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On the point spectrum of a relativistic electron in an electric and magnetic field

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Abstract
A Mourre-type estimate is derived for the pseudorelativistic Brown–Ravenhall operator describing an atomic electron in a specific magnetic field of constant direction. As a consequence it is shown that its point spectrum is finite in $\mathbb{R}\backslash\{m\}$ if the Coulomb potential strength γ is below $\frac{1}{2}$. An extension of the Mourre-type estimate to the exact block-diagonalized Dirac operator is also discussed.

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1. Introduction

We consider a relativistic electron in the Coulomb field $V = -\gamma/x$ of a point nucleus with charge Z fixed at the origin (we have $\gamma = Ze^2$ with $e^2 \approx 1/137.04$ the fine structure constant). In addition, we allow for the presence of an external magnetic field, $\mathbf{B} = \nabla \times \mathbf{A}$ with vector potential $\mathbf{A}$. The electron is described by the Dirac operator (in relativistic units, $\hbar = c = 1$),

$$H = D_A + V, \qquad D_A = \boldsymbol{\alpha}(\mathbf{p} - e\mathbf{A}) + \beta m, \tag{1.1}$$

where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are Dirac matrices and m is the electron mass. $\mathbf{x}$ and $\mathbf{p}$ denote, respectively, the coordinate and the momentum of the electron, and $x = |\mathbf{x}|$ is the modulus of $\mathbf{x}$. H is defined in the Hilbert space $L_2(\mathbb{R}^3) \otimes \mathbb{C}^4$ [1].

It is well known that the spectrum of H extends to minus infinity because of the existence of the positronic states. There are, however, many situations where pair creation plays no role and where the negative continuum states can be disregarded. One of the current methods to get rid of these states, i.e. to remedy the unboundedness of H from below, is to work with pseudorelativistic no-pair operators instead. An operator of widespread interest is the Brown–Ravenhall operator [2–4] because it is simply the projection of H onto the electron's positive spectral subspace defined for $\gamma = 0$. This operator can be identified [5] as the first-order term (in γ) of the Douglas–Kroll series resulting from a unitary transformation scheme [6, 7] applied to H in order to decouple the spectral subspaces of electron and positron up to a given order in γ. An exact block diagonalization of H was recently achieved (for $\mathbf{A} = \mathbf{0}$) by Siedentop and Stockmeyer [8] who established the convergence of the Douglas–Kroll series for $\gamma \leqslant 0.38$.

If a (classical) magnetic field is admitted the investigations of the pseudorelativistic operators are scarce, in contrast to the multitude of studies concerning the Schrödinger or Pauli operators (for those see the comprehensive review by Erdös [9]). There are investigations on the stability of matter ([10], see also [11] for a pseudorelativistic scalar operator) as well as on the localization of the essential spectrum [12, 13] within the Brown–Ravenhall model. Some spectral analysis was also done for the Jansen–Hess operator (which is the second-order term of the Douglas–Kroll series [14]).

For a more detailed description of the spectrum of operators the Mourre estimate [15, 16] has proven to be a powerful tool. In the case of Schrödinger operators it was used to prove the absence of positive eigenvalues and the absence of the singular continuous spectrum (see e.g. [17]). It was also derived for Hamilton operators where the kinetic energy is a more general function of the particle momentum [18]. In all this work, the relative compactness of the potential with respect to the kinetic energy is an essential condition. For the pseudorelativistic operators matters are complicated by the fact that they enjoy only relative boundedness instead of relative compactness. It is shown below that for a pure Coulomb potential V (and some restrictions on the vector potential) a Mourre-type estimate can nevertheless be established in the single-particle case. However, bounds on the potential strength γ become necessary.

The paper is organized as follows. In section 2 the Brown–Ravenhall operator is introduced and the relevant boundedness properties are stated. The Mourre-type estimate for this operator (proposition 1) is derived in section 3 and is subsequently used to prove the absence of accumulation points of eigenvalues and of eigenvalues of infinite multiplicity in $\mathbb{R}\backslash\{m\}$ (theorem 1, section 4). The application of the Mourre-type estimate for related operators in the field-free case ($A = 0$) is discussed in section 5. In particular, the absence of eigenvalues above m (when $Z \leqslant 35$) is provided for the exact (block-diagonalized) Dirac operator (theorem 2). The paper is concluded with a remark on $A \neq 0$ results for this operator.

2. The Brown–Ravenhall operator and its boundedness properties

We start this section by introducing the Brown–Ravenhall operator H^{BR}, acting on the four-dimensional spinor space. Its derivation in terms of the above-mentioned projection or alternatively, from a unitary transformation scheme, exists in the literature for the case of $A = 0$ (see e.g. [3, 5, 7]). The inclusion of a magnetic field is straightforward [19, 14]. Thus we restrict ourselves to that part of the formalism which is necessary to introduce the quantities to be used in the subsequent estimates.

The first unitary transformation in the Douglas–Kroll scheme is the Foldy–Wouthuysen transformation $U_0 = A_E\big(1 + \beta\frac{\alpha(\mathbf{p}-e\mathbf{A})}{E_A+m}\big)$ with $A_E = \big(\frac{E_A+m}{2E_A}\big)^{1/2}$. Its application to H block diagonalizes the kinetic part D_A and results in [6]

$$\begin{aligned} &U_0 H U_0^{-1} = \beta E_A + \mathcal{E}_1 + \mathcal{O}_1 \\ &E_A := |D_A| = \sqrt{(\mathbf{p} - e\mathbf{A})^2 - e\boldsymbol{\sigma}\mathbf{B} + m^2} \geqslant m \\ &\mathcal{E}_1 := U_0 \tfrac{1}{2}(V + \tilde{D}_A V \tilde{D}_A) U_0^{-1}, \qquad \mathcal{O}_1 := U_0 \tfrac{1}{2}(V - \tilde{D}_A V \tilde{D}_A) U_0^{-1}, \end{aligned} \tag{2.1}$$

where $\tilde{D}_A = D_A/E_A$ and $\boldsymbol{\sigma}$ is the vector of Pauli matrices. We note that the transformed potential, $U_0 V U_0^{-1} = \mathcal{E}_1 + \mathcal{O}_1$, has been separated into its (block) diagonal term $\mathcal{E}_1$ and the off-diagonal term $\mathcal{O}_1$. We also recall that $E_A^2 - m^2 = (\boldsymbol{\sigma}(\mathbf{p} - e\mathbf{A}))^2$ is the Pauli operator. The Brown–Ravenhall operator is defined by the diagonal part of (2.1) projected onto its upper block,

$$H^{\mathrm{BR}} = \frac{1+\beta}{2} U_0 H U_0^{-1} \frac{1+\beta}{2} = \frac{1+\beta}{2} (E_A + \mathcal{E}_1) \frac{1+\beta}{2} \tag{2.2}$$

where $\beta^2 = 1$ is used.

Since by construction, H^{BR} is a 4×4 matrix-valued operator with only one 2×2 entry, termed h^{BR}, i.e. $H^{\mathrm{BR}} = \left(\begin{smallmatrix} h^{\mathrm{BR}} & 0 \\ 0 & 0 \end{smallmatrix}\right)$, it is often convenient to work in the reduced two-dimensional spinor space instead. This is done by setting $\varphi := \left(\begin{smallmatrix} u \\ 0 \end{smallmatrix}\right)$ with a two-spinor u and identifying [3, 7]

$$(u, h^{\mathrm{BR}} u) = (\varphi, H^{\mathrm{BR}} \varphi). \tag{2.3}$$

The analysis of an operator which can be decomposed into a kinetic and a potential part is considerably simplified if the potential is controlled by the kinetic part (allowing for a 'perturbative' treatment of the potential). This control is expressed by means of the relative boundedness (or form boundedness) of the potential with respect to the kinetic part with bound less than one. It guarantees a self-adjoint extension of the operator when its kinetic part has this property.

For example, we may consider $e\boldsymbol{\sigma}\mathbf{B}$ in (2.1) as a potential added to the Schrödinger kinetic energy $(\mathbf{p} - e\mathbf{A})^2$. Let us assume that $\mathbf{A} \in L_{2,\mathrm{loc}}(\mathbb{R}^3)$ and $\int_{|\mathbf{x}-\mathbf{y}|\leqslant 1} |\mathbf{B}(\mathbf{y})|^2 \,\mathrm{d}\mathbf{y} < \infty$ for $\mathbf{x} \in \mathbb{R}^3$ such that $\mathbf{B}$ is $(\mathbf{p} - e\mathbf{A})^2$-bounded with bound zero [20]. Then E_A with domain $\mathcal{D}(E_A) = H_1(\mathbb{R}^3) \otimes \mathbb{C}^4$ (where H_r denotes the Sobolev spaces) extends to a self-adjoint operator in $L_2(\mathbb{R}^3) \otimes \mathbb{C}^4$ [21, 14]. The condition on $\mathbf{B}$ at infinity can, however, be avoided if $\mathbf{A} \in L_{3,\mathrm{loc}}(\mathbb{R}^3)$ [1, p 113, notes 4.3] or if $\mathbf{A}$ is a C^2-function (according to the theory of first-order elliptic differential operators [22, p 54, 112, problem 45]). This relies on the fact that the self-adjointness of the Dirac operator D_A is transferred to $E_A = \sqrt{D_A^2}$.

Turning to the Brown–Ravenhall operator which can be split according to $H^{\mathrm{BR}} =: T_A + V_A$ we have the kinetic part $T_A = \frac{1+\beta}{2} E_A \frac{1+\beta}{2}$ related to E_A and the potential part V_A according to (2.2). The T_A-boundedness of V_A will be needed explicitly in the proof of theorem 1 once the Mourre-type estimate has been established. In order to show this boundedness property we will use estimates which rely on the diamagnetic inequality and on the relative boundedness of the potential in the $A = 0$ case. For $\psi \in L_2(\mathbb{R}^3)$ and $\mathbf{A} \in L_{2,\mathrm{loc}}(\mathbb{R}^3)$, the diamagnetic inequality estimates the Schrödinger-type operator $S_A^2 = (\mathbf{p} - e\mathbf{A})^2 + m^2$ by the field-free $(A = 0)$ kinetic energy operator $E_p^2 = p^2 + m^2$ (with $p = |\mathbf{p}|$) in the following way, $\left|\left(\mathrm{e}^{-tS_A^2}\psi\right)(\mathbf{x})\right| \leqslant \left(\mathrm{e}^{-tE_p^2}|\psi|\right)(\mathbf{x})$ ([23, 24], see also [21] and references therein). Using the integral representations $\mathrm{e}^{-t\tilde{A}} = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{\mathrm{d}\tau}{\sqrt{\tau}} \,\mathrm{e}^{-\tau}\, \mathrm{e}^{-(t^2/4\tau)\tilde{A}^2}$ [11] and $\tilde{A}^{-1} = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-t\tilde{A}}$ we get as an immediate consequence,

$$\left| \left(\frac{1}{S_A^{2/n}} \psi \right)(\mathbf{x}) \right| \leqslant \left(\frac{1}{E_p^{2/n}} |\psi| \right)(\mathbf{x}), \qquad n = 2^{\tilde{m}}, \quad \tilde{m} = 0, 1, \ldots. \tag{2.4}$$

For the sake of demonstration we give the proof of (2.4) when $\tilde{m} = 0$:

$$\begin{aligned} \left| \left(\frac{1}{S_A^2} \psi \right)(\mathbf{x}) \right| &= \left| \int_0^\infty \mathrm{d}t \left(\mathrm{e}^{-tS_A^2}\psi\right)(\mathbf{x}) \right| \leqslant \int_0^\infty \mathrm{d}t \left| \left(\mathrm{e}^{-tS_A^2}\psi\right)(\mathbf{x}) \right| \\ &\leqslant \int_0^\infty \mathrm{d}t \left(\mathrm{e}^{-tE_p^2}|\psi|\right)(\mathbf{x}) = \left(\frac{1}{E_p^2} |\psi| \right)(\mathbf{x}). \end{aligned} \tag{2.5}$$

For $\tilde{m} > 0$ we choose $\tilde{A} := S_A^{2/n}$ and proceed by successively applying the first integral representation until we arrive at $\mathrm{e}^{-\tilde{t}S_A^2}$ (with some $\tilde{t}$). After having used the diamagnetic inequality all integrals are performed in the reversed order.

