ON THE POSITIVITY OF THE JANSEN-HESS OPERATOR FOR ARBITRARY MASS.

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Abstract. The Jansen-Heß operator is an approximate (pseudo-)relativistic no-pair Hamiltonian in the Furry picture which is used in the physics literature to describe heavy atoms. Within the single-particle Coulomb model we prove that their energy, and thus the resulting self-adjoint operator and its spectrum, is positive for $Z \leq 114$.

1. Introduction

Consider a relativistic electron in the Coulomb field V, described by the Dirac operator (in relativistic units, $\hbar = c = 1$)

$$H = D_0 + V, \qquad D_0 := -i\boldsymbol{\alpha}\, \partial/\partial\mathbf{x} + \beta m, \quad V(x) := -\frac{\gamma}{x} \tag{1}$$

acting on the Hilbert space $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$, where $\gamma := Ze^2$, Z the nuclear charge number, $e^2 = (137.04)^{-1}$ the fine structure constant, $\boldsymbol{\alpha}$ and β the Dirac matrices and $x := |\mathbf{x}|$.

It is well-known that H is not bounded from below. As long as pair creation is neglected, the conventional way to circumvent this deficiency is the introduction of the semibounded operator $P_+ H P_+$ where P_+ projects onto the positive spectral subspace of H (Furry picture, see Sucher [10] and [11] for a review).

Jansen and Heß [8], based on work by Douglas and Kroll [3] suggested an approximate operator which is derived from a Foldy-Wouthuysen-type transformation scheme. It is a second-order operator in the potential strength γ. It can be written in the form $\Lambda_+(D_0 + V + \frac{i}{2}[W_1, B_1])\,\Lambda_+$ on $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$ where Λ_+ projects onto the positive spectral subspace of the *free* Dirac operator D_0 while W_1 and B_1 are operators linear in γ [7]. Alternatively, as in [4, 2], it can be reduced to an operator acting on two-spinors $\varphi \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$

$$b_m := b_{0m} + b_{1m} + b_{2m} := \mathcal{B} + \gamma^2 \tilde{K} \tag{2}$$

where $b_{0m} + b_{1m} := \mathcal{B}$ is the Brown-Ravenhall operator, and $b_{2m} := \gamma^2 \tilde{K}$ is the second-order term in γ.

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For the massless case ($m = 0$) Brummelhuis, Siedentop and Stockmeyer [2] could prove positivity, i.e.

$$(\varphi, b_m \varphi) \geq 0 \qquad \text{for } \gamma \leq \gamma_c \tag{3}$$

with $\gamma_c = 1.006$ (corresponding to nuclear charge numbers $Z \leq 137$), where γ_c was found to be solution of $1 - \frac{\gamma}{2}(\frac{\pi}{2} + \frac{2}{\pi}) + \frac{\gamma^2}{8}(\frac{\pi}{2} - \frac{2}{\pi})^2 = 0$. For $m \neq 0$, they could prove boundedness from below for $\gamma \leq \gamma_c$ which they obtained from the relative boundedness of the massive Jansen-Heß operator with respect to the massless one. From their proof, positivity was found to hold for $Z \leq 25$.

The aim of the present work is to show positivity of b_m for higher coupling constants. We will choose the momentum representation and we set $\hat{\varphi}(\mathbf{p}) := \int_{\mathbb{R}^3} e^{-i\mathbf{p}\cdot\mathbf{x}} \varphi(\mathbf{x}) d\mathbf{x}/(2\pi)^{3/2}$ for the Fourier transform of φ. Following [4] and [2] we expand φ in terms of spherical spinors Ω_ν

$$\hat{\varphi}(\mathbf{p}) = \sum_{\nu \in I} p^{-1} \hat{f}_\nu(p) \Omega_\nu(\hat{\mathbf{p}}), \qquad \nu = (l, M, s) \tag{4}$$

such that $(\varphi, b_m \varphi) = \sum_{\nu \in I} (f_\nu, b_{lsm} f_\nu) \geq 0$ is equivalent to proving positivity for each component ν. Here, the index set $I := \{\nu = (l, M, s)|\ l \in \mathbb{N}_0,\ M = -l - \frac{1}{2}, ..., l + \frac{1}{2},\ s = \pm\frac{1}{2},\ l + s > 0,\ \Omega_\nu \neq 0\}$, $\hat{\mathbf{p}} := \mathbf{p}/p$, $p := |\mathbf{p}|$, and

$$\sum_{\nu \in I} \int_0^\infty |\hat{f}_\nu(p)|^2 dp = \int_{\mathbb{R}^3} |\hat{\varphi}(\mathbf{p})|^2 d\mathbf{p}. \tag{5}$$

In this partial wave decomposition we define according to (2)

$$b_{lsm} := b_{0m} + b^{(1)}_{lsm} + b^{(2)}_{lsm}, \tag{6}$$

where explicitly ([2], [6])

$$b_{0m} := e(p) := \sqrt{p^2 + m^2}$$

$$b^{(1)}_{lsm}(p, p') := -\frac{\gamma}{\pi}\ [q_l(\frac{p}{p'})\ + h(p)h(p') q_{l+2s}(\frac{p}{p'})]\ A(p)A(p') \tag{7}$$

$$b^{(2)}_{lsm}(p, p') := \frac{\gamma^2}{2\pi^2} \int_0^\infty dp'' N(p, p', p'') A(p)A(p')\ (F_1 + F_2 - F_3 - F_4) \tag{8}$$

with

$$N(p, p', p'') := \left[\frac{1}{e(p') + e(p'')} + \frac{1}{e(p) + e(p'')}\right] A^2(p'')$$

$$h(p) := \frac{p}{e(p) + m}, \qquad A^2(p) := \frac{e(p) + m}{2e(p)} \tag{9}$$

$$F_1 := q_l(\frac{p''}{p}) q_l(\frac{p''}{p'})\ h^2(p''), \qquad F_2 := q_{l+2s}(\frac{p''}{p}) q_{l+2s}(\frac{p''}{p'})\ h(p)h(p')$$

$$F_3 := q_l(\frac{p''}{p})q_{l+2s}(\frac{p''}{p'})\ h(p'')h(p'), \qquad F_4 := q_{l+2s}(\frac{p''}{p})q_l(\frac{p''}{p'})\ h(p)h(p'').$$

Here we have introduced reduced Legendre functions $q_l(x) := Q_l(\frac{1}{2}(x+\frac{1}{x}))$, Q_l being the Legendre function of the second kind (see Stegun, pages 331–353, in [1]). From the properties of Q_l (see [4]) it follows that $F_i \geq 0$, $i = 1, ..., 4$. Moreover, we show that $F_1 + F_2 - F_3 - F_4 \geq 0$, i.e. the kernel $b^{(2)}_{lsm}(p, p')$ is positive (Section 2).

Then one can prove the following.

Proposition 1. *Let $\gamma < \gamma_{c_1} = 0.5929$ $(Z \leq 81)$. Then $b_{lsm} > 0$ for all $l \in \mathbb{N}_0$, $s = \pm\frac{1}{2}$ and all masses $m \neq 0$.*
(The proof is analytical).

