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On the spectrum of