Let $f > 0$ be a function in coordinate space such that $f E_p^{-2/n}$ is bounded by c_n. Then from (2.4) $f S_A^{-2/n}$ has the same bound (which is a generalization of [21, theorem 2.4]),

$$\left\| f \frac{1}{S_A^{2/n}} \psi \right\|^2 \leqslant \left\| f \frac{1}{E_p^{2/n}} |\psi| \right\|^2 \leqslant c_n^2 \|\psi\|^2. \tag{2.6}$$

Choosing $f(\mathbf{x}) = \frac{1}{x}$, $n = 2$ and $f(\mathbf{x}) = \frac{1}{\sqrt{x}}$, $n = 4$, respectively, and taking $\varphi_1 = S_A^{-1}\psi$ and $\varphi_2 = S_A^{-1/2}\psi$, (2.6) leads to the estimates (upon using the Hardy and Kato inequalities for c_n),

$$\begin{aligned} &\|V\varphi_1\| \leqslant 2\gamma \|\sqrt{(\mathbf{p} - e\mathbf{A})^2 + m^2}\varphi_1\| \\ &(\varphi_2, V\varphi_2) \leqslant \frac{\gamma\pi}{2}(\varphi_2, \sqrt{(\mathbf{p} - e\mathbf{A})^2 + m^2}\varphi_2). \end{aligned} \tag{2.7}$$

We note that these estimates are readily extended to several particles since the diamagnetic inequality holds in arbitrary dimension ν [25, p 163]. Considering for example two particles (denoted by $k = 1, 2$ such that $\nu = 6$) and choosing $f(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|^{1/2}}$, $n = 4$, one obtains for $\varphi \in H_{1/2}(\mathbb{R}^6)$,

$$\begin{aligned} \left(\varphi, \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|}\varphi\right) &\leqslant c_4^2 \left(\varphi, \sqrt{\sum_{k=1}^2 (\mathbf{p}_k - e\mathbf{A}(\mathbf{x}_k))^2 + 2m^2}\varphi\right) \\ &\leqslant c_4^2 \left(\varphi, \sum_{k=1}^2 \sqrt{(\mathbf{p}_k - e\mathbf{A}(\mathbf{x}_k))^2 + m^2}\varphi\right) \end{aligned} \tag{2.8}$$

with $c_4^2 = \frac{\pi}{2}$ from the estimate (see e.g. [12])

$$\left(\varphi, \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|}\varphi\right) \leqslant \frac{\pi}{2}(\varphi, p_1\varphi) \leqslant \frac{\pi}{2}(\varphi, \sqrt{p_1^2 + p_2^2 + 2m^2}\varphi). \tag{2.9}$$

All these estimates also hold for $m = 0$.

For later use (in the proof of the Mourre-type estimate) we mention that the inclusion of a magnetic field preserves compactness [17, p 117]. This is also a consequence of the diamagnetic inequality and may be shown as follows. Let us assume that $f \frac{1}{E_p^{2/n}}$ is compact, i.e. f is $E_p^{2/n}$-bounded with bound zero. From (2.6) it follows that f is also $S_A^{2/n}$-bounded with bound zero. Lemma 11.5 from [26] implies that if in addition, $\left\|\chi_R f \frac{1}{S_A^{2/n}}\right\| \to 0$ as $R \to \infty$ (where χ_R is the characteristic function on the set $\{x \in \mathbb{R}^3 : |x| > R\}$) then $f \frac{1}{S_A^{2/n}}$ is compact[1].

Assume $f \to 0$ as $x \to \infty$. From (2.6) with f replaced by $\chi_R f$ we have indeed

$$\left\|\chi_R f \frac{1}{S_A^{2/n}}\right\| \leqslant \left\|\chi_R f \frac{1}{E_p^{2/n}}\right\| \leqslant \|\chi_R f\| \left\|\frac{1}{E_p^{2/n}}\right\| \to 0 \tag{2.10}$$

as $R \to \infty$ since $E_p^{-2/n} \leqslant m^{-2/n}$ is bounded and since $|\chi_R f| < \epsilon$ is arbitrarily small for R sufficiently large.

Let us in the following consider only bounded magnetic fields $\mathbf{B}$, i.e. $B = |\mathbf{B}| \leqslant B_0$ and derive the T_A-boundedness of V_A for that case. With $\beta E_A = E_A\beta$ (because E_A is block diagonal) and $\varphi = \binom{u}{0} \in H_1(\mathbb{R}^3) \otimes \mathbb{C}^4$ we have $\|T_A\varphi\| = \|E_A\varphi\|$. Since U_0 and $\tilde{D}_A$ have norm unity,

$$\|V_A\varphi\| = \left\|\frac{1+\beta}{2}\mathcal{E}_1\frac{1+\beta}{2}\varphi\right\| \leqslant \frac{1}{2}\left\|VU_0^{-1}\varphi\right\| + \frac{1}{2}\left\|V\tilde{D}_A U_0^{-1}\varphi\right\|. \tag{2.11}$$

[1] Estimates (2.7)–(2.10) should replace the estimates in [14, 12] derived from the inequality $(\varphi_1, p^2\varphi_1) \leqslant (\varphi_1, (\mathbf{p} - e\mathbf{A})^2\varphi_1)$ which is not generally valid [24]. The results given in these papers are not affected.

From (2.7) one easily obtains [14] $\|V\tilde{\varphi}\| \leqslant 2\gamma\|E_A\tilde{\varphi}\| + 2\gamma\sqrt{eB_0}\|\tilde{\varphi}\|$. Also, E_A commutes with $\tilde{D}_A$ and with U_0. In fact, we can decompose the commutator $[U_0, E_A] = A_E[\beta, E_A]\frac{\boldsymbol{\alpha}(\mathbf{p}-e\mathbf{A})}{E_A+m} + A_E\beta\frac{1}{E_A+m}[\boldsymbol{\alpha}(\mathbf{p}-e\mathbf{A}), E_A]$. We have $[\beta, E_A] = 0$ and so $[\boldsymbol{\alpha}(\mathbf{p}-e\mathbf{A}), E_A] = [D_A, E_A] - m[\beta, E_A] = 0$. Thus, setting $\tilde{\varphi} = U_0^{-1}\varphi$ and, respectively, $\tilde{\varphi} = \tilde{D}_A U_0^{-1}\varphi$ we get

$$\|V_A\varphi\| \leqslant 2\gamma\|E_A\varphi\| + 2\gamma\sqrt{eB_0}\|\varphi\|. \tag{2.12}$$

It follows that V_A is E_A-bounded and thus T_A-bounded with bound smaller than one if $\gamma < \frac{1}{2}$, implying $\mathcal{D}(H^{\mathrm{BR}}) = \mathcal{D}(E_A) = H_1(\mathbb{R}^3)\otimes\mathbb{C}^4$. We note that this bound is more restrictive than the respective form bound, $\gamma < \frac{2}{\pi}$ [10, 14], necessary to guarantee the self-adjointness of H^{BR} by means of the Friedrichs extension.

It is also possible to show the E_A-boundedness of V_A without a constant term on the rhs. This fact relies on an estimate introduced by Balinsky *et al* [27] which relates the Schrödinger operator to the Pauli operator (when zero-modes are absent). That estimate is extended in [12, lemma 7] for any $\mathbf{A} \in L_{2,\mathrm{loc}}(\mathbb{R}^3)$ to

$$\begin{aligned} &E_A^2 \geqslant \delta_m^2(B)[(\mathbf{p}-e\mathbf{A})^2 + m^2] = \delta_m^2(B)S_A^2,\\ &\delta_m(B) = \inf_{\|\varphi\|=1}\|(1-S_m^*S_m)\varphi\| \end{aligned} \tag{2.13}$$

with $S_m := (eB)^{\frac{1}{2}}\left(E_A^2 + eB\right)^{-\frac{1}{2}}$ and where $0 < \delta_m(B) \leqslant 1$. When $\|\mathbf{B}\|_\infty = B_0$, one can make use of $S_mS_m^* = eB^{\frac{1}{2}}\frac{1}{E_A^2+eB}B^{\frac{1}{2}} \leqslant \frac{eB}{m^2+eB} \leqslant \frac{eB_0}{m^2+eB_0}$. This leads to an improved lower bound, $\frac{m^2}{m^2+eB_0} \leqslant \delta_m(B) \leqslant 1$.

One obtains from (2.7) and (2.13),

$$\|V\varphi\| \leqslant \frac{2\gamma}{\delta_m(B)}\|E_A\varphi\|, \tag{2.14}$$

which results in $\|V_A\varphi\| \leqslant \frac{2\gamma}{\delta_m(B)}\|E_A\varphi\|$ in place of (2.12). Note that one has to pay for the omission of the constant term by an inferior bound, $\gamma < \frac{1}{2}\delta_m(B)$.

3. The Mourre-type estimate for the Brown–Ravenhall operator

The Mourre estimate tells us that a suitable commutator of an (unbounded) operator is strictly positive in a given spectral interval Δ, apart from some compact remainder. As a consequence, the operator will not have eigenvalues accumulating in that interval. It is the aim of this section to derive such an estimate for h^{BR} with a slight weakening of the compactness condition.

Proposition 1. *Let h^{BR} be the Brown–Ravenhall operator with magnetic field of constant direction generated by a vector potential $\mathbf{A}$ satisfying*

(i) $\mathbf{A} \in L_{2,\mathrm{loc}}(\mathbb{R}^3)$, $\nabla\cdot\mathbf{A} = 0$;
(ii) $\nabla\times\mathbf{A}$ *bounded and continuous;*
(iii) $f_A := \boldsymbol{\alpha}e\mathbf{A} + e(\mathbf{x}\nabla)(\boldsymbol{\alpha}\mathbf{A})$ *as a function of* $\mathbf{x}$ *bounded,* $(E_A+\mu)^{-1}f_A(E_A+\mu)^{-1}$ *compact for some* $\mu \geqslant 0$.