For the massless case it was shown [2] that $l = 0, s = \frac{1}{2}$ is the ground-state configuration of the Jansen-Heß operator. When $m \neq 0$ and s is fixed, the lowest-energy configurations are found to be $l = 0$ $(s > 0)$ and $l = 1$ $(s < 0)$, respectively (Section 3). This leads to

Proposition 2. *Let γ_{c_2} be the solution of $1 - \frac{\gamma}{2}(\frac{\pi}{2} + \frac{2}{\pi}) - \frac{\gamma^2}{8}(\frac{\pi}{2} - \frac{2}{\pi})^2 = 0$ $(\gamma_{c_2} = 0.8368$, $Z \leq 114)$. Then one has $b_{lsm} > 0$ for $\gamma < \gamma_{c_2}$ and all $l \in \mathbb{N}_0$, $s = \pm\frac{1}{2}$ and all masses $m \neq 0$.*
(The proof is numerical).

The plan of the paper is as follows: we start by considering some properties of the *kernel* of the operator $b^{(2)}_{lsm}$ in (6). In Section 2 we prove that it is positive. In Section 3 we study the monotonicity properties of the kernel of $b^{(2)}_{lsm}$ with respect to the orbital quantum number l. These properties are used in Sections 4 and 5, where we prove the positivity of the Jansen-Heß operator (Propositions 1 and 2).

2. Positivity of the kernel of the Jansen-Hess operator

Proposition 3. *For all $l \in \mathbb{N}_0$, $s = \pm\frac{1}{2}$ and $p, p' > 0$ we have $b^{(2)}_{lsm}(p, p') > 0$, and $b^{(2)}_{lsm}(0, p') = b^{(2)}_{lsm}(p, 0) = b^{(2)}_{lsm}(0, 0) = 0$.*

Proof: We write the sum $F_1 + F_2 - F_3 - F_4$ as a product in the following way:

$$\begin{aligned} &F_1 + F_2 - F_3 - F_4 = \\ &= q_l\left(\frac{p''}{p}\right) q_l\left(\frac{p''}{p'}\right) h^2(p'') + q_{l+2s}\left(\frac{p''}{p}\right) q_{l+2s}\left(\frac{p''}{p'}\right) h(p)h(p') - \\ &- q_l\left(\frac{p''}{p}\right) q_{l+2s}\left(\frac{p''}{p'}\right) h(p'')h(p') - q_{l+2s}\left(\frac{p''}{p}\right) q_l\left(\frac{p''}{p'}\right) h(p)h(p'') = \\ &= \left(q_l\left(\frac{p''}{p}\right) h(p'') - q_{l+2s}\left(\frac{p''}{p}\right) h(p)\right) \cdot \left(q_l\left(\frac{p''}{p'}\right) h(p'') - q_{l+2s}\left(\frac{p''}{p'}\right) h(p')\right). \end{aligned}$$

With

$$g_{l,s}(p, p'') := q_l\left(\frac{p''}{p}\right) h(p'') - q_{l+2s}\left(\frac{p''}{p}\right) h(p) \tag{10}$$

we have

$$b^{(2)}_{lsm}(p,p') = \frac{\gamma^2}{2\pi^2}\int_0^\infty dp'' N(p,p',p'')A(p)A(p')\cdot g_{l,s}(p,p'')\cdot g_{l,s}(p',p''). \tag{11}$$

Proposition 3 follows from the following lemma:

Lemma 1. *For all* $p,p'>0$ *and* $m\geq 0$,

$$g_{l,s}(p,p')>0 \text{ for } s=1/2;$$
$$g_{l,s}(p,p')<0 \text{ for } s=-1/2.$$

For any $p,p'\geq 0$ *and* $m>0$, *we have* $g_{l,s}(0,p')=g_{l,s}(p,0)=g_{l,s}(0,0)=0$.

Proof of Lemma: Using the definitions (9), we write explicitly

$$g_{l,s}(p,p') = q_l\left(\frac{p'}{p}\right)\frac{p'}{e(p')+m} - q_{l+2s}\left(\frac{p'}{p}\right)\frac{p}{e(p)+m},$$

where

$$q_l\left(\frac{p'}{p}\right) = Q_l(t) := \frac{1}{2}\int_{-1}^{1}\frac{P_l(s)}{t-s}ds, \qquad t=\frac{1}{2}\left(\frac{p}{p'}+\frac{p'}{p}\right), \tag{12}$$

where the P_l are Legendre polynomials.

We consider first the limit case: either $p=0$ and $p'>0$ or $p'=0$ and $p>0$. Taking the limit $t\to\infty$, i.e. either $p'\to 0$ and $p>0$ or $p\to 0$ and $p'>0$, we get $q_l\left(\frac{p'}{p}\right)\to 0$, and thus $g_{l,s}(0,p')=0$, $g_{l,s}(p,0)=0$, for all $p,p'>0$.

If $p=p'>0$, then

$$\begin{aligned} g_{l,s}(p,p) =& \frac{p}{e(p)+m}\left(q_l(1)-q_{l+2s}(1)\right) = \\ =& \frac{p}{e(p)+m}\left(Q_l(1)-Q_{l+2s}(1)\right) > 0 \text{ for } s=1/2 \text{ and } <0 \text{ for } s=-1/2. \end{aligned} \tag{13}$$

This follows from the following formulæ proven in the Appendix,

$$Q_l(1)-Q_{l+1}(1) = \frac{1}{l+1} > 0 \qquad \forall\, l=0,1,2,\dots \text{ and} \tag{14}$$

$$Q_l(1)-Q_{l-1}(1) = -\frac{1}{l} < 0 \qquad \forall\, l=1,2,\dots, \tag{15}$$

using the representation of Q_l in terms of hypergeometric functions [5, p. 999]. In the limit $p=p'\to 0$, we get $g_{l,s}(p,p')\to 0$ if $m\neq 0$. Thus the limit case in Lemma 1 is proved.

If $p\neq p',\ p,p'>0$, we can use the following representation of the Legendre function of the second kind (as in [4]) :

$$q_l\left(\frac{p'}{p}\right) = Q_l(t) = \int_{t+(t^2-1)^{1/2}}^{\infty}\frac{z^{-l-1}}{\sqrt{1-2tz+z^2}}dz, \qquad t=\frac{1}{2}\left(\frac{p}{p'}+\frac{p'}{p}\right), \tag{16}$$

which is valid for $t>1$.

