}\mathbf{A}) f(\mathbf{x})|^2 d\mathbf{x} \\ &\qquad \geq \sum_{k=1}^{K} \left(\int_{B_k} \left(\frac{1}{4|\mathbf{x}-\mathbf{R}_k|^2} - \frac{1}{d_k^2}(1 + \frac{|\mathbf{x}-\mathbf{R}_k|^2}{4d_k^2}) \right) |f(\mathbf{x})|^2 d\mathbf{x} \right). \qquad (16) \end{aligned}$$

Using this inequality we are able to control the $|\mathbf{x}-\mathbf{R}_k|^{-2}$ singularities for V_{eff}^2 in balls of radius d_k around $\mathbf{R}_k$ by a piece of $(-i\nabla + \sqrt{\alpha}\mathbf{A})^2$. This gives

$$\begin{aligned} T \;\;\geq\;\; -\,\mathrm{tr}\Bigg\{ \Bigg[&\left(1-\epsilon-\frac{\pi^2\alpha^2}{16} - 4(\frac{1}{\epsilon}-1)\alpha^2 Z^2\right)|-i\nabla + \sqrt{\alpha}\mathbf{A}|^2 - (1-\epsilon)\sqrt{\alpha}|\mathbf{B}| \\ &-(\frac{1}{\epsilon}-1)\alpha^2 Z^2 \sum_{k=1}^{K} \left(\frac{\chi_{\Upsilon_k \setminus B_k}(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_k|^2} - \frac{4}{d_k^2}(1+\frac{|\mathbf{x}-\mathbf{R}_k|^2}{4d_k^2})\chi_{B_k}(\mathbf{x}) \right) \Bigg]_-^{\frac{1}{2}} \Bigg\} \end{aligned}$$

The Lieb-Thirring inequality for the moment $1/2$ implies

$$\begin{aligned} T &\geq \frac{-L_{1/2,3}}{\left(1-\epsilon-\frac{\pi^2\alpha^2}{16}-4(\frac{1}{\epsilon}-1)\alpha^2Z^2\right)^{3/2}}\int_{\mathbb{R}^3}\Bigg\{(\frac{1}{\epsilon}-1)\alpha^2Z^2\Bigg[\sum_{k=1}^K\frac{\chi_{\Upsilon_k\setminus B_k}(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_k|^2} \\ &\quad +4\sum_{k=1}^K\frac{1}{d_k^2}\left(1+\frac{|\mathbf{x}-\mathbf{R}_k|^2}{4d_k^2}\right)\chi_{B_k(\mathbf{x})}\Bigg]+\sqrt{\alpha}(1-\epsilon)|B|\Bigg\}^2 d\mathbf{x} \\ &\geq \frac{-L_{1/2,3}}{\left(1-\epsilon-\frac{\pi^2\alpha^2}{16}-4(\frac{1}{\epsilon}-1)\alpha^2Z^2\right)^{3/2}}\Bigg\{(1+\epsilon')(\frac{1}{\epsilon}-1)^2\alpha^4Z^4 \\ &\quad \times\Bigg[\sum_{k=1}^K\int_{\mathbb{R}^3}\frac{\chi_{\Upsilon_k\setminus B_k}(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_k|^4}d\mathbf{x}+16\sum_{k=1}^K\frac{1}{d_k^4}\int_{\mathbb{R}^3}\left(1+\frac{|\mathbf{x}-\mathbf{R}_k|^2}{4d_k^2}\right)^2\chi_{B_k(\mathbf{x})}d\mathbf{x}\Bigg] \\ &\quad +(1+\frac{1}{\epsilon'})(1-\epsilon)^2\alpha\int_{\mathbb{R}^3}B^2d\mathbf{x}\Bigg\}. \end{aligned}$$

Collecting all terms and using the previous inequality gives with $\delta := 3+64(1/3+1/10+1/112)$ – for any $\epsilon'\in(0,\infty)$ and under assumptions (12)-(14) –