Let E_Δ be the spectral projection for h^{BR} onto an open interval $\Delta \subset \mathbb{R}$. Then there exists a constant $\alpha_0 > 0$ and an operator k_A with $(E_A+\mu)^{-1}k_A(E_A+\mu)^{-1}$ compact such that for $m \notin \Delta$,

$$E_\Delta \mathrm{i}[h^{\mathrm{BR}}, a_A]E_\Delta \geqslant \alpha_0 E_\Delta + E_\Delta k_A E_\Delta \tag{3.1}$$

where $[h^{\mathrm{BR}}, a_A] = h^{\mathrm{BR}}a_A - a_Ah^{\mathrm{BR}}$ is the commutator with a suitably chosen self-adjoint operator a_A.

We note that all assumptions are satisfied if $\mathbf{A} \in C^1(\mathbb{R}^3)$ with $A \to 0$ as $x \to \infty$ and with $\operatorname{div} \mathbf{A} = 0$. Then $\mathbf{A}$ and its derivative are bounded, and also f_A is bounded and vanishes at infinity. This assures the compactness of $f_A(E_p + \mu)^{-1}$ and thus of $f_A(E_A + \mu)^{-1} = f_A(S_A + \mu)^{-1} \cdot (S_A + \mu)(E_A + \mu)^{-1}$ for $\mu \geqslant 0$ due to (2.10) and (2.13).

We shall construct the operator a_A from the generator $\mathcal{A}$ of dilations (which is used in the Mourre estimate for Schrödinger operators), recalling that $\mathbf{p} = -\mathrm{i}\boldsymbol{\nabla}$ and $\mathbf{px} = \mathbf{xp} - 3\mathrm{i}$,

$$\mathcal{A} = \frac{1}{2}(\mathbf{xp} + \mathbf{px}) = \mathbf{xp} - \frac{3\mathrm{i}}{2}. \tag{3.2}$$

The domain of $\mathcal{A}$ is $C_0^\infty(\mathbb{R}^3)$. One easily verifies, using the invariance $\mathrm{i}[\boldsymbol{\alpha}\mathbf{p} + V, \mathcal{A}] = \boldsymbol{\alpha}\mathbf{p} + V$, the commutator relation for the Dirac operator (1.1),

$$\mathrm{i}[H, \mathcal{A}] = H - \beta m + \boldsymbol{\alpha} e\mathbf{A} + e(\mathbf{x}\boldsymbol{\nabla})(\boldsymbol{\alpha}\mathbf{A}). \tag{3.3}$$

In order to derive the commutator of h^{BR} we apply the Foldy–Wouthuysen transformation U_0 to this equation. Then, separating $U_0 H U_0^{-1}$ from (2.1) into its block-diagonal and off-diagonal part, i.e. $U_0 H U_0^{-1} = \tilde{H}^{\mathrm{BR}} + \mathcal{O}_1$ with $\tilde{H}^{\mathrm{BR}} := \beta E_A + \mathcal{E}_1$, we get

$$\begin{aligned} &\mathrm{i}[\tilde{H}^{\mathrm{BR}}, A_U] + \mathrm{i}[\mathcal{O}_1, A_U] = \tilde{H}^{\mathrm{BR}} + \mathcal{O}_1 - mC_1 + U_0 f_A U_0^{-1}, \\ &A_U := U_0 \mathcal{A} U_0^{-1}, \end{aligned} \tag{3.4}$$

where the domain of A_U is $M_A := \left\{U_0\varphi : \varphi \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4\right\}$ and f_A is defined in proposition 1. The operator $C_1 := U_0 \beta U_0^{-1}$ is unitary and self-adjoint, $C_1^* C_1 = C_1^2 = 1$. From the block structure of the matrix-valued symmetric operators,

$$\tilde{H}^{\mathrm{BR}} = \begin{pmatrix} h^{\mathrm{BR}} & 0 \\ 0 & h_{22} \end{pmatrix}, \qquad A_U = \begin{pmatrix} a_{11} & a_{12} \\ a_{12}^* & a_{22} \end{pmatrix}, \qquad \mathcal{O}_1 = \begin{pmatrix} 0 & o_{12} \\ o_{12}^* & 0 \end{pmatrix}, \tag{3.5}$$

we obtain the upper left block of (3.4) in the following form:

$$\begin{aligned} &\mathrm{i}[h^{\mathrm{BR}}, a_{11}] = h^{\mathrm{BR}} - mc_{11} + k_A, \\ &k_A := \left(U_0 f_A U_0^{-1}\right)_{11} - \mathrm{i}[\mathcal{O}_1, A_U]_{11}, \end{aligned} \tag{3.6}$$

where $c_{11} = (C_1)_{11}$ and the subscript 11 denotes the respective upper left block. From (3.6) it follows that $\tilde{B} := \mathrm{i}[h^{\mathrm{BR}}, a_{11}] - h^{\mathrm{BR}} - k_A = -mc_{11}$ is a bounded operator. Thus for $\psi \in L_2(\mathbb{R}^3) \otimes \mathbb{C}^2$, using that c_{11} is self-adjoint and bounded by 1 (since C_1 is), we have the estimate

$$(\psi, \tilde{B}\psi) = -m(\psi, c_{11}\psi) \geqslant -m|(\psi, c_{11}\psi)| \geqslant -m(\psi, \psi) \tag{3.7}$$

such that $\tilde{B} \geqslant -m$. Applying E_Δ to this inequality we get

$$E_\Delta \mathrm{i}[h^{\mathrm{BR}}, a_{11}] E_\Delta \geqslant E_\Delta (h^{\mathrm{BR}} - m) E_\Delta + E_\Delta k_A E_\Delta. \tag{3.8}$$

In order to prove the Mourre-type estimate (3.1), identifying a_A with a_{11}, we first have to show the compactness of $(E_A + \mu)^{-1} k_A (E_A + \mu)^{-1}$. We recall that U_0 commutes with E_A such that $(E_A + \mu)^{-1} U_0 f_A U_0^{-1} (E_A + \mu)^{-1}$ is compact by assumption (iii) which is then also true for its upper left block.

The compactness of $(E_A + \mu)^{-1} \mathrm{i}[\mathcal{O}_1, A_U](E_A + \mu)^{-1}$ is proven in the following way. From (2.1) and (3.2) we have

$$\begin{aligned} \mathrm{i}[\mathcal{O}_1, A_U] &= \frac{\mathrm{i}}{2} U_0 [V - \tilde{D}_A V \tilde{D}_A, \mathbf{xp}] U_0^{-1} \\ &= \frac{1}{2} U_0 (V - \mathrm{i}[\tilde{D}_A, \mathbf{xp}] V \tilde{D}_A - \tilde{D}_A V \tilde{D}_A - \tilde{D}_A V \mathrm{i}[\tilde{D}_A, \mathbf{xp}]) U_0^{-1}. \end{aligned} \tag{3.9}$$

Since E_A commutes with $\tilde{D}_A$, the compactness concerning the first and third terms is easily shown. In fact,

$$\frac{1}{E_A+\mu}U_0(V-\tilde{D}_A V\tilde{D}_A)U_0^{-1}\frac{1}{E_A+\mu}$$
$$= -\gamma U_0\left(\frac{1}{E_A+\mu}\frac{1}{x}\frac{1}{E_A+\mu} - \tilde{D}_A\frac{1}{E_A+\mu}\frac{1}{x}\frac{1}{E_A+\mu}\tilde{D}_A\right)U_0^{-1}. \tag{3.10}$$

As $\frac{1}{x^{1/2}}(E_p+\mu)^{-1}$ is a compact operator according to Herbst [28], the operator $(E_A+\mu)^{-1}\frac{1}{x^{1/2}}\frac{1}{x^{1/2}}(E_A+\mu)^{-1}$ is compact (by (2.10) and (2.13)) and thus (3.10) represents a compact operator.

The fourth term in (3.9) is the Hermitean conjugate of the second term and thus need not be discussed separately. From (3.3) and $\tilde{D}_A = D_A\frac{1}{E_A}$ we have

$$\mathrm{i}[\tilde{D}_A, \mathbf{xp}] = (D_A(m=0)+f_A)\frac{1}{E_A} + \mathrm{i}D_A\left[\frac{1}{E_A}, \mathbf{xp}\right] \tag{3.11}$$

where $D_A(m=0) = \boldsymbol{\alpha}(\mathbf{p}-e\mathbf{A})$. The first term of (3.11), inserted into the second term of (3.9), leads to the following operator,

$$K_1 := \frac{\gamma}{2}U_0\frac{1}{E_A+\mu}(D_A(m=0)+f_A)\left\{\frac{1}{E_A}\frac{1}{x}\frac{1}{E_A+\mu}\right\}\tilde{D}_A U_0^{-1}. \tag{3.12}$$

$E_A^{-1}\frac{1}{x}(E_A+\mu)^{-1}$ is compact as discussed above. $(E_A+\mu)^{-1}D_A(m=0)$ is bounded as is f_A according to the assumption (iii). Thus K_1 is compact.

The remaining term K_2, arising from the commutator contribution in (3.11), can be cast into the form

$$K_2 := \frac{\gamma}{2}\left(U_0\frac{1}{E_A+\mu}D_A\right)\mathrm{i}\left[\frac{1}{E_A}, \mathbf{xp}\right]E_A\left\{\frac{1}{E_A}\frac{1}{x}\frac{1}{E_A+\mu}\right\}\left(\tilde{D}_A U_0^{-1}\right) \tag{3.13}$$

where the operators in round brackets are bounded and in curly brackets compact. K_2 is compact if $\mathrm{i}\left[\frac{1}{E_A}, \mathbf{xp}\right]E_A = -\frac{\mathrm{i}}{E_A}[E_A, \mathbf{xp}]$ is bounded. (For $A=0$ this is trivial since $\mathrm{i}[E_p^{-1}, \mathbf{xp}] = -p^2/E_p^3$.) In order to show this we express the commutator in terms of $[D_A, \mathbf{xp}]$ which is known from (3.3). We use a formula [29, (C.1.4)] generalized to positive self-adjoint operators $\tilde{A}$,

$$[\mathrm{e}^{-t\tilde{A}}, \tilde{B}] = -t\int_0^1 \mathrm{d}\tau\, \mathrm{e}^{-\tau t\tilde{A}}[\tilde{A}, \tilde{B}]\,\mathrm{e}^{-(1-\tau)t\tilde{A}}, \tag{3.14}$$

where $\tilde{B}$ is self-adjoint and $t \geqslant 0$. This formula is obtained with the help of the formal derivative of $\tilde{B}(\tau) := \mathrm{e}^{-\tau t\tilde{A}}\tilde{B}\,\mathrm{e}^{\tau t\tilde{A}}\,\mathrm{e}^{-t\tilde{A}}$ for $0<\tau<1$ which subsequently is integrated.