Let $x = p/p' > 0$. Then

$$t^2 - 1 = \left(\frac{1}{2}\left(x - \frac{1}{x}\right)\right)^2, \ \sqrt{t^2-1} = \frac{1}{2}\left|x - \frac{1}{x}\right|,$$

$$t + (t^2-1)^{1/2} = \frac{1}{2}\left(x + \frac{1}{x} + \left|x - \frac{1}{x}\right|\right) = \begin{cases} x, & x > 1 \Leftrightarrow 0 < p' < p \\ 1/x, & x < 1 \Leftrightarrow 0 < p < p' \\ 1, & x = 1 \Leftrightarrow 0 < p = p'. \end{cases} \tag{17}$$

We have

$$t + (t^2-1)^{1/2} > 1 \text{ for all } p \neq p', \ p, p' > 0. \tag{18}$$

Then,

$$\text{for } s > 0, \text{ we have } q_{l+2s}\left(\frac{p'}{p}\right) \leq q_l\left(\frac{p'}{p}\right)\left(t + (t^2-1)^{1/2}\right)^{-2s}, \tag{19}$$

as for $s > 0$ we have:

$$q_{l+2s}\left(\frac{p'}{p}\right) = \int_{t+(t^2-1)^{1/2}}^{\infty} \frac{z^{-l-1}}{\sqrt{1-2tz+z^2}} \cdot z^{-2s} dz \leq q_l\left(\frac{p'}{p}\right)\left(t + (t^2-1)^{1/2}\right)^{-2s};$$

$$\text{for } s < 0, \text{ we have } q_l\left(\frac{p'}{p}\right) \leq q_{l+2s}\left(\frac{p'}{p}\right)\left(t + (t^2-1)^{1/2}\right)^{2s}, \tag{20}$$

since for $s < 0$ we have

$$q_l\left(\frac{p}{p'}\right) = \int_{t+(t^2-1)^{1/2}}^{\infty} \frac{z^{-l-1-2s}}{\sqrt{1-2tz+z^2}} \cdot z^{2s} dz \leq q_{l+2s}\left(\frac{p}{p'}\right)\left(t + (t^2-1)^{1/2}\right)^{2s}.$$

For $s > 0$, using equation (19), we get

(21)

$$\begin{aligned} g_{l,s}(p,p') =& \frac{p'}{e(p')+m}\left(q_l\left(\frac{p'}{p}\right) - q_{l+2s}\left(\frac{p'}{p}\right)\frac{(e(p')+m)}{(e(p)+m)}\frac{p}{p'}\right) \\ &\geq \frac{p'}{e(p')+m} q_l\left(\frac{p'}{p}\right) \cdot \left(1 - \left(t + (t^2-1)^{1/2}\right)^{-2s} \cdot \frac{(e(p')+m)}{(e(p)+m)}\frac{p}{p'}\right) \\ &=: \frac{p'}{e(p')+m} q_l\left(\frac{p'}{p}\right) \theta_s(p,p'). \end{aligned}$$

Suppose that $p' > p > 0$. Then according to (17)

$$\theta_s(p,p') = 1 - \left(\frac{p'}{p}\right)^{-2s} \cdot \frac{(e(p')+m)p}{(e(p)+m)p'} = 1 - \frac{p^{2s+1}}{p'^{2s+1}} \cdot \frac{e(p')+m}{e(p)+m} = 1 - \frac{f(p)}{f(p')},$$

where $f(p) := \dfrac{p^{2s+1}}{e(p)+m}$. Since $f(0) = 0$ and

$$f'(p) = \frac{p^{2s}\left((2s+1)(e(p)+m)e(p) - p^2\right)}{e(p)(e(p)+m)^2} > 0 \qquad \text{for } p > 0,$$

we have $f(p') > f(p) > 0$ for $p' > p > 0$. This implies

$$\text{for } s > 0 \text{ and } 0 < p < p',\ g_{l,s}(p,p') \geq \frac{p'}{e(p')+m}\, q_l\left(\frac{p'}{p}\right)\left(1 - \frac{f(p)}{f(p')}\right) > 0.$$

We have thus proved the first statement in Lemma 1 for $p' > p > 0$ and $s > 0$.

Suppose now that $p > p' > 0$. The first statement in Lemma 1 then follows using (17):

$$\begin{aligned}\theta_s(p,p') =& 1 - \left(\frac{p}{p'}\right)^{-2s} \cdot \frac{(e(p')+m)p}{(e(p)+m)p'} = 1 - \left(\frac{p'}{p}\right)^{2s-1} \cdot \frac{e(p')+m}{e(p)+m} > \\ &> 1 - \left(\frac{p'}{p}\right)^{2s-1} = 0,\ \text{for } s = 1/2.\end{aligned}$$

Let now $s < 0$. Then we get, using the bound (20),

(22)

$$\begin{aligned}-g_{l,s}(p,p') =& \frac{p}{e(p)+m}\left(q_{l+2s}\left(\frac{p'}{p}\right) - q_l\left(\frac{p'}{p}\right)\frac{(e(p)+m)}{e(p')+m}\frac{p'}{p}\right) \\ &\geq \frac{p}{e(p)+m} q_{l+2s}(\frac{p'}{p}) \cdot \left(1 - \left(t + (t^2-1)^{1/2}\right)^{2s} \cdot \frac{(e(p)+m)}{(e(p')+m)}\frac{p'}{p}\right) \\ &= \frac{p}{e(p)+m} q_{l+2s}(\frac{p'}{p})\theta_{-s}(p',p) > 0,\end{aligned}$$

using the bound on θ_{-s} for $-s > 0$.

The proof of Lemma 1 and therefore the proof of Proposition 3 is finished.

□

3. The lowest energy configurations

In this section we prove a useful pointwise bound on the kernel of the Jansen-Heß part of the operator in (6):

Lemma 2. *For all* $p, p' > 0$, $l \in \mathbb{N}_0$ *and* $s = \pm\frac{1}{2}$ *we have*
$b^{(2)}_{lsm}(p,p') < b^{(2)}_{0sm}(p,p')$ *for* $s = 1/2,\ l > 0$;
$b^{(2)}_{lsm}(p,p') < b^{(2)}_{1sm}(p,p')$, *for* $s = -1/2,\ l > 1$.

Note that, if either p or p' is zero, then all $b^{(2)}_{lsm}(p,p') = 0$, by Proposition 3.

Proof: Let first $p \neq p'$, $p, p' > 0$ and $s = \frac{1}{2}$. By Lemma 1 we know that $g_{l,s}(p,p') > 0$ and by equation (11) it is enough to prove that $g_{l,s}(p,p') < g_{0,s}(p,p')$ for all $p \neq p'$, $p, p' > 0$, $l \in \mathbb{N}$ and $s = \frac{1}{2}$. As $g_{l,s}$ is a C^∞ function of $l \geq 0$ we prove that $(g_{l,s}(p,p'))'_l < 0$.

We use

(23)

$$q_l'\left(\frac{p'}{p}\right) = \int_{t+(t^2-1)^{1/2}}^{\infty} (-\ln(z)) \cdot \frac{z^{-l-1}}{\sqrt{1-2tz+z^2}} dz < 0, \text{for } t = \frac{1}{2}\left(\frac{p'}{p} + \frac{p}{p'}\right) > 1,$$

where q_l' means derivative with respect to l, and we get the bound

$$-q_{l+2s}'\left(\frac{p'}{p}\right) < -q_l'\left(\frac{p'}{p}\right)\left(t+(t^2-1)^{1/2}\right)^{-2s},\ s>0,\ t>1,$$

in the same way as the bound (19).