$$\begin{aligned} \mathcal{E}_{\mathbf{A},V,\alpha} &\geq \operatorname{tr}\left[(D^{\mathbf{A},0}+\alpha V_{\mathrm{eff}})\gamma\right]-\frac{\alpha}{2}\int\frac{|\gamma(x,y)|^2}{|\mathbf{x}-\mathbf{y}|}dxdy+\frac{\alpha Z^2}{8}\sum_{k=1}^K d_k^{-1}+\int_{\mathbb{R}^3}\mathbf{B}^2 \\ &\geq \frac{\alpha Z^2}{8}\left[1-\frac{8\pi\delta L_{1/2,3}(\frac{1}{\epsilon}-1)^2(1+\epsilon')\alpha^3Z^2}{\left(1-\epsilon-\frac{\pi^2\alpha^2}{16}-4(\frac{1}{\epsilon}-1)\alpha^2Z^2\right)^{3/2}}\right]\sum_{k=1}^K d_k^{-1} \\ &\quad +\frac{1}{8\pi}\left[1-\frac{8\pi L_{1/2,3}(1-\epsilon)^2(1+\frac{1}{\epsilon'})\alpha}{\left(1-\epsilon-\frac{\pi^2\alpha^2}{16}-4(\frac{1}{\epsilon}-1)\alpha^2Z^2\right)^{3/2}}\right]\int_{\mathbb{R}^3}\mathbf{B}^2. \end{aligned}$$

□

A Inequalities

BKS Inequality Let $p\geq 1$ and consider two non-negative self-adjoint linear operators C and D such that $[C^p-D^p]_-^{1/p}$ is trace class. Then $[C-D]_-$ is trace class

$$\operatorname{tr}[C-D]_-\leq\operatorname{tr}[C^p-D^p]_-^{1/p}$$

(Birman, Koplienko, and Solomyak [3], see also [9]).

Diamagnetic Inequalities Let $\mathbf{A}\in L^2_{loc}(\mathbb{R}^3,\mathbb{R}^3)$, then, for all u with $|u|\in H^1(\mathbb{R}^3)$

$$\int_{\mathbb{R}^3}(\nabla|u|)^2\leq\int_{\mathbb{R}^3}|(-i\nabla-\mathbf{A})u|^2$$

(Simon [13]) and for all $u\in\mathcal{D}(|p|)$

$$(|u|,\,|p|\,|u|)\leq(u,\,|p+\mathbf{A}|\,u)$$

(see [8, Formula (5.7)]). (Note that we allow for the right side to be infinite.)

Electrostatic Inequality Let ν be any bounded Borel measure on $\mathbb{R}^3$, then with the notations of Theorem 1 we have [12, Lemma 1]

$$\frac{\alpha}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{d\nu(\mathbf{x})d\nu(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}-\alpha\int_{\mathbb{R}^3}(V(\mathbf{x})-V_{\text{eff}}(\mathbf{x}))d\nu(\mathbf{x})+\alpha U\geq\frac{\alpha Z^2}{8}\sum_{k=1}^{K}\frac{1}{d_k}.$$

Kato's Inequality Let H_0 be the closure of the essentially self-adjoint operator $-\Delta$ on $C_0^\infty(\mathbb{R}^3)$. Then for $u\in\mathcal{D}(H_0^{1/2})$ and $\mathbf{a}\in\mathbb{R}^3$, ([7, chap. V, §5, Formula (5.33)])

$$\int_{\mathbb{R}^3}|\mathbf{x}-\mathbf{a}|^{-1}|\,u(\mathbf{x})|^2d\mathbf{x}\leq\frac{\pi}{2}\int_{\mathbb{R}^3}|\mathbf{k}|\,|\hat{u}(\mathbf{k})|^2d\mathbf{k}\leq\frac{\pi}{2}(|H_0|u,\,u).$$

Localized Hardy Inequality Let $\mathbf{R}$ be any point in $\mathbb{R}^3$ and d any positive real number. If $B_d(\mathbf{R})$ denotes the ball in $\mathbb{R}^3$ with center $\mathbf{R}$ and radius d, then, for any $f\in L^2(B_d(R))$ such that $\nabla f\in L^2(B_d(R))$ we have [12, Formula (5.2)]

$$\int_{B_d(\mathbf{R})}|\nabla f(\mathbf{x})|^2d\mathbf{x}\geq\frac{1}{d^2}\int_{B_d(\mathbf{R})}\left(\frac{d^2}{4|\mathbf{x}-\mathbf{R}|^2}-(1+\frac{|\mathbf{x}-\mathbf{R}|^2}{4d^2})\right)|f(\mathbf{x})|^2d\mathbf{x}.$$

Lieb-Thirring Inequality ($d=3$, $\gamma=1/2$) Given a positive constant μ, a real vector field $\mathbf{A}$ with square integrable gradients, and a real valued function V in $L^2(\mathbb{R}^3)$, we have for $V_+ := (|V|+V)/2$

$$\operatorname{tr}\left\{\left[(-i\mu\nabla-\mathbf{A})^2-V\right]_-^{1/2}\right\}\leq\frac{L_{1/2,3}}{\mu^3}\int_{\mathbb{R}^3}V_+^2$$

(see Lieb and Thirring [11] for the case $\mathbf{A}=\mathbf{0}$ and Avron, Herbst, and Simon [1] for the general case).