We will also need a heat kernel estimate, proven in the Schrödinger case for magnetic fields of constant direction by Loss and Thaller [30]. It concerns the estimate of the kernel of $\mathrm{e}^{-tE_A^2}$ by the respective kernel of the field-free operator. This kernel is given by $\mathrm{e}^{-t(p^2+m^2)}(\mathbf{x},\mathbf{x}') = (4\pi t)^{-\frac{3}{2}}\,\mathrm{e}^{-(\mathbf{x}-\mathbf{x}')^2/4t}\,\mathrm{e}^{-tm^2}$ (see e.g. [25, p 161] for $m=0$), with the important property that it is positive.

Proposition 2. *Let* $\mathbf{B}(\mathbf{x})$ *with* $0 < B(\mathbf{x}) \leqslant B_0$ *be a continuous magnetic field of constant direction. Then the heat kernel of* E_A^2 *satisfies the following bound,*

$$\left|\mathrm{e}^{-tE_A^2}(\mathbf{x},\mathbf{x}')\right| \leqslant \frac{1}{\sqrt{4\pi t}}\frac{eB_0}{4\pi\,\sinh(eB_0 t)}\,\mathrm{e}^{-(\mathbf{x}-\mathbf{x}')^2/(4t)}\,\mathrm{e}^{eB_0 t}\,\mathrm{e}^{-m^2 t}. \tag{3.15}$$

As a consequence,

$$\left|\mathrm{e}^{-tE_A^2}(\mathbf{x},\mathbf{x}')\right| \leqslant c(B_0)\,\mathrm{e}^{-t\tilde{E}_p^2}(\mathbf{x},\mathbf{x}') \tag{3.16}$$

where $\tilde{E}_p := \sqrt{p^2+(m-\epsilon)^2}$ *with* $0<\epsilon<m$.

The proof of (3.15) is indicated in appendix A. The step from (3.15) to (3.16) follows from $\frac{eB_0 t\, \mathrm{e}^{eB_0 t}}{\sinh(eB_0 t)} \leqslant 1 + 2eB_0 t$ and $t\,\mathrm{e}^{-m^2 t} \leqslant c\,\mathrm{e}^{-(m-\epsilon)^2 t}$.

Let us proceed with the boundedness proof of $\frac{\mathrm{i}}{E_A}[E_A, \mathbf{xp}]$. We write $E_A = \lim_{t\to 0}\big(1 - \mathrm{e}^{-tE_A^2}\big)\big/(tE_A)$ and apply the integral representation [21] $E_A^{-1} = \pi^{-1/2}\int_0^\infty \mathrm{d}\tau\,\tau^{-1/2}\,\mathrm{e}^{-\tau E_A^2}$. Then, with (3.14) as well as $E_A^2 = D_A^2$,

$$
\begin{aligned}
\mathrm{i}[E_A, \mathbf{xp}] &= \lim_{t\to 0}\frac{1}{\sqrt{\pi}}\frac{1}{t}\int_0^\infty \frac{\mathrm{d}\tau}{\sqrt{\tau}}\big(\mathrm{i}\big[\mathrm{e}^{-\tau E_A^2}, \mathbf{xp}\big] - \mathrm{i}\big[\mathrm{e}^{-(t+\tau)E_A^2}, \mathbf{xp}\big]\big) \\
&= -\lim_{t\to 0}\frac{1}{\sqrt{\pi}}\frac{1}{t}\int_0^\infty \frac{\mathrm{d}\tau}{\sqrt{\tau}}(\tau I_1 - tI_2)
\end{aligned}
\tag{3.17}
$$

where

$$
\begin{aligned}
I_1 &:= \int_0^1 \mathrm{d}\mu\,\mathrm{e}^{-\mu\tau E_A^2}\big(\mathrm{i}\big[D_A^2, \mathbf{xp}\big]\,\mathrm{e}^{-(1-\mu)\tau E_A^2} - \mathrm{e}^{-\mu t E_A^2}\mathrm{i}\big[D_A^2, \mathbf{xp}\big]\,\mathrm{e}^{-(1-\mu)(t+\tau)E_A^2}\big) \\
I_2 &:= \int_0^1 \mathrm{d}\mu\,\mathrm{e}^{-\mu(t+\tau)E_A^2}\mathrm{i}\big[D_A^2, \mathbf{xp}\big]\,\mathrm{e}^{-(1-\mu)(t+\tau)E_A^2}.
\end{aligned}
\tag{3.18}
$$

From (3.3) we have $\mathrm{i}\big[D_A^2, \mathbf{xp}\big] = (D_A(m=0) + f_A)D_A + D_A(D_A(m=0) + f_A)$ which consists of four summands, each of which will be treated separately.

The boundedness resulting from $(a) D_A(m=0)D_A$ is easily obtained since this operator commutes with E_A. Using that $\lim_{t\to 0}\frac{1}{t}(f(0) - f(t)) = -f'(0)$ we get for the contribution (a) to the commutator,

$$
\lim_{t\to 0}\frac{1}{t}(\tau I_1 - tI_2)_{(a)} = D_A(m=0)D_A\,\mathrm{e}^{-\tau E_A^2}\big(\tau E_A^2 - 1\big)
\tag{3.19}
$$

such that $\frac{\mathrm{i}}{E_A}[E_A, \mathbf{xp}]_{(a)} = \frac{D_A(m=0)D_A}{2E_A^2}$ is bounded. The same holds true when $D_A(m=0)D_A$ is replaced by $(b) D_A D_A(m=0)$.

For the term $(c) D_A f_A$ we first study the contribution from I_2 and define the operator

$$
\mathcal{O}_a := \frac{D_A}{E_A\sqrt{\pi}}\int_0^\infty \frac{\mathrm{d}\tau}{\sqrt{\tau}}\int_0^1 \mathrm{d}\mu\,\mathrm{e}^{-\mu\tau E_A^2} f_A\,\mathrm{e}^{-(1-\mu)\tau E_A^2},
\tag{3.20}
$$

and prove the boundedness of $\mathcal{O}_a^*$. Using the representation of $\mathrm{e}^{-\mu\tau E_A^2}$ by its kernel together with proposition 2 we obtain for $\tilde{\varphi} := \tilde{D}_A\varphi \in L_2(\mathbb{R}^3)\otimes\mathbb{C}^4$,

$$
\begin{aligned}
|(\mathcal{O}_a^*\varphi)(\mathbf{x})| &\leqslant \frac{1}{\sqrt{\pi}}\int_0^\infty \frac{\mathrm{d}\tau}{\sqrt{\tau}}\int_0^1 \mathrm{d}\mu\int_{\mathbb{R}^6}\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{y}'\big|\mathrm{e}^{-(1-\mu)\tau E_A^2}(\mathbf{x},\mathbf{y})\big||f_A(\mathbf{y})|\cdot\big|\mathrm{e}^{-\mu\tau E_A^2}(\mathbf{y},\mathbf{y}')\big||\tilde{\varphi}(\mathbf{y}')| \\
&\leqslant \frac{c^2(B_0)}{\sqrt{\pi}}\|f_A\|_\infty\int_0^\infty \frac{\mathrm{d}\tau}{\sqrt{\tau}}\int_0^1 \mathrm{d}\mu\int_{\mathbb{R}^3}\mathrm{d}\mathbf{y}'\,\mathrm{e}^{-\tau\tilde{E}_p^2}(\mathbf{x},\mathbf{y}')|\tilde{\varphi}(\mathbf{y}')| \\
&= \tilde{c}\left(\frac{1}{\tilde{E}_p}|\tilde{\varphi}|\right)(\mathbf{x})
\end{aligned}
\tag{3.21}
$$

with some B_0-dependent constant $\tilde{c}$. Therefore $\|\mathcal{O}_a^*\varphi\| \leqslant \tilde{c}\big\|\frac{1}{\tilde{E}_p}\big\|\|\tilde{D}_A\varphi\| \leqslant \tilde{C}\|\varphi\|$, which implies that also $\mathcal{O}_a$ is bounded.

Let us now investigate the contribution from I_1 which can be expressed as a sum of two operators, using that $\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{-\mu(t+\tau)E_A^2}|_{t=0} = -\mu E_A^2\,\mathrm{e}^{-\mu\tau E_A^2}$,

$$
\begin{aligned}
\mathcal{O}_{b_1} + \mathcal{O}_{b_2} := \frac{D_A}{E_A\sqrt{\pi}}\int_0^\infty \sqrt{\tau}\,\mathrm{d}\tau\int_0^1 \mathrm{d}\mu\big(\mu E_A^2\,\mathrm{e}^{-\mu\tau E_A^2} f_A\,\mathrm{e}^{-(1-\mu)\tau E_A^2} \\
+\,\mathrm{e}^{-\mu\tau E_A^2} f_A(1-\mu)E_A^2\,\mathrm{e}^{-(1-\mu)\tau E_A^2}\big).
\end{aligned}
\tag{3.22}
$$

For $\mathcal{O}_{b_1}$ we obtain the estimate, taking $\varphi, \psi \in L_2(\mathbb{R}^3) \otimes \mathbb{C}^4$,

$$\left|\left(\psi, \mathcal{O}_{b_1}\varphi\right)\right| \leqslant \frac{1}{\sqrt{\pi}} \|\tilde{D}_A\psi\| \left\| E_A^2 \int_0^1 \mu\, \mathrm{d}\mu \int_0^\infty \sqrt{\tau}\, \mathrm{d}\tau\, \mathrm{e}^{-\mu\tau E_A^2} \tilde{\varphi} \right\| \tag{3.23}$$

where $\tilde{\varphi} := f_A\, \mathrm{e}^{-(1-\mu)\tau E_A^2}\varphi$. The integral $E_A^2 \int_0^1 \mu\, \mathrm{d}\mu \int_0^\infty \sqrt{\tau}\, \mathrm{d}\tau\, \mathrm{e}^{-\mu\tau E_A^2} = E_A^2 \int_0^1 \mu\, \mathrm{d}\mu \frac{\sqrt{\pi}}{2\mu^{3/2}E_A^3} = \frac{\sqrt{\pi}}{E_A}$ is bounded, and $\tilde{\varphi}$ with $\|\tilde{\varphi}\| \leqslant \|f_A\|_\infty \|\varphi\|$ does not change its convergence properties. Thus $\left|\left(\psi, \mathcal{O}_{b_1}\varphi\right)\right| \leqslant C\|\psi\|\|\varphi\|$ with some constant C. In the same way (substituting $\tilde{\mu} := 1-\mu$) one shows the boundedness of $\mathcal{O}_{b_2}^*$. Thus $\frac{\mathrm{i}}{E_A}[E_A, \mathbf{xp}]_{(c)} = \mathcal{O}_a + \mathcal{O}_{b_1} + \mathcal{O}_{b_2}$ is bounded.