Writing $g_{l,s}(p,p')$ as in (21) and taking the derivative with respect to l we get as in the previous section

$$(24)\qquad (g_{l,s}(p,p'))_l' = \frac{p'}{e(p')+m}\left(q_l'\left(\frac{p'}{p}\right) - q_{l+2s}'\left(\frac{p'}{p}\right)\frac{(e(p')+m)}{(e(p)+m)}\frac{p}{p'}\right)$$
$$< -\frac{p'}{e(p')+m}\cdot q_l'\left(\frac{p'}{p}\right)\cdot\left(-1+\left(t+(t^2-1)^{1/2}\right)^{-2s}\cdot\frac{(e(p')+m)}{(e(p)+m)}\frac{p}{p'}\right)<0.$$

We have

(25)

$$\left(b_{lsm}^{(2)}(p,p')\right)_l' = \frac{\gamma^2}{2\pi^2}\int_0^\infty N(p,p',p'')A(p)A(p')\cdot$$
$$\cdot\left[(g_{l,s}(p,p''))_l'\cdot g_{l,s}(p',p'') + g_{l,s}(p,p'')\cdot(g_{l,s}(p',p''))_l'\right]dp''<0$$

and thus the statement of Lemma 2 for $p\neq p'$, $p,p'>0$, $s=1/2$ and $l>0$.

When $s=-\frac{1}{2}$, we have $g_{l,s}(p,p')<0$ and as in (22) we can prove that $-(g_{l,s}(p,p'))_l'<0$. From this it follows that $|g_{l,s}(p,p')| < |g_{1,s}(p,p')|$ for $l>1$. Equation (25) then shows again that $\left(b_{lsm}^{(2)}(p,p')\right)_l'<0$. This leads to $b_{lsm}^{(2)}(p,p') < b_{1sm}^{(2)}(p,p')$ for $p\neq p'$, $p,p'>0$.

When $p=p'$, we use $|g_{ls}(p,p'')| < |g_{\lambda s}(p,p'')|$ for $p\neq p''$ and $p,p''>0$ where $\lambda=0,\ l>0$ for $s=\frac{1}{2}$ and $\lambda=1,\ l>1$ for $s=-\frac{1}{2}$. Insertion into (11) shows that $b_{lsm}^{(2)}(p,p) < b_{\lambda sm}^{(2)}(p,p)$.

The proof of Lemma 2 is thus finished. □

Lemma 2 provides some information on the lowest energy configuration which we formulate in a Proposition below. Note that this Proposition will not be used in the proof of our main results Propositions 1 and 2 in the next sections.

Proposition 4. *We have*

$$(26)\quad \inf\left\{(\varphi,b_m\varphi)|\ (1+p^{1/2})|\varphi|\in L^2(\mathbb{R}^3),\ \|\varphi\|=1\right\}\geq$$
$$\inf\left\{(f,b_{0,\frac{1}{2},m}^{-}f)+(g,b_{1,-\frac{1}{2},m}^{-}g)|\ (1+p^{1/2})|f|,\ (1+p^{1/2})|g|\in L^2(\mathbb{R}_+),\ \|f\|^2+\|g\|^2=1\right\},$$

where the last infimum can in addition be restricted to positive functions f,g, and where

$$(27)\qquad b_{lsm}^{-} := b_{0m}+b_{lsm}^{(1)}-b_{lsm}^{(2)}.$$

Proof: For any given $f \in L^2(\mathbb{R}_+)$ we have the following bound from below:

$$(f, b_{lsm} f) = (f, (b_{0m} + b_{lsm}^{(1)} + b_{lsm}^{(2)}) f) \;\geq (f, b_{0m} f) \;-(f, -b_{lsm}^{(1)} f) \;-\; |(f, b_{lsm}^{(2)} f)|$$

$$\geq (|f|, b_{0m}|f|) \;-(|f|, -b_{lsm}^{(1)}|f|) \;-\; (|f|, b_{lsm}^{(2)}|f|) \;= (|f|, b_{lsm}^{-}|f|), \tag{28}$$

where we have used that the kernel (7) of $-b_{lsm}^{(1)}$ is positive, and that according to Proposition 3 the kernel of $b_{lsm}^{(2)}$ is positive as well, allowing the bound

$$|(f, b_{lsm}^{(2)} f)| \;\leq \int_0^\infty \int_0^\infty dp\, dp' \;|\hat{f}(p)|\; b_{lsm}^{(2)}(p,p')\; |\hat{f}(p')|. \tag{29}$$

Note that the operator b_{lsm}^{-} defined in (27) differs from b_{lsm} by a minus sign of the last term. Therefore in contrast to the Brown-Ravenhall case [4], the inequalities (28) *do not* assure a positive ground-state configuration for the original Hamiltonian b_m. However, applying Lemma 2 to the right hand side of (28) and using [4], we have the bound from below

$$(|f|, b_{lsm}^{-}|f|) \;\geq\; (|f|, b_{\lambda sm}^{-}|f|), \tag{30}$$

with $\lambda = 0$ for $s = \frac{1}{2}$ and $\lambda = 1$ for $s = -\frac{1}{2}$. Hence we may follow the argumentation of [4] by assuming that the coefficients f_ν in (4) are zero unless $\nu = (0, \frac{1}{2}, \frac{1}{2})$ or $\nu = (1, \frac{1}{2}, -\frac{1}{2})$ when minimizing.

According to (28) and (4), (5) we get

$$\inf\{(\varphi, b_m \varphi)\} = \inf\{\sum_{\nu \in I} (f_\nu, b_{lsm} f_\nu)\} \geq \inf\{|f|, b_{0,\frac{1}{2},m}^{-}|f|) + (|g|, b_{1,-\frac{1}{2},m}^{-}|g|)\}, \tag{31}$$

where φ, f and g obey the restrictions given in (26).

Equation (31) shows that as in [4] we may and shall restrict ourselves to positive functions when evaluating the infimum. □

4. Proof of Proposition 1

Let us consider the following estimate of the energy in a state characterised by ν. Then from (28) and (29)

$$(f_\nu, (b_{0m} + b_{lsm}^{(1)} + b_{lsm}^{(2)}) f_\nu) \tag{32}$$

$$\geq (f_\nu, b_{0m} f_\nu) \;-(|f_\nu|, -b_{lsm}^{(1)}|f_\nu|) \;- \int_0^\infty \int_0^\infty dp\, dp' \;|\hat{f}_\nu(p)|\; b_{lsm}^{(2)}(p,p')\; |\hat{f}_\nu(p')|.$$

Thereby positivity of $b_{lsm}^{(2)}(p,p')$ allows for keeping the four terms F_i from (8) with their respective sign. In the following we will estimate the last term in (32) by means of the Lieb and Yau formula [9] for a symmetric and nonnegative kernel $k(p,p')$

$$\int_0^\infty \int_0^\infty dp\, dp' \;|\hat{\varphi}(p)|\; k(p,p')\; |\hat{\varphi}(p')| \;\leq \int_0^\infty dp\; |\hat{\varphi}(p)|^2 \int_0^\infty dp' k(p,p') \; \left| \frac{f(p)}{f(p')} \right|^2 \tag{33}$$

with a convergence generating function $f(p) > 0$ for $p > 0$. Below, we will always use $f(p) = p^{\frac{1}{2}}$. Factors of the kernel which depend symmetrically on p and p' may be absorbed into the functions $\hat{\varphi}(p)$ and $\hat{\varphi}(p')$, respectively.