B Notations

We collect some additional notation that was already used in [2]:

Fock Space and Field Operators For a given orthogonal decomposition $L^2(\mathbb{R}^3)\otimes\mathbb{R}^4=\mathfrak{H}_+\oplus\mathfrak{H}_-$ into the one-particle electron and positron subspace, one constructs, following [14] (see also [6] and [2]), the Fock space $\mathfrak{F}$. We denote the orthogonal projections onto $\mathfrak{H}_+$ and $\mathfrak{H}_-$ are denoted by $P_{\mathfrak{H}_+}$ and $P_{\mathfrak{H}_-}$ respectively. For any $f\in\mathfrak{H}$, we also denote the particle annihilation (respectively creation) operator by $a(f)$ (respectively $a^*(f)$) and the antiparticle annihilation (respectively creation) operator by $b(f)$ (respectively $b^*(f)$). (Note that – according to the convention used in [6] and also here – $a(f)=a(P_{\mathfrak{H}_+}f)$ and $b(f)=b(P_{\mathfrak{H}_-}f)$.) They fulfill the canonical anticommutation relations for all f and g in $\mathfrak{H}$

$$\{a(f),\,a(g)\}=\{a^*(f),\,a^*(g)\}=\{b(f),b(g)\}=\{b^*(f),\,b^*(g)\}=0,\qquad(17)$$

$$\{a(f),\,a^*(g)\}=(f,\,P_{\mathfrak{H}_+}g)\,,\ \{b^*(f),b(g)\}=(f,\,P_{\mathfrak{H}_-}g)\qquad(18)$$

where $\{\ ,\ \}$ denotes the anticommutator.

For any $f \in \mathfrak{H}$, the field operator is the antilinear bounded operator

$$\Psi(f) := a(f) + b^*(f)$$

acting in $\mathfrak{F}$. Its adjoint is linear and equal to $\Psi^*(f) = a^*(f) + b(f)$. Given an orthonormal basis $\{\dots, e_{-2}, e_{-1}, e_0, e_1, \dots\}$ of $\mathfrak{H}$, where vectors with negative indices are in $\mathfrak{H}_-$ and vectors with nonnegative indices are in $\mathfrak{H}_+$, we denote $a_i := a(e_i)$, $a_i^* := a^*(e_i)$, $b_i := b(e_i)$, $b_i^* := b^*(e_i)$, $\Psi_i := a_i + b_i^*$ and $\Psi_i^* := a_i^* + b_i$.

ONE-PARTICLE DENSITY MATRIX A trace class operator Γ on $\mathfrak{H} \times \mathfrak{H}$ is called a one-particle density operator (1-pdm), if

- $\Gamma = \Gamma^*$ and $-1 \le \Gamma \le 1$.
-
$$\Gamma = \begin{pmatrix} \gamma & \upsilon \\ \upsilon^* & -\overline{\gamma} \end{pmatrix} \tag{19}$$

  with

$$\gamma^* = \gamma \text{ and } \upsilon^t = -\upsilon \tag{20}$$

  where the superscript t refers to transposition, i.e., given our basis fixed initially, the matrix elements of B^t are $(B^t)_{i,j} := B_{j,i}$.

Since the Hilbert space $\mathfrak{H}$ is the orthogonal sum of $\mathfrak{H}_+$ and $\mathfrak{H}_-$, we can write

$$\Gamma = \begin{pmatrix} \gamma_{++} & \gamma_{+-} & \upsilon_{++} & \upsilon_{+-} \\ \gamma_{-+} & \gamma_{--} & \upsilon_{-+} & \upsilon_{--} \\ \upsilon^*_{++} & \upsilon^*_{-+} & -\bar{\gamma}_{++} & -\bar{\gamma}_{+-} \\ \upsilon^*_{+-} & \upsilon^*_{--} & -\bar{\gamma}_{-+} & -\bar{\gamma}_{--} \end{pmatrix}$$

with $\gamma_{++} := P_{\mathfrak{H}_+}\gamma P_{\mathfrak{H}_+}$, $\gamma_{+-} := P_{\mathfrak{H}_+}\gamma P_{\mathfrak{H}_-}$, $\gamma_{-+} := P_{\mathfrak{H}_-}\gamma P_{\mathfrak{H}_+} = \gamma^*_{+-}$, and $\gamma_{--} := P_{\mathfrak{H}_-}\gamma P_{\mathfrak{H}_-}$ appropriately restricted. Similarly $\upsilon_{++} := P_{\mathfrak{H}_+}\upsilon P_{\mathfrak{H}_+}$, $\upsilon_{+-} := P_{\mathfrak{H}_+}\upsilon P_{\mathfrak{H}_-}$, $\upsilon_{-+} := P_{\mathfrak{H}_-}\upsilon P_{\mathfrak{H}_+} = -\upsilon^t_{+-}$, and $\upsilon_{--} := P_{\mathfrak{H}_-}\upsilon P_{\mathfrak{H}_-}$ also appropriately restricted.