For $(d)\, f_A D_A$ we write the operator relating to I_1 as a sum $\mathcal{O}_{d_1} + \mathcal{O}_{d_2}$ in analogy to (3.22) and make for $\mathcal{O}_{d_1}$ the following decomposition,

$$\left(\psi, \mathcal{O}_{d_1}\varphi\right) = \frac{1}{\sqrt{\pi}} \int_0^\infty \mathrm{d}\tau \int_0^1 \mathrm{d}\mu \left(\tau^{\frac{1}{4}} \mu^{\frac{1}{2}} \frac{1}{\tilde{\mu}^{\frac{3}{8}}}\, \mathrm{e}^{-\mu\tau E_A^2} E_A\psi,\, f_A \tau^{\frac{1}{4}} \mu^{\frac{1}{2}} \tilde{\mu}^{\frac{3}{8}} D_A\, \mathrm{e}^{-\tilde{\mu}\tau E_A^2}\varphi \right). \tag{3.24}$$

Upon using the Schwarz inequality and the boundedness of f_A we can estimate $\left|\left(\psi, \mathcal{O}_{d_1}\varphi\right)\right| \leqslant \pi^{-\frac{1}{2}}\left(I_1^2 \cdot I_2^2\right)^{\frac{1}{2}}$ where

$$\begin{aligned} I_2^2 &\leqslant \|f_A\|_\infty^2 \left(\varphi, \int_0^1 \mathrm{d}\mu\, \mu \tilde{\mu}^{\frac{3}{4}} \int_0^\infty \mathrm{d}\tau\, \tau^{\frac{1}{2}} E_A^2\, \mathrm{e}^{-2\tilde{\mu}\tau E_A^2}\varphi \right) \\ &= \|f_A\|_\infty^2 \frac{\sqrt{\pi}}{4\sqrt{2}} \int_0^1 \mathrm{d}\mu \frac{\mu}{(1-\mu)^{\frac{3}{4}}} \left(\varphi, \frac{1}{E_A}\varphi\right) \leqslant c_2\|\varphi\|^2. \end{aligned} \tag{3.25}$$

Likewise, $I_1^2 \leqslant \frac{\sqrt{\pi}}{4\sqrt{2}} \int_0^1 \mathrm{d}\mu \mu^{-\frac{1}{2}}(1-\mu)^{-\frac{3}{4}}\left(\psi, \frac{1}{E_A}\psi\right) \leqslant c_1\|\psi\|^2$. For the operator $\mathcal{O}_{d_2}$ we consider $(\psi, \mathcal{O}_{d_2}^*\varphi)$ and proceed as in (3.23)ff to prove its boundedness (by introducing $\tilde{\varphi}_d$ with $\|\tilde{\varphi}_d\| = \left\| f_A\, \mathrm{e}^{-\mu\tau E_A^2} E_A^{-1}\varphi \right\| \leqslant c\|\varphi\|$). In the same way the contribution from I_2 is handled (relying on the boundedness of $D_A \int_0^1 \mathrm{d}\mu \int_0^\infty \mathrm{d}\tau\tau^{-1/2}\, \mathrm{e}^{-\tilde{\mu}\tau E_A^2} = 2\sqrt{\pi} D_A/E_A$). Collecting results, we thus have shown the boundedness of $\frac{\mathrm{i}}{E_A}[E_A, \mathbf{xp}]$. This establishes the compactness of $(E_A+\mu)^{-1}\mathrm{i}[\mathcal{O}_1, A_U](E_A+\mu)^{-1}$ and hence of $(E_A+\mu)^{-1}k_A(E_A+\mu)^{-1}$. See endnote 2

The last part in the proof of the Mourre-type estimate (3.1) is the search for a positive constant α_0 on the rhs of (3.8) if $m \notin \Delta$.

Let first Δ be an open interval on the real line such that $\inf\Delta > m$. Then $E_\Delta(h^{\mathrm{BR}} - m)E_\Delta \geqslant E_\Delta \alpha_0 E_\Delta = \alpha_0 E_\Delta$ with $\alpha_0 := \inf\Delta - m > 0$.

If $\Delta \subset (-\infty, m)$ we have $\sigma_{\mathrm{ess}}(E_A) \cap \Delta = \emptyset$ since $E_A \geqslant m$. Moreover it was shown in [14] that $\sigma_{\mathrm{ess}}(h^{\mathrm{BR}}) = \sigma_{\mathrm{ess}}(E_A)$ for $\gamma < \frac{1}{2}$ (in the proof of [14, theorem 2] one has to drop all second-order terms in γ). This means that $\sigma(h^{\mathrm{BR}}) \cap \Delta$ is discrete and E_Δ is compact. Then one trivially has an $\alpha_0 > 0$ because the rhs of (3.8) can be rearranged, $E_\Delta(h^{\mathrm{BR}} - m)E_\Delta + E_\Delta k_A E_\Delta = \alpha_0 E_\Delta + E_\Delta \tilde{k} E_\Delta$ with $\tilde{k} := k_A - E_\Delta(\alpha_0 + m)E_\Delta + E_\Delta h^{\mathrm{BR}} E_\Delta$. The operator $h^{\mathrm{BR}} E_\Delta$ is bounded such that $E_\Delta h^{\mathrm{BR}} E_\Delta$ is compact. The same is true for $(\alpha_0 + m)E_\Delta$. Thus (3.8) turns into (3.1) with $\tilde{k}$ substituted for k_A.

We note that proposition 1 differs from the conventional Mourre estimate [15, 17, p 62] in that the latter requires the compactness of $E_\Delta k_A E_\Delta$ itself. For the pseudorelativistic operators it will turn out that $E_\Delta k_A E_\Delta$ is only compact for sufficiently small potential strength γ. As shown below, this restriction on γ results from the requirement that the potential is E_A-bounded with bound < 1. Also conditions on the domain of a_A and on the range of the commutator (to define it in the form sense) are usually included in the Mourre estimate. Here, these conditions will appear in the context of proposition 3.

4. Finite point spectrum

In this section we show that the following theorem is a consequence of the Mourre-type estimate.

Theorem 1. *Let h^{BR} be the Brown–Ravenhall operator with magnetic field of constant direction generated by a vector potential* $\mathbf{A}$ *subject to the conditions of proposition 1.*

Then for $\gamma < \frac{1}{2}(Z \leqslant 68)$, h^{BR} has in $\mathbb{R}\backslash\{m\}$ at most isolated eigenvalues of finite multiplicity.

For the proof of theorem 1 we proceed as follows. First we establish that the expectation value of the lhs of the Mourre-type estimate (3.1) vanishes, if taken with any eigenfunction of h^{BR}. Then we make use of the fact that for a sequence of eigenfunctions converging weakly to zero the expectation value of a compact operator goes to zero. This leaves us with a positive expectation value of the rhs of (3.1), a contradiction.

The first item is guaranteed by Mourre's proposition [15, proposition II.4, 17, theorem 4.6].

Proposition 3 (Mourre)**.** *Let H and $\mathcal{A}$ be self-adjoint operators acting in the Hilbert space L_2 and satisfying*

(a) $\mathcal{D}(\mathcal{A}) \cap \mathcal{D}(H)$ is a core for H.
(b) $\mathrm{i}[H, \mathcal{A}]$ defined on $\mathcal{D}(\mathcal{A}) \cap \mathcal{D}(H)$ is a bounded map from H_1 into H_{-1} (where $\mathcal{D}(H) = H_1$ and $\psi \in H_{-1}$ if $\left\| \frac{1}{|H|+1} \psi \right\| < \infty$).
(c) There is a self-adjoint operator H_0 with $\mathcal{D}(H_0) = \mathcal{D}(H)$ such that $\mathrm{i}[H_0, \mathcal{A}]$ is a bounded map from H_1 into L_2, and $\mathcal{D}(\mathcal{A}) \cap \mathcal{D}(H_0\mathcal{A})$ is a core for H_0.

Then, if ψ is an eigenfunction of H and $\tilde{\mu} > 0$,

$$(\psi, [H, \mathcal{A}]\psi) = \lim_{\tilde{\mu}\to\infty} \left(\psi, \left[H, \mathrm{i}\tilde{\mu}\mathcal{A}\frac{1}{\mathcal{A} + \mathrm{i}\tilde{\mu}} \right] \psi \right) = 0. \tag{4.1}$$

In order to apply proposition 3 we have to verify the conditions (a)–(c) for our operators under consideration. It is the conditions (a) and (b) that are conventionally included in the Mourre estimate.

(a) We recall that $\mathcal{D}(H^{\mathrm{BR}}) = \mathcal{D}(E_A) = H_1(\mathbb{R}^3) \otimes \mathbb{C}^4$. The domain M_A of A_U defined below (3.4) is dense in L_2. In fact, let $\psi_0 \in L_2(\mathbb{R}^3) \otimes \mathbb{C}^4$. Then $U_0^{-1}\psi_0 \in L_2(\mathbb{R}^3) \otimes \mathbb{C}^4$ and there is $\varphi_n \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4$ such that $\left\| U_0^{-1}\psi_0 - \varphi_n \right\| < \epsilon$. Consequently, $\|\psi_0 - U_0\varphi_n\| = \left\| U_0\left(U_0^{-1}\psi_0 - \varphi_n\right) \right\| < \epsilon$.
Moreover, M_A is a subset of H_1, the domain of E_A, as for any $\psi = U_0\varphi \in M_A$ we have $\|E_A\psi\| = \|U_0E_A\varphi\| \leqslant \|E_A\varphi\| < \infty$. From $\overline{M_A} = \overline{H_1} = L_2$ it follows that $M_A = \mathcal{D}(A_U) \cap \mathcal{D}(H^{\mathrm{BR}})$ is a core for H^{BR}.

(b) We have to show that for $\psi \in H_1$, $\mathrm{i}[\tilde{H}^{\mathrm{BR}}, A_U]\psi \in H_{-1}$ by investigating all operators of (3.4) which constitute the commutator. The bounded operators $U_0 f_A U_0^{-1}$ and mC_1 as well as $\tilde{H}^{\mathrm{BR}}$ map into $L_2 \subset H_{-1}$. So does $\mathcal{O}_1$ (by (2.11) and (2.12)). The remaining operator $\mathrm{i}[\mathcal{O}_1, A_U]$ maps into H_{-1} which can be shown by considering $\psi \in M_A \subset H_1(\mathbb{R}^3) \otimes \mathbb{C}^4$ such that $(E_A + \mu)\psi \in L_2(\mathbb{R}^3) \otimes \mathbb{C}^4$. We decompose

$$\mathrm{i}[\mathcal{O}_1, A_U]\psi = (E_A + \mu)\tilde{K}(E_A + \mu)\psi =: (E_A + \mu)\tilde{\varphi} \tag{4.2}$$

where $\tilde{K} := (E_A + \mu)^{-1}\mathrm{i}[\mathcal{O}_1, A_U](E_A + \mu)^{-1}$ is compact, in particular bounded. Therefore, $\tilde{\varphi} \in L_2(\mathbb{R}^3) \otimes \mathbb{C}^4$ such that $(E_A + \mu)\tilde{\varphi}$ is in H_{-1} by definition, relying on (2.12).