For the proof of Proposition 1 we will use strong estimates that allow for an analytical evaluation of the integrals. One has

$$N(p,p',p'') \leq \left[\frac{1}{m+e(p'')} + \frac{1}{m+e(p'')}\right] \frac{e(p'')+m}{2e(p'')} = \frac{1}{e(p'')} \leq \frac{1}{p''}. \tag{34}$$

Moreover, the negative terms $-F_3, -F_4$ in (8) are estimated by zero. Then applying (33) with $\hat{\varphi} := A(p)\hat{f}_\nu(p)$, the contribution to $b^{(2)}_{lsm}(p,p')$ from F_1 is estimated by

$$\begin{aligned} &\frac{\gamma^2}{2\pi^2}\int_0^\infty\int_0^\infty dp\,dp'\ |\hat{f}_\nu(p)|\ A(p)\ \int_0^\infty dp'' N(p,p',p'')\ F_1\ A(p')\ |\hat{f}_\nu(p')| \\ &\leq \frac{\gamma^2}{2\pi^2}\int_0^\infty dp\ |\hat{f}_\nu(p)|^2\ A^2(p)\ \int_0^\infty \frac{p}{p'}dp'\ \int_0^\infty \frac{dp''}{p''}\ q_l(\frac{p''}{p})q_l(\frac{p''}{p'})\ h^2(p''). \end{aligned} \tag{35}$$

Let us first consider states with $s = \frac{1}{2}$. Then we estimate $h^2(p'') \leq 1$ and make use of the fact that $0 \leq q_l(x) \leq \ldots \leq q_1(x) \leq q_0(x) \quad \forall l \geq 1,\ \ x \in \mathbb{R}_+$ (see [4] for $x \neq 1$ and the Appendix for $x = 1$) to get

$$\begin{aligned} I_1(p) &:= \int_0^\infty \frac{p}{p'}dp' \int_0^\infty \frac{dp''}{p''}\ q_l(\frac{p''}{p})q_l(\frac{p''}{p'})\ h^2(p'') \\ &\leq \int_0^\infty \frac{dp''}{p''}\ q_0(\frac{p''}{p})\ \int_0^\infty \frac{p}{p'}dp'\ q_0(\frac{p''}{p'}). \end{aligned} \tag{36}$$

Successively, we substitute $z := p'/p''$ for p' and then $\zeta := p''/p$ for p'' and use the formula (noting that $q_l(z) = q_l(1/z)$ for $l \geq 0$)

$$\int_0^\infty \frac{dz}{z}\ q_0(z)\ = 2\int_0^1 \frac{dz}{z}\ q_0(z)\ = \frac{\pi^2}{2} \qquad \text{with } q_0(z) = \ln\left|\frac{1+z}{1-z}\right|. \tag{37}$$

Then the two integrals decouple and one obtains

$$I_1(p) \leq\ p\ \left(\frac{\pi^2}{2}\right)^2. \tag{38}$$

According to (35) the second term of $b^{(2)}_{lsm}(p,p')$ resulting from F_2 is estimated by

$$\frac{\gamma^2}{2\pi^2}\int_0^\infty dp\ |\hat{f}_\nu(p)|^2\ A^2(p)h^2(p)\int_0^\infty \frac{p}{p'}dp'\int_0^\infty \frac{dp''}{p''}\ q_{l+1}(\frac{p''}{p})q_{l+1}(\frac{p''}{p'}). \tag{39}$$

Estimating q_{l+1} by q_1 and using (as in [4])

(40)

$$\int_0^\infty \frac{dx}{x}\ q_1(x)\ = 2\int_0^1 \frac{dx}{x}\ q_1(x)\ = 2 \qquad \text{with } q_1(x) = \frac{1}{2}(x+\frac{1}{x})\ \ln\left|\frac{1+x}{1-x}\right| - 1$$

one obtains

$$I_2(p) := \int_0^\infty \frac{dp''}{p''}\ q_{l+1}(\frac{p''}{p})\int_0^\infty \frac{p}{p'}dp'\ q_{l+1}(\frac{p''}{p'})\ \leq 4p. \tag{41}$$

The first-order term $b_{lsm}^{(1)}$ is estimated in a similar way, following [4]. According to (32) and (33), since $-b_{lsm}^{(1)}(p,p') > 0$ for $p, p' > 0$,

$$\int_0^\infty \int_0^\infty dp\, dp'\, |\hat{f}_\nu(p)|\; - b_{lsm}^{(1)}(p,p')\, |\hat{f}_\nu(p')| \tag{42}$$

$$\le \frac{\gamma}{\pi} \int_0^\infty dp\, |\hat{f}_\nu(p)|^2\, A^2(p)\, \left\{ \int_0^\infty \frac{p}{p'} dp'\, q_l(\frac{p}{p'}) \; + h^2(p) \int_0^\infty \frac{p}{p'} dp'\, q_{l+2s}(\frac{p}{p'}) \right\}\, .$$

We restrict ourselves to $s = \frac{1}{2}$ and estimate by setting $l = 0$ as before. Then, making the substitution $z := p'/p$ and evaluating the integrals by means of (37) and (40) we find

$$I_0 := \int_0^\infty \frac{p}{p'} dp'\, q_l(\frac{p}{p'}) \; + h^2(p) \int_0^\infty \frac{p}{p'} dp'\, q_{l+1}(\frac{p}{p'}) \tag{43}$$

$$\le \int_0^\infty \frac{p}{p'} dp'\, q_0(\frac{p}{p'}) \; + h^2(p) \int_0^\infty \frac{p}{p'} dp'\, q_1(\frac{p}{p'}) \; = \; p\, (\frac{\pi^2}{2} \; + h^2(p) \cdot 2)\, .$$

Collecting results, the expectation value of the Jansen-Heß operator is estimated by

$$(f_\nu, b_{l\frac{1}{2}m} f_\nu) \;\ge \int_0^\infty dp\, |\hat{f}_\nu(p)|^2\, e(p) \cdot G_{0\frac{1}{2}}(p), \tag{44}$$

$$G_{0\frac{1}{2}}(p) := \; 1 - \frac{\gamma}{\pi}\, \frac{p}{e(p)}\, A^2(p) \left(\frac{\pi^2}{2} \; + 2h^2(p) \right) - \frac{\gamma^2}{2\pi^2}\, \frac{p}{e(p)}\, A^2(p) \left(\frac{\pi^4}{4} \; + 4h^2(p) \right).$$