For each state $\rho \in \mathfrak{D}$, we define the associated 1-pdm Γ_ρ by its matrix elements as

$$(h, \Gamma_\rho g) = \rho\Big(:[\Psi^*(g_1) + \Psi(\tilde{g}_2)][\Psi(h_1) + \Psi^*(\tilde{h}_2)]:\Big) \tag{21}$$

where $h := (h_1, h_2) \in \mathfrak{H}^2$, $g := (g_1, g_2) \in \mathfrak{H}^2$ and given $f = \sum_{k\in\mathbb{Z}} \lambda_k e_k$, we define $\tilde{f} = \sum_{k\in\mathbb{Z}} \overline{\lambda_k} e_k$. The colons denote normal ordering, i.e., anticommuting all stared operators to the left ignoring the anticommutators. Note that for a fixed basis, Γ_ρ is uniquely defined. The matrix elements of Γ_ρ are thus $\gamma_{i,j} = \rho(:\Psi_j^*\Psi_i:)$, $(\gamma_{++})_{i,j} = \rho(a_j^* a_i)$, $(\gamma_{+-})_{i,j} = \rho(b_j a_i)$, $(\gamma_{--})_{i,j} = -\rho(b_i^* b_j)$ and $\upsilon_{i,j} = \rho(:\Psi_j\Psi_i:)$, $(\upsilon_{++})_{i,j} = \rho(a_j a_i)$, $(\upsilon_{+-})_{i,j} = \rho(b_j^* a_i)$, $(\upsilon_{--})_{i,j} = \rho(b_j^* b_i^*)$.

We also recall that

$$\gamma_{++}^2 + \gamma_{+-}\gamma_{-+} \leq \gamma_{++}, \quad (22)$$
$$\gamma_{-+}\gamma_{+-} + \gamma_{--}^2 \leq -\gamma_{--}. \quad (23)$$

holds [2].

States – Generalized Hartree-Fock States A state is a bounded positive linear form ρ on the space of bounded operators on $\mathfrak{F}$ with $\rho(1) = 1$. The set of generalized Hartree-Fock states (or quasi-free states with finite particle number) is the set of states ρ that fulfill

i) For all finite sequences of operators $d_1, d_2, \cdots, d_{2K}$, where d_i stands for $a(f)$, $a^*(f)$, $b(f)$, or $b^*(f)$, we have $\rho(d_1 d_2 \cdots d_{2K-1}) = 0$ and

$$\rho(d_1 d_2 \cdots d_{2K}) = \sum_{\sigma \in S} \operatorname{sgn}(\sigma) \rho(d_{\sigma(1)} d_{\sigma(2)}) \cdots \rho(d_{\sigma(2K-1)} d_{\sigma(2K)})$$

where S is the set of permutations σ such that $\sigma(1) < \sigma(3) < \cdots < \sigma(2K-1)$ and $\sigma(2i-1) < \sigma(2i)$ for all $1 \leq i \leq K$. This implies in particular

$$\rho(d_1 d_2 d_3 d_4) = \rho(d_1 d_2)\rho(d_3 d_4) - \rho(d_1 d_3)\rho(d_2 d_4) + \rho(d_1 d_4)\rho(d_2 d_3). \quad (24)$$

ii) The state ρ has a finite particle number, i.e., if $N := \sum_{i \in \mathbb{Z}} (a_i^* a_i + b_i^* b_i)$ denotes the particle number operator, we have $\rho(N) < \infty$, or equivalently, written in terms of the one-particle density matrix, $\operatorname{tr}(\gamma_{++} - \gamma_{--}) < \infty$.

We write $\mathfrak{D}_{HF}$ for the set of all generalized Hartree-Fock states ρ with finite kinetic energy, i.e., $\sum_{i,j \in \mathbb{Z}} (D^{0,0})_{i,j} \rho(:\Psi_i^* \Psi_j:)$ is absolutely convergent.

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