(c) We identify H_0 with E_A. Setting $V = 0$ in (3.4), the commutator reduces to

$$\mathrm{i}[\beta E_A, A_U] = \beta E_A - mC_1 + U_0 f_A U_0^{-1}. \tag{4.3}$$

For $\psi \in M_A \subset H_1(\mathbb{R}^3) \otimes \mathbb{C}^4$ we thus have $\|\mathrm{i}[\beta E_A, A_U]\psi\| < \infty$ implying that $\mathrm{i}[\beta E_A, A_U]$ maps from H_1 into L_2. It is easily seen that A_U leaves M_A invariant. One has for $\psi = U_0\varphi \in M_A$,

$$A_U\psi = U_0 \mathcal{A} U_0^{-1} U_0 \varphi = U_0 \tilde{\psi} \in M_A \tag{4.4}$$

since $\tilde{\psi} := \mathcal{A}\varphi \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4$. Therefore, $\mathcal{D}(E_A A_U) = M_A$ and $\mathcal{D}(A_U) \cap \mathcal{D}(E_A A_U) = M_A$ is a core for E_A.

All these results hold necessarily for the upper left block of the operators under consideration, establishing the applicability of proposition 3.

The remaining proof of theorem 1 follows Mourre [15], see also [17, proof of theorem 4.7]. Let $\Delta \in \mathbb{R}$ be an open interval on which the Mourre-type estimate holds. Let $(\lambda_n)_{n\in\mathbb{N}} \in \Delta$ be an infinite sequence of eigenvalues of h^{BR} converging to $\lambda \in \Delta$, or let λ be an eigenvalue of infinite multiplicity (represented by $\lambda_n = \lambda$ for all $n \in \mathbb{N}$). We will show that such λ cannot exist.

Let $(\psi_n)_{n\in\mathbb{N}}$ be the orthonormal sequence of eigenfunctions to $(\lambda_n)_{n\in\mathbb{N}}$ (which converges weakly to zero). We claim that $(\psi_n, E_\Delta k_A E_\Delta \psi_n) \to 0$ as $n \to \infty$. Define $\tilde{\psi}_n := (h^{\mathrm{BR}} + \mu)E_\Delta \psi_n$ and choose μ such that $h^{\mathrm{BR}} + \mu$ is invertible (note that h^{BR} is bounded from below for $\gamma < \frac{2}{\pi}$). Then we decompose

$$(\psi_n, E_\Delta k_A E_\Delta \psi_n) = \left(\tilde{\psi}_n, \frac{1}{h^{\mathrm{BR}} + \mu}(E_A + \mu)\left\{\frac{1}{E_A + \mu} k_A \frac{1}{E_A + \mu}\right\}(E_A + \mu)\frac{1}{h^{\mathrm{BR}} + \mu}\tilde{\psi}_n\right). \tag{4.5}$$

We have $E_\Delta \psi_n = \psi_n$ and $\tilde{\psi}_n = (\lambda_n + \mu)\psi_n \overset{w}{\rightharpoonup} 0$ as $n \to \infty$. ($\tilde{\psi}_n$ is normalizable since $\|\tilde{\psi}_n\| = \lambda_n + \mu \to \lambda + \mu \in \mathbb{R}_+$ as $n \to \infty$.) Moreover, $(E_A + \mu)(h^{\mathrm{BR}} + \mu)^{-1}$ is bounded for $\gamma < \frac{1}{2}$ because of the relative boundedness (2.12). Thus the operator in (4.5) is compact and turns $(\tilde{\psi}_n)_{n\in\mathbb{N}}$ into a strongly convergent sequence. Therefore the rhs of (4.5) goes to zero as $n \to \infty$.

Finally we get from the Mourre-type estimate (3.1), using proposition 3,

$$\mathrm{i} \lim_{n\to\infty} (\psi_n, [h^{\mathrm{BR}}, a_{11}]\psi_n) \geqslant \alpha_0 + \lim_{n\to\infty} (\psi_n, E_\Delta k_A E_\Delta \psi_n), \tag{4.6}$$

i.e. $0 \geqslant \alpha_0$, a contradiction. Since (3.1) holds in $\mathbb{R}\backslash\{m\}$ this proves theorem 1.

5. Application to related operators

We shall first concentrate on the special case $A = 0$ and later turn to the general case. When magnetic fields are absent in the Brown–Ravenhall operator it can be shown that theorem 1, based on the Mourre-type estimate, holds even for $\gamma < \frac{3}{4}$ (see [31, (II.6.29)] for this bound). It is also readily possible to derive a Mourre-type estimate for the pseudorelativistic operators of higher order in γ. We have done so for the (second-order) Jansen–Hess operator which is well defined for $\gamma < 1.006$ [5]. The proof relies on the explicit expression for the kernel of the second unitary transformation U_1 which follows the Foldy–Wouthuysen transformation U_0 (for $A = 0$) in the Douglas–Kroll scheme. It obeys $U_1U_0 = U_0\,\mathrm{e}^{-\mathrm{i}B_1}$, $B_1(\mathbf{p}, \mathbf{p}') = -\frac{\mathrm{i}\gamma}{(2\pi)^2} \frac{1}{(\mathbf{p}-\mathbf{p}')^2} \frac{1}{E_p + E_{p'}} (\tilde{D}_0(\mathbf{p}) - \tilde{D}_0(\mathbf{p}'))$ with $\tilde{D}_0 = (\boldsymbol{\alpha}\mathbf{p} + \beta m)/E_p$ [7]. By applying U_1U_0 to the Dirac operator there arise additional (remainder) terms—in contrast to the Brown–Ravenhall case—but it can be shown that they have the required compactness property. Since the potential of the Jansen–Hess operator is E_p-bounded (with bound < 1) for $\gamma \leqslant 0.67$ [31], the Mourre-type estimate establishes a finite point spectrum up to this value. It should be noted, however, that different methods (relying on the virial theorem for the Brown–Ravenhall operator [4, 31] and on dilation analyticity for the Jansen–Hess operator [32]) provide better bounds for the absence of eigenvalues (for h^{BR}) respectively accumulation points of eigenvalues (for the latter) above m ($\gamma < 0.906$ [3] respectively $\gamma < 1.006$) because they only require the E_p-form boundedness of the respective potentials.

A case of interest is, however, the exact block-diagonalized Dirac operator. The block diagonalization of H is achieved by the unitary transformation $\tilde{U} = U_0 U$ with U_0 as above and U given by [8]

$$U = [1 - (\Lambda_- - \Lambda_+)(P_+ - \Lambda_+)]\,(1 - (P_+ - \Lambda_+)^2)^{-\frac{1}{2}}. \tag{5.1}$$

P_+ is the projector onto the positive spectral subspace of H while $\Lambda_\pm = \frac{1}{2}(1 \pm \tilde{D}_0) = P_\pm(\gamma = 0)$ with $P_- = 1 - P_+ . U$ (and hence $\tilde{U}$) exist for $\|P_+ - \Lambda_+\| < 1$, i.e. for $\gamma < 0.685$. The domain of $H_{\mathrm{ex}} := \tilde{U} H \tilde{U}^{-1}$ is $\mathcal{D}(H_{\mathrm{ex}}) = \{\tilde{U}\varphi : \varphi \in H_1(\mathbb{R}^3) \otimes \mathbb{C}^4\}$ since H is self-adjoint on $\mathcal{D}(E_p) = H_1(\mathbb{R}^3) \otimes \mathbb{C}^4$ (for $\gamma < \frac{1}{2}$ [1, p 112]). If $\tilde{U}$ leaves H_1 invariant then $\mathcal{D}(H_{\mathrm{ex}}) = H_1(\mathbb{R}^3) \otimes \mathbb{C}^4$.

This invariance, which is needed for the applicability of proposition 3 (see below), requires for $\varphi \in H_1(\mathbb{R}^3) \otimes \mathbb{C}^4$ that $\|E_p \tilde{U} \varphi\| = \left\| U_0 \left(E_p U E_p^{-1}\right) E_p \varphi \right\| < \infty$. This holds true since $E_p U E_p^{-1}$ is bounded (which is proven in appendix B for $\gamma \leqslant \gamma_c = 0.257$).

Applying $\tilde{U}$ to the commutator equation (3.3) for $A = 0$ we get, defining $A_{\tilde{U}} := \tilde{U} \mathcal{A} \tilde{U}^{-1}$,

$$\mathrm{i}[H_{\mathrm{ex}}, A_{\tilde{U}}] = H_{\mathrm{ex}} - m \tilde{U} \beta \tilde{U}^{-1}. \tag{5.2}$$

This leads to the following estimate for its upper left block (according to (3.5)–(3.7)),

$$\mathrm{i}[h_{\mathrm{ex}}, \tilde{a}_{11}] - h_{\mathrm{ex}} \geqslant -m \tag{5.3}$$

where h_{ex} and $\tilde{a}_{11}$ denote the upper left block of H_{ex} and $A_{\tilde{U}}$, respectively.

Now let λ be an eigenvalue of h_{ex} and $\psi_\lambda \in H_1(\mathbb{R}^3) \otimes \mathbb{C}^2$ the normalized eigenfunction to λ. Then we get from (5.3),

$$(\psi_\lambda, \mathrm{i}[h_{\mathrm{ex}}, \tilde{a}_{11}]\psi_\lambda) \geqslant \lambda - m. \tag{5.4}$$

The application of Mourre's proposition (4.1)–(5.4) results in $\lambda \leqslant m$, which proves:

Theorem 2. *Let $\gamma \leqslant \gamma_c = 0.257 (Z \leqslant 35)$ and $A = 0$. Then h_{ex} and hence the Dirac operator H has no eigenvalues above m.*

The assumptions (a)–(c) in proposition 3 are readily verified. For (a) we have $\mathcal{D}(A_{\tilde{U}}) =: \tilde{M} = \left\{\tilde{U}\varphi : \varphi \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4\right\}$ which is dense in L_2. Moreover, $\tilde{M} \subset H_1$ since for $\psi = \tilde{U}\varphi \in \tilde{M}$ we have $\|E_p \psi\| = \left\|\left(E_p \tilde{U} E_p^{-1}\right) E_p \varphi\right\| < \infty$ from appendix B. Thus $\tilde{M} = \mathcal{D}(A_{\tilde{U}}) \cap \mathcal{D}(H_{\mathrm{ex}})$ is a core for H_{ex}.

(b) holds since from (5.2), $\mathrm{i}[H_{\mathrm{ex}}, A_{\tilde{U}}]$ even maps from H_1 into L_2. For (c) we set $H_0 := H_{\mathrm{ex}}$. We have $\tilde{M} \subset \mathcal{D}(H_{\mathrm{ex}} A_{\tilde{U}})$ since for $\varphi \in C_0^\infty$, $\|H_{\mathrm{ex}} A_{\tilde{U}} \tilde{U} \varphi\| = \|H_{\mathrm{ex}} \tilde{U} \mathcal{A} \varphi\| < \infty$. This is so because $\mathcal{A}$ leaves $C_0^\infty \subset H_1$ invariant. Thus $D(A_{\tilde{U}}) \cap \mathcal{D}(H_{\mathrm{ex}} A_{\tilde{U}}) = \tilde{M}$.