Following the argumentation at the end of section 3, the minimizing function f_ν can be chosen with $\nu = (0, \frac{1}{2}, \frac{1}{2})$.

m-invariance of $G_{0\frac{1}{2}}(p)$ is provided by means of introducing $p := mx$ (for $m \neq 0$). Then, using the definition (9) of $A(p)$ and $h(p)$ one obtains with $e(p) = m\sqrt{x^2+1}$

$$G_{0\frac{1}{2}}(x) = 1 - \frac{\gamma}{\pi} x \left\{ \frac{\sqrt{x^2+1}+1}{x^2+1} \left(\frac{\pi^2}{4} + \frac{\gamma \pi^3}{16} \right) + \frac{x^2}{(\sqrt{x^2+1}+1)(x^2+1)} \left(1 + \frac{\gamma}{\pi} \right) \right\}. \tag{45}$$

If $G_{0\frac{1}{2}}(x) > 0$ then $b_{l\frac{1}{2}m} > 0$. One easily derives $G_{0\frac{1}{2}}(x) = 1$ for $x = 0$ and $G_{0\frac{1}{2}}(x) \to 1 - \frac{\gamma}{\pi}\,(1 + \frac{\pi^2}{4} + \frac{\gamma}{\pi} + \gamma \frac{\pi^3}{16})$ for $x \to \infty$ which is positive for sufficiently small γ. Our strategy is to look for $\min_{x \in \mathbb{R}_+} G_{0\frac{1}{2}}(x)$ as a function of γ and subsequently determine γ_{c_1} by requiring that this minimum is zero.

The requirement $G'_{0\frac{1}{2}}(x) = 0$ gives the following equation for the minimum value x_0

$$\alpha x_0^2 \; = \; \alpha\, (1 + \sqrt{x_0^2+1}\,) \; + \; \beta\, \frac{3x_0^2\sqrt{x_0^2+1} + x_0^4 + 3x_0^2}{(\sqrt{x_0^2+1}+1)^2} \tag{46}$$

with $\alpha := \frac{\pi^2}{4} + \frac{\gamma\pi^3}{16}$ and $\beta := 1 + \frac{\gamma}{\pi}$. Defining $z_0 := \sqrt{x_0^2+1}$ this results in a quadratic equation for z_0,

$$(z_0 - 2)\,(z_0 + 1)\,\alpha \;=\; \beta\,(z_0 - 1)\,(z_0 + 2) \tag{47}$$

with the solution (since $z_0 \geq 1$ and $\alpha > \beta$)

$$z_0 \;=\; \frac{\alpha + \beta + \sqrt{9\alpha^2 + 9\beta^2 - 14\alpha\beta}}{2(\alpha - \beta)}\;. \tag{48}$$

From this one can calculate

$$G_{0\frac{1}{2}}(x_0) \;=\; 1 \;-\frac{\gamma}{\pi}\,x_0\,\frac{1}{z_0^2}\,[\alpha\,(z_0+1) \;+\beta\,(z_0-1)] \;\overset{!}{=}\; 0 \tag{49}$$

resulting in $\gamma_{c_1} = 0.5929$.

In the second step of the proof of Proposition 1, we have to investigate the $s = -\frac{1}{2}$ states. For these states, one can again use $q_{l-1}(x) \leq q_0(x)$ to estimate the expectation values of $b_{lsm}^{(1)}$ and $b_{lsm}^{(2)}$ by those for $l = 1$ and $s = -\frac{1}{2}$. The subsequent method of calculation is the same as for the states with $l = 0,\ s = \frac{1}{2}$, only that $q_0(x)$ and $q_1(x)$ are interchanged. Instead of (44) one now obtains

$$(f_\nu, b_{l-\frac{1}{2}m} f_\nu) \;\geq\; \int_0^\infty dp\;|\hat{f}_\nu(p)|^2\;e(p)\cdot G_{1-\frac{1}{2}}(p), \tag{50}$$

$$G_{1-\frac{1}{2}}(p) := \;1 - \frac{\gamma}{\pi}\;\frac{p}{e(p)}\;A^2(p)\left(2\;+\frac{\pi^2}{2}h^2(p)\right) - \frac{\gamma^2}{2\pi^2}\;\frac{p}{e(p)}\;A^2(p)\left(4 + \frac{\pi^4}{4}h^2(p)\right).$$

We will show that (with $p := mx$)

$$G_{1-\frac{1}{2}}(x) = 1 - \frac{\gamma}{\pi}x\left\{\frac{\sqrt{x^2+1}+1}{x^2+1}(1+\frac{\gamma}{\pi}) + \frac{\sqrt{x^2+1}-1}{x^2+1}(\frac{\pi^2}{4}+\frac{\gamma\pi^3}{16})\right\} \tag{51}$$

is monotonically decreasing, attaining its infimum at $x \to \infty$, namely $G_{1-\frac{1}{2}}(x) \to 1 - \frac{\gamma}{\pi}\,(1 + \frac{\pi^2}{4}) - \frac{\gamma^2}{\pi^2}\,(1 + \frac{\pi^4}{16})$. This limit value is again strictly decreasing with γ, and at $\gamma = \gamma_{c_1} = 0.5929$, it equals $0.0932 > 0$. This shows that $(f_\nu, b_{l,-\frac{1}{2},m} f_\nu) > 0$ for $\gamma \leq \gamma_{c_1}$ such that we have finally proved $(f_\nu, b_{lsm} f_\nu) > 0$ for $\gamma < \gamma_{c_1}$.

The derivative of $G_{1-\frac{1}{2}}(x)$ can be cast into the form

$$-G'_{1-\frac{1}{2}}(x) \;=\; \frac{\gamma}{\pi}\frac{1}{(x^2+1)^2}\left\{x^2\left(\frac{\pi^2}{4}-1\right) + \sqrt{x^2+1}\left(1+\frac{\pi^2}{4}\right) + 1 - \frac{\pi^2}{4}\right.$$
$$\left. +\;\gamma\left[x^2\left(\frac{\pi^3}{16}-\frac{1}{\pi}\right) + \sqrt{x^2+1}\left(\frac{1}{\pi}+\frac{\pi^3}{16}\right) + \frac{1}{\pi} - \frac{\pi^3}{16}\right]\right\} \tag{52}$$

The r.h.s. of (52) is positive for all $x \in \mathbb{R}_+$ since $\sqrt{x^2+1} \geq 1$, showing that $G_{1-\frac{1}{2}}(x)$ is monotonically decreasing. □

5. Proof of Proposition 2

In order to improve on γ_{c_1}, all contributions to the expectation value of $b^{(2)}_{lsm}$ are retained. Also, the estimates introduced after the application of the Lieb and Yau formula are not made. Moreover, for the Brown-Ravenhall operator, an improved estimate for the $l=0,\ s=\frac{1}{2}$ states provided by Tix [12] is used ($p=mx$)

$$(f_\nu, (b_{0m}+b^{(1)}_{lsm})\, f_\nu) \;\geq \int_0^\infty dp\; |\hat{f}_\nu(p)|^2\; e(p)\cdot T_{0\frac{1}{2}}(x), \tag{53}$$

$$T_{0\frac{1}{2}}(x) :=\; 1\; - \frac{\gamma}{2}\left\{ (\sqrt{x^2+1}+1)\; \frac{\arctan x}{x} \;+\; \frac{(\sqrt{x^2+1}-1)(x-\arctan x)}{(x^2+1)\,\arctan x - x} \right\}.$$

valid for all l,s according to [4].