When a magnetic field is included $H = D_A + V$ can be block diagonalized in exactly the same way by $\tilde{U} = U_0 U_A$, where U_A is defined in (5.1) with the replacements $\Lambda_\pm \mapsto \Lambda_{A,\pm} = \frac{1}{2}(1 \pm \tilde{D}_A)$ and $P_+ \mapsto P_{A,+}$ (the projector relating to $D_A + V$). The existence of U_A requires a bound on γ which will depend on the magnetic field. Incidentally this B-dependence enters in a very simple way as shown presently. Like in the $A = 0$ case the bound on γ is determined from the requirement $\|P_{A,+} - \Lambda_{A,+}\| < 1$. It is calculated with the help of the diamagnetic inequality in form (2.6),

$$\left\| \frac{1}{x^{1/2}} \frac{1}{S_A^{1/2}} \psi \right\| \leqslant \left\| \frac{1}{x^{1/2}} \frac{1}{E_p^{1/2}} \right\| \|\psi\| \leqslant \sqrt{\frac{\pi}{2}} \|\psi\| \tag{5.5}$$

and with an estimate of $|H|$ by E_A from below, using (2.14),

$$\|H\psi\| \geqslant \|D_A\psi\| - \|V\psi\| \geqslant \left(1 - \frac{2\gamma}{\delta_m(B)}\right) \|E_A\psi\|. \tag{5.6}$$

Using the representation $P_{A,+} - \Lambda_{A,+} = \frac{\gamma}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\eta (D_A + \mathrm{i}\eta)^{-1} \frac{1}{x} (H + \mathrm{i}\eta)^{-1}$ [8] we get for $f, g \in L_2(\mathbb{R}^3) \otimes \mathbb{C}^4$ from the Schwarz inequality,

$$|(f, (P_{A,+} - \Lambda_{A,+})g)| \leqslant \frac{\gamma}{2\pi} \left(\int_{-\infty}^{\infty} \mathrm{d}\eta \left\| \frac{1}{x^{\frac{1}{2}}} \frac{1}{D_A - \mathrm{i}\eta} f \right\|^2 \right)^{\frac{1}{2}} \left(\int_{-\infty}^{\infty} \mathrm{d}\eta \left\| \frac{1}{x^{\frac{1}{2}}} \frac{1}{H + \mathrm{i}\eta} g \right\|^2 \right)^{\frac{1}{2}}. \tag{5.7}$$

With (5.5) we obtain

$$\left\| \frac{1}{x^{1/2}} \frac{1}{H + \mathrm{i}\eta} g \right\| \leqslant \sqrt{\frac{\pi}{2}} \left\| S_A^{1/2} \frac{1}{E_A^{1/2}} \right\| \left\| E_A^{1/2} \frac{1}{|H|^{1/2}} \right\| \left\| \frac{|H|^{1/2}}{H + \mathrm{i}\eta} g \right\|. \tag{5.8}$$

Further we have $\|S_A^{1/2} E_A^{-1/2}\| \leqslant (\delta_m(B))^{-1/2}$ by (2.13) and estimate $E_A^{1/2}$ by $|H|^{1/2}$ for $\gamma < \delta_m(B)/2$ from (5.6). For the last term in (5.8) we profit from $\int_{-\infty}^{\infty} \mathrm{d}\eta \| |\tilde{A}|^{1/2} (\tilde{A} \pm \mathrm{i}\eta)^{-1} g\|^2 = \pi \|g\|^2$ for any operator $\tilde{A}$ [8] such that, using the same technique for both factors in (5.7),

$$|(f, (P_{A,+} - \Lambda_{A,+})g)| \leqslant \frac{\gamma\pi}{4\delta_m(B)} \left(1 - \frac{2\gamma}{\delta_m(B)}\right)^{-1/2} \|f\| \|g\|. \tag{5.9}$$

We define the scaled parameter $\tilde{\gamma} = \gamma/\delta_m(B)$, and get $\|P_{A,+} - \Lambda_{A,+}\| < 1$ if $\tilde{\gamma} \frac{\pi}{4} (1 - 2\tilde{\gamma})^{-1/2} < 1$. This results in $\tilde{\gamma} \leqslant 0.44$, i.e. $\gamma \leqslant 0.44\delta_m(B)$. For $B = 0 (\delta_m(B) = 1)$ this bound is smaller than that obtained in [8] (by a different estimate which, however, is inferior if $B \neq 0$).

In conclusion, we remark that a Mourre-type estimate (3.1) with Δ above m can also be established for the block-diagonalized Dirac operator h_{ex} when $A \neq 0$. Since on the rhs of (5.3) there will appear the additional term $\tilde{k}_A := (\tilde{U} f_A \tilde{U}^{-1})_{11}$, only the absence of eigenvalues of infinite multiplicity or of accumulation points of eigenvalues of h_{ex} in Δ can be inferred (as for the Brown–Ravenhall operator). The assumptions on $\mathbf{A}$ are, however, different from those stated in proposition 1. The first condition in (iii) as well as the restrictions posed by proposition 2 (except $B \leqslant B_0$) have to be replaced by the requirement that $\mathbf{A}$ is bounded, its bound being sufficiently small such that the E_A-boundedness of E_p is assured. Moreover, the necessary bound on the potential strength γ is much more restrictive than that given above (for the existence of U_A) and depends on the particular choice of the magnetic field.

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Appendix A. Estimate of the heat kernel of E_A^2 for bounded $B \leqslant B_0$

With the assumption that **B** has constant direction in space we can restrict ourselves to a two-dimensional problem, i.e. $\mathbf{A} = (A_1(x_1, x_2), A_2(x_1, x_2), 0)$ such that $\mathbf{B} = (0, 0, B(x_1, x_2))$. Accounting for the required boundedness of B, we can take $0 < B(x_1, x_2) \leqslant B_0$. We assume that the reader is acquainted with the work of Loss and Thaller [30] for the estimate of the heat kernel of the Schrödinger operator $H_s := (\mathbf{p}_\perp - e\mathbf{A})^2$ where $\mathbf{p}_\perp = (p_1, p_2, 0)$ and will only indicate the necessary modifications of their proof. We have $E_A^2 = H_s + p_3^2 - e\sigma_3 B + m^2$. Since there is no dependence on x_3, the heat kernel relating to the third dimension reduces to the free heat kernel in one dimension, $\mathrm{e}^{-tp_3^2}(x_3, x_3') = (4\pi t)^{-\frac{1}{2}}\,\mathrm{e}^{-(x_3 - x_3')^2/4t}$ [25, p 35], as a multiplicative factor.

Given an initial state $u_0(\mathbf{x})$, its time evolution is defined by

$$u(\mathbf{x}, t) = \mathrm{e}^{-t\tilde{E}_A^2} u_0(\mathbf{x}) \tag{A.1}$$

where here and in the following $\mathbf{x} = (x_1, x_2)$ and $\tilde{E}_A^2 = E_A^2 - p_3^2$. From (A.1) we obtain $\frac{\mathrm{d}u}{\mathrm{d}t} = -\tilde{E}_A^2 u$ and u_0 is the solution of this equation at $t = 0$ (which is a Gaussian function for a constant field $B(x_1, x_2) = B_0$ [33]).

We have $\frac{\mathrm{d}}{\mathrm{d}t}|u|^2 = \overline{u}\frac{\mathrm{d}u}{\mathrm{d}t} + \frac{\mathrm{d}\overline{u}}{\mathrm{d}t}u$ which, following [30, section 3] and using $\overline{u}\sigma_3 u \leqslant |u|^2$, leads to the estimate

$$\begin{aligned}\frac{1}{2}\int_{\mathbb{R}^2} \mathrm{d}\mathbf{x}|u|^{r-2}\frac{\mathrm{d}}{\mathrm{d}t}|u|^2 &\leqslant -(r-1-c^2)\int_{\mathbb{R}^2}\mathrm{d}\mathbf{x}|u|^{r-2}(\nabla|u|)^2 \\ &\quad - \frac{2ec}{r}\int_{\mathbb{R}^2}\mathrm{d}\mathbf{x}\, B|u|^r + \int_{\mathbb{R}^2}\mathrm{d}\mathbf{x}|u|^r(eB - m^2)\end{aligned} \tag{A.2}$$

where $r = r(t) \geqslant 2$ and c is a constant with $0 < c < \sqrt{r-1}$. We remark that due to the definition of our operator, the changes with respect to the work of Loss and Thaller concern the replacements $\mathbf{A} \mapsto -e\mathbf{A}$, $\frac{t}{2} \mapsto t$. The negative sign of **A** can be compensated by a negative sign in the auxiliary function ∇S of [30] which has dropped out in (A.2). So the first two terms in (A.2) are (up to a factor of 2 from the definition of t) identical to those of [30], while the last term is an additional term arising from the structure of $\tilde{E}_A^2$.

Since $c < \sqrt{r-1} \leqslant \frac{r}{2}$ for all $r \geqslant 1$, we can estimate further, using the normalization $\int_{\mathbb{R}^2}\mathrm{d}\mathbf{x}|u|^r = 1$ and $0 < B \leqslant B_0$,

$$\int_{\mathbb{R}^2}\mathrm{d}\mathbf{x}|u|^r eB\left(1 - \frac{2c}{r}\right) - m^2 \leqslant -\frac{2c}{r}eB_0 + (eB_0 - m^2). \tag{A.3}$$

Upon insertion into (A.2) one gets, apart from the constant term $(eB_0 - m^2)$, the identical expression of [30]. Therefore,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\ln\|u\|_r &\leqslant \frac{r'}{r^2}\int_{\mathbb{R}^2}\mathrm{d}\mathbf{x}|u|^r\ln|u|^r - (r-1-c^2)\int_{\mathbb{R}^2}\mathrm{d}\mathbf{x}|u|^{r-2}(\nabla|u|)^2 \\ &\quad - \frac{2c}{r}eB_0 + (eB_0 - m^2) \leqslant -2L(r, r') + (eB_0 - m^2)\end{aligned} \tag{A.4}$$

where $L(r, r')$ is the function obtained by [30] for the optimal choice of c such that the rhs of the first inequality in (A.4) under the absence of $(eB_0 - m^2)$ is minimized. Integrating (A.4) from 0 to t with the choice of r such that $r(0) = p$, $r(t) = q$, and then exponentiating, leads to

$$\left\|\mathrm{e}^{-t\tilde{E}_A^2}\right\|_{L_p\to L_q} = \sup_{u\in L_p}\frac{\left\|\mathrm{e}^{-t\tilde{E}_A^2}u\right\|_q}{\|u\|_p} \leqslant \mathrm{e}^{-2\int_0^t \mathrm{d}t\, L(r,r')}\cdot \mathrm{e}^{eB_0 t - m^2 t}. \tag{A.5}$$

The further reasoning from [30, remark 2 and theorem 1.3] then provides

$$\left|\mathrm{e}^{-t\tilde{E}_A^2}(\mathbf{x},\mathbf{x}')\right| \leqslant \frac{eB_0}{4\pi\,\sinh(eB_0t)}\,\mathrm{e}^{-(\mathbf{x}-\mathbf{x}')^2/4t}\,\mathrm{e}^{eB_0t-m^2t} \tag{A.6}$$

for two-dimensional $\mathbf{x}, \mathbf{x}'$, which completes the proof of proposition 2.

Appendix B. Boundedness of $E_pUE_p^{-1}$

We shall prove the boundedness of the adjoint operator $E_p^{-1}U^*E_p$. From (5.1) we have

$$E_p^{-1}U^*E_p = E_p^{-1}(1-(P_+-\Lambda_+)^2)^{-\frac{1}{2}}E_p\left[1-E_p^{-1}(P_+-\Lambda_+)E_p(\Lambda_--\Lambda_+)\right]. \tag{B.1}$$

Noting that $\|\Lambda_- - \Lambda_+\| = \|\tilde{D}_0\| = 1$ we will first show that $E_p^{-1}(P_+-\Lambda_+)E_p$ can be bounded below unity if γ is small enough. Using the integral representation $P_+ - \Lambda_+ = -\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\eta(D_0+\mathrm{i}\eta)^{-1}V(H+\mathrm{i}\eta)^{-1}$ we follow the strategy of [8] and estimate for $f, g \in H_1(\mathbb{R}^3)\otimes\mathbb{C}^4$ by means of the Schwarz inequality, introducing $W := E_p^{-\frac{5}{4}}\frac{1}{x}E_p^{\frac{1}{4}}$,

$$\begin{aligned}\left|\left(f, E_p^{-1}(P_+-\Lambda_+)E_pg\right)\right| &= \frac{\gamma}{2\pi}\left|\int_{-\infty}^{\infty}\mathrm{d}\eta\left(f, E_p^{-1}\frac{|\eta|^{\frac{1}{4}}}{D_0+\mathrm{i}\eta}E_p^{\frac{5}{4}}WE_p^{-\frac{1}{4}}\frac{|\eta|^{-\frac{1}{4}}}{H+\mathrm{i}\eta}E_pg\right)\right| \\ &\leqslant \frac{\gamma}{2\pi}\left(\int_{-\infty}^{\infty}\mathrm{d}\eta\left\|E_p^{\frac{5}{4}}\frac{|\eta|^{\frac{1}{4}}}{D_0-\mathrm{i}\eta}E_p^{-1}f\right\|^2\right)^{\frac{1}{2}}\|W\|\left(\int_{-\infty}^{\infty}\mathrm{d}\eta\left\|E_p^{-\frac{1}{4}}\frac{|\eta|^{-\frac{1}{4}}}{H+\mathrm{i}\eta}E_pg\right\|^2\right)^{\frac{1}{2}}.\end{aligned} \tag{B.2}$$

Let us assume for the moment that W is bounded by c_w. In the first factor we can use the integral formula, introducing $\tilde{f} = E_p^{\frac{1}{4}}f$ and $y = \eta/E_p$ [34, p 354],

$$\begin{aligned}\int_{-\infty}^{\infty}\mathrm{d}\eta\left\|\frac{|\eta|^{\frac{1}{4}}}{D_0-\mathrm{i}\eta}E_p^{\frac{1}{4}}f\right\|^2 &= \left(\tilde{f}, \int_{-\infty}^{\infty}\mathrm{d}\eta\frac{|\eta|^{\frac{1}{2}}}{D_0^2+\eta^2}\tilde{f}\right) \\ &= 2\int_0^{\infty}\mathrm{d}y\,\frac{y^{\frac{1}{2}}}{1+y^2}\left(\tilde{f}, \frac{1}{E_p^{\frac{1}{2}}}\tilde{f}\right) = \pi\sqrt{2}\|f\|^2.\end{aligned} \tag{B.3}$$

In order to treat the second factor in the same way we estimate E_p^{-1} by $|H|^{-1}$ with the help of Hardy's inequality,

$$\|Hg\| \leqslant \|D_0g\| + \|Vg\| \leqslant (1+2\gamma)\|E_pg\| \tag{B.4}$$

and consequently $E_p^{-\frac{1}{2}} \leqslant (1+2\gamma)^{\frac{1}{2}}|H|^{-\frac{1}{2}}$ (note that $|H| \geqslant \nu_\gamma E_p > 0$ for $\gamma < \frac{\sqrt{3}}{2}$ with $\nu_\gamma = \frac{1}{3}\sqrt{1-\gamma^2}(\sqrt{4\gamma^2+9}-4\gamma)$[35]). Then with $\tilde{g} = E_pg$ and $\eta = |H|\tilde{\eta}$,

$$\begin{aligned}\int_{-\infty}^{\infty}\mathrm{d}\eta\left\|E_p^{-\frac{1}{4}}\frac{|\eta|^{-\frac{1}{4}}}{H+\mathrm{i}\eta}E_pg\right\|^2 &\leqslant (1+2\gamma)^{\frac{1}{2}}\left(\tilde{g}, |H|^{-\frac{1}{2}}\int_{-\infty}^{\infty}\mathrm{d}\eta\frac{|\eta|^{-\frac{1}{2}}}{H^2+\eta^2}\tilde{g}\right) \\ &\leqslant 2(1+2\gamma)^{\frac{1}{2}}\int_0^{\infty}\mathrm{d}\tilde{\eta}\frac{1}{\tilde{\eta}^{\frac{1}{2}}(1+\tilde{\eta}^2)}(\tilde{g}, |H|^{-2}\tilde{g}) \leqslant \pi\sqrt{2}(1+2\gamma)^{\frac{1}{2}}\frac{1}{\nu_\gamma^2}\|g\|^2\end{aligned} \tag{B.5}$$

where in the last inequality $|H|^{-2} \leqslant \frac{1}{\nu_\gamma^2}E_p^{-2}$ was used.

Insertion into (B.2) leads to the desired estimate,

$$\left|\left(f, E_p^{-1}(P_+-\Lambda_+)E_pg\right)\right| \leqslant c_w\frac{\gamma}{\sqrt{2}\nu_\gamma}(1+2\gamma)^{\frac{1}{4}}\|f\|\|g\| =: c_0\|f\|\|g\|. \tag{B.6}$$

For $\gamma < \gamma_c$ (see below) we have $c_0 < 1$. With the same argumentation as [8, proof of lemma 5] this proves the boundedness of $E_p^{-1}(1-(P_+ - \Lambda_+)^2)^{-\frac{1}{2}} E_p$ as well. Thus $E_p^{-1} U^* E_p$ is bounded.

It remains to show the boundedness of W and to find the constant c_w. According to the Lieb and Yau formula which is related to the Schur test for the boundedness of integral operators [36] (see also [7]), the integrals over the kernel k_W of W, multiplied by suitable nonnegative convergence generating functions h,

$$\begin{aligned} I(\mathbf{p}) &:= \int_{\mathbb{R}^3} \mathrm{d}\mathbf{p}' |k_W(\mathbf{p},\mathbf{p}')| \frac{h(p)}{h(p')} \\ J(\mathbf{p}') &:= \int_{\mathbb{R}^3} \mathrm{d}\mathbf{p} |k_W(\mathbf{p},\mathbf{p}')| \frac{h(p')}{h(p)} \end{aligned} \tag{B.7}$$

have to be finite. Using the Fourier representation of $\frac{1}{x}$ we get $k_W(\mathbf{p},\mathbf{p}') = \frac{1}{2\pi^2} E_p^{-\frac{5}{4}} \frac{1}{|\mathbf{p}-\mathbf{p}'|^2} E_{p'}^{\frac{1}{4}}$. We choose $h(p) = p^{\frac{3}{2}}$ and use $\int_{S^2} \mathrm{d}\omega' \frac{1}{|\mathbf{p}-\mathbf{p}'|^2} = \frac{2\pi}{pp'} \ln \frac{p+p'}{|p-p'|}$ for the angular integral. Then

$$\begin{aligned} I(p) &= \frac{1}{\pi} \frac{1}{pE_p^{\frac{5}{4}}} \int_0^\infty \mathrm{d}p'\, p' \ln \frac{p+p'}{|p-p'|} E_{p'}^{\frac{1}{4}} \frac{p^{\frac{3}{2}}}{p'^{\frac{3}{2}}} \\ J(p') &= \frac{1}{\pi} \frac{E_{p'}^{\frac{1}{4}}}{p'} \int_0^\infty p\, \mathrm{d}p \ln \frac{p+p'}{|p-p'|} \frac{1}{E_p^{\frac{5}{4}}} \frac{p'^{\frac{3}{2}}}{p^{\frac{3}{2}}}. \end{aligned} \tag{B.8}$$

We make the substitutions $p' = pq'$ in I and $p = p'q$ in J and introduce the parameters $\xi_1 = p/m$ and $\xi_2 = p'/m$. Then, using the estimates $\frac{\xi^2 q'^2 + 1}{\xi^2+1} = \frac{\xi^2 q'^2}{\xi^2+1} + \frac{1}{\xi^2+1} \leqslant q'^2 + 1$ and $(a+b)^{\frac{1}{n}} \leqslant a^{\frac{1}{n}} + b^{\frac{1}{n}}$ for $a, b \geqslant 0$ and $n \in \mathbb{N}$, we obtain

$$\begin{aligned} I(m\xi_1) &\leqslant \frac{1}{\pi} \int_0^\infty \frac{\mathrm{d}q'}{q'^{\frac{1}{2}}} \ln \frac{1+q'}{|1-q'|} \left(1 + q'^{\frac{1}{4}}\right) \\ J(m\xi_2) &\leqslant \frac{1}{\pi} \int_0^\infty \frac{\mathrm{d}q}{q^{\frac{3}{2}}} \ln \frac{1+q}{|1-q|} \left(1 + \frac{1}{q^{\frac{1}{4}}}\right). \end{aligned} \tag{B.9}$$

These integrals can be evaluated analytically with the help of a formula from [5], and they provide the same bound for I and J. Hence,

$$\left\| E_p^{-\frac{5}{4}} \frac{1}{x} E_p^{\frac{1}{4}} \right\| \leqslant \sup_{\xi_1,\xi_2 \geqslant 0} [I(m\xi_1) J(m\xi_2)]^{\frac{1}{2}} \leqslant 2 + \frac{4}{3\tan\left(\frac{\pi}{8}\right)} =: c_w \approx 5.22. \tag{B.10}$$

If inserted into (B.6) we get $c_0 < 1$ for $\gamma < 0.187$. A numerical evaluation of the integrals (B.8) shows that their maximum value is attained for $p, p' \to \infty$, providing the upper bound $I(m\xi_1), J(m\xi_2) \leqslant \frac{4}{3\tan(\pi/8)} \approx 3.22$. This leads to $\gamma_c = 0.257$ corresponding to $Z = 35$. This bound is inferior to the bound $\gamma_c = 0.382$ obtained by [8] for the invariance of $H_{1/2}$ by $\tilde{U}$.

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Endnotes

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