Together with Lemma 2 this allows for the following representation of (32) for $s=\frac{1}{2}$,

$$\begin{aligned}
&(f_\nu, (b_{0m}+b^{(1)}_{lsm}+b^{(2)}_{lsm})f_\nu)\\
&\geq (f_\nu,(b_{0m}+b^{(1)}_{lsm})f_\nu) - \int_0^\infty\!\!\int_0^\infty dp dp' |\hat{f}_\nu(p)| b^{(2)}_{lsm}(p,p')|\hat{f}_\nu(p')|\\
&\geq \int_0^\infty dp\; |\hat{f}_\nu(p)|^2\; e(p)\cdot T_{0\frac{1}{2}}(x) \;-\; \int_0^\infty\!\!\int_0^\infty dp\, dp'\; |\hat{f}_\nu(p)|\; b^{(2)}_{0\frac{1}{2}m}(p,p')\; |\hat{f}_\nu(p')|\;.
\end{aligned} \tag{54}$$

The second-order term is estimated by means of the Lieb and Yau formula (33)

$$\begin{aligned}
&\int_0^\infty\!\!\int_0^\infty dp\, dp'\; |\hat{f}_\nu(p)|\; b^{(2)}_{0\frac{1}{2}m}(p,p')\; |\hat{f}_\nu(p')| \;\leq\; \frac{\gamma^2}{2\pi^2} \int_0^\infty dp\; |\hat{f}_\nu(p)|^2\; A^2(p) \int_0^\infty dp'\; \frac{p}{p'}\\
&\cdot \int_0^\infty dp''\; N(p,p',p'') \left[q_0\left(\frac{p''}{p}\right) q_0\left(\frac{p''}{p'}\right) h^2(p'') \;+\; q_1\left(\frac{p''}{p}\right) q_1\left(\frac{p''}{p'}\right) h(p)h(p') \right.\\
&\left. \quad -\, q_0\left(\frac{p''}{p}\right) q_1\left(\frac{p''}{p'}\right) h(p'')h(p') \;-\; q_1\left(\frac{p''}{p}\right) q_0\left(\frac{p''}{p'}\right) h(p)h(p'')\right].
\end{aligned} \tag{55}$$

Again, the two successive substitutions $z:=p'/p''$ for p' and $\zeta := p''/p$ for p'' are made. Inserting (9) for $A^2(p)$ and $h(p)$ and setting $p=mx$ as before, (54) with (55) is cast into the form

$$(f_\nu, b_{lsm} f_\nu) \;\geq\; \int_0^\infty dp\; |\hat{f}_\nu(p)|^2\; e(p)\cdot \tilde{G}_{0\frac{1}{2}}(x) \tag{56}$$

$$\begin{aligned}
\tilde{G}_{0\frac{1}{2}}(x) :=\; T_{0\frac{1}{2}}(x) \;-\; \frac{\gamma^2}{8\pi^2}\; x^4\; \frac{\sqrt{x^2+1}+1}{x^2+1}\; &\left(\tilde{I}_1(x) \;+\; \frac{1}{\sqrt{x^2+1}+1}\; \tilde{I}_2(x) \right.\\
&\left. -\, \tilde{I}_3(x) \;-\; \frac{1}{\sqrt{x^2+1}+1}\; \tilde{I}_4(x) \right),
\end{aligned}$$

where we have defined

$$\tilde{I}_1(x) := \int_0^\infty d\zeta \, \frac{\zeta^2}{\sqrt{x^2\zeta^2+1}\,(\sqrt{x^2\zeta^2+1}+1)} \, q_0(\zeta) \int_0^\infty \frac{dz}{z} \, \tilde{N} \, q_0(z) \tag{57}$$

$$\tilde{I}_2(x) := \int_0^\infty \zeta d\zeta \, \frac{\sqrt{x^2\zeta^2+1}+1}{\sqrt{x^2\zeta^2+1}} \, q_1(\zeta) \int_0^\infty \frac{dz}{\sqrt{x^2\zeta^2 z^2+1}+1} \, \tilde{N} \, q_1(z)$$

$$\tilde{I}_3(x) := \int_0^\infty d\zeta \frac{\zeta^2}{\sqrt{x^2\zeta^2+1}} \, q_0(\zeta) \int_0^\infty \frac{dz}{\sqrt{x^2\zeta^2 z^2+1}+1} \, \tilde{N} \, q_1(z)$$

$$\tilde{I}_4(x) := \int_0^\infty \zeta d\zeta \, \frac{1}{\sqrt{x^2\zeta^2+1}} \, q_1(\zeta) \int_0^\infty \frac{dz}{z} \, \tilde{N} \, q_0(z)\,.$$

$$\text{with} \qquad \tilde{N} := \frac{1}{\sqrt{x^2\zeta^2 z^2+1}+\sqrt{x^2\zeta^2+1}} \; + \; \frac{1}{\sqrt{x^2+1}+\sqrt{x^2\zeta^2+1}}\,.$$

For the numerical evaluation, the integration interval is reduced to $[0,1]$ by means of splitting the integrals at 1 and making a variable substitution $z \mapsto 1/z$. It is found numerically that $\tilde{G}_{0\frac{1}{2}}(x)$ is a monotonically decreasing function of x, attaining its infimum at $x \to \infty$. From (56) and (57) one derives

$$\inf_{x\in\mathbb{R}_+} \tilde{G}_{0\frac{1}{2}}(x) \; = \; 1 \, - \frac{\gamma}{2}\,[\frac{\pi}{2}+\frac{2}{\pi}] \; - \; \frac{\gamma^2}{8\pi^2}\,[\frac{\pi^4}{4}+4-\pi^2-\pi^2]\,. \tag{58}$$

The limit $x \to \infty$ of Tix's [12] approximation (53) is the same as for the estimate (45) of the linear term in γ introduced in the previous section. The critical value of γ is obtained from

$$1 \; - \; \frac{\gamma}{2}\left(\frac{\pi}{2}+\frac{2}{\pi}\right) \; - \; \frac{\gamma^2}{8}\left(\frac{\pi}{2}-\frac{2}{\pi}\right)^2 \; = \; 0 \tag{59}$$

and is given by $\gamma_{c_2} = 0.8368$. For $\gamma < \gamma_{c_2}$, the l.h.s. of (59) is positive. From (56) it therefore follows that $b_{l,\frac{1}{2},m} > 0$ for $\gamma < \gamma_{c_2}$.

For $s = -\frac{1}{2}$, we have in place of (54)

$$(f_\nu, (b_{0m} + b^{(1)}_{lsm} + b^{(2)}_{lsm})\, f_\nu)$$

$$\geq \; (f_\nu, (b_{0m} + b^{(1)}_{1,-\frac{1}{2},m})\, f_\nu) \; - \; \int_0^\infty \!\! \int_0^\infty dp\, dp' \, |\hat{f}_\nu(p)| \, b^{(2)}_{1,-\frac{1}{2},m}(p,p') |\hat{f}_\nu(p')|\,. \tag{60}$$

For the linear term, again a better estimate than the one given in (50) is needed. In contrast to (42), the factor $h(p)h(p')$ is kept in the kernel when applying the Lieb and Yau formula (33). Then

$$\int_0^\infty \!\! \int_0^\infty dpdp' \, |\hat{f}_\nu(p)| \, - b^{(1)}_{1,-\frac{1}{2},m}(p,p') \, |\hat{f}_\nu(p')| \; \leq \; \frac{\gamma}{\pi} \int_0^\infty dp \, |\hat{f}_\nu(p)|^2 A^2(p) \tag{61}$$

$$\cdot \left(\int_0^\infty \frac{p}{p'} dp' \, q_1\left(\frac{p}{p'}\right) \; + \; h(p) \int_0^\infty \frac{p}{p'} dp' \; h(p') \; q_0\left(\frac{p}{p'}\right) \right) \,.$$

The first of the integrals over p' equals $2p$ as before, and for the second one the substitution $z := p'/p$ and $p = mx$ are used. One finds

$$(f_\nu, b_{lsm} f_\nu) \;\geq\; \int_0^\infty dp\, |\hat{f}_\nu(p)|^2 \, e(p)\, \tilde{G}_{1-\frac{1}{2}}(x), \tag{62}$$

$$\tilde{G}_{1-\frac{1}{2}}(x) := \; 1 \;-\; \frac{\gamma}{\pi} x \left(\frac{\sqrt{x^2+1}+1}{x^2+1} \;+\; \frac{x^2}{2(x^2+1)}\, \tilde{J}_0(x) \right) \;-\; \frac{\gamma^2}{8\pi^2}\, x^4 \, \frac{\sqrt{x^2+1}+1}{x^2+1}$$

$$\cdot \left(\tilde{J}_1(x) \;+\; \frac{1}{\sqrt{x^2+1}+1}\, \tilde{J}_2(x) -\; \tilde{J}_3(x) \;-\; \frac{1}{\sqrt{x^2+1}+1}\, \tilde{J}_4(x) \right),$$

where $\tilde{J}_i(x), \quad i = 1, ..., 4$ is obtained from $\tilde{I}_i(x)$ by interchanging q_0 with q_1 everywhere, and

$$\tilde{J}_0(x) := \int_0^\infty dz\; q_0(z)\; \frac{1}{\sqrt{x^2z^2+1}+1}.$$

$\tilde{G}_{1-\frac{1}{2}}(x)$ is numerically found to decrease monotonically in x with its infimum (at ∞) again given by the r.h.s. of (58). Moreover, one always has $\tilde{G}_{1-\frac{1}{2}}(x) > \tilde{G}_{0\frac{1}{2}}(x)$. Thus $\tilde{G}_{1-\frac{1}{2}}(x) > 0$ if $\gamma < \gamma_{c_2}$ where γ_{c_2} is determined from $\inf_{x\in\mathbb{R}_+} \tilde{G}_{1-\frac{1}{2}}(x) = \lim_{x\to\infty} \tilde{G}_{1-\frac{1}{2}}(x) = 0$. This shows by means of (62) that $b_{l,-\frac{1}{2},m} > 0$ for $\gamma < \gamma_{c_2}$. Collecting results, we have $b_{lsm} > 0$ for $s = \pm\frac{1}{2}$ and $\gamma < \gamma_{c_2}$, which proves Proposition 2. □

The present proof of positivity by means of the Lieb and Yau formula cannot be extended to provide critical coupling constants beyond γ_{c_2}. This is lower than the Brown-Ravenhall critical coupling constant [4] $\tilde{\gamma}_c = 0.906$ $(Z \leq 124)$, derived from (58) by dropping the quadratic term.

A comparison of (59) with the defining equation of the critical coupling constant $\gamma_c = 1.006$ for $m = 0$ [2] reveals that these equations only differ in the sign of the quadratic term. This sign, however, has been made negative by force in the course of our proof in order to allow for the subsequent estimates. Hence we conjecture that also for $m \neq 0$, positivity holds for $\gamma < \gamma_c$ and not just for $\gamma < \gamma_{c_2}$.

Appendix

We derive an analytical expression for the difference $Q_l(x) - Q_{l+2s}(x)$ of the Legendre functions of the second kind for the limit $x \to 1$ from above.

From the representation of $Q_l(x)$ in terms of hypergeometric functions ${}_2F_1$ one has [5, p.999]

$$Q_l(1) \;=\; \lim_{x\to 1} \frac{\Gamma(l+1)\Gamma(\frac{1}{2})}{2^{l+1}\Gamma(l+\frac{3}{2})}\, x^{-l-1}\; {}_2F_1(\frac{l+2}{2}, \frac{l+1}{2}, l+\frac{3}{2}, \frac{1}{x^2})$$

$$=\; \lim_{z\to 1} \frac{\Gamma(l+1)\Gamma(\frac{1}{2})}{2^{l+1}\Gamma(\frac{l+2}{2})\Gamma(\frac{l+1}{2})}\; [2\psi(1) - \psi(\frac{l+2}{2}) - \psi(\frac{l+1}{2}) - \ln(1-z)]$$

with $z := 1/x^2$ where the continuation of the hypergeometric function near $z = 1$ in terms of Euler's psi function has been used [1, p.559].

From this representation, one obtains with the help of the functional equation for the gamma function, $\Gamma(x+1) = x\Gamma(x)$, in the case of $s = \frac{1}{2}$,

$$Q_l(1) - Q_{l+1}(1) \;=\; \frac{\Gamma(l+1)\Gamma(\frac{1}{2})}{2^{l+1}\Gamma(\frac{l+2}{2})\Gamma(\frac{l+1}{2})}\,[-\psi(\frac{l+1}{2}) + \psi(\frac{l+3}{2})]$$

since the logarithmic terms drop out. With the help of the functional equation for the psi function [5, p.945], $\psi(x+1) - \psi(x) = 1/x$, and the product formula for the gamma function [5, p.938] one finds

$$Q_l(1) - Q_{l+1}(1) \;=\; \frac{\Gamma(l+1)\Gamma(\frac{1}{2})}{2^{l}\Gamma(\frac{l+2}{2})\Gamma(\frac{l+1}{2})} \cdot \frac{1}{l+1} \;=\; \frac{1}{l+1}\,. \tag{63}$$

Reducing l by 1 one recovers from (63) the result for $s = -\frac{1}{2}$,

$$Q_l(1) \;-\; Q_{l-1}(1) \;=\; -\,\frac{1}{l}$$

which proves the assertions (14) and (15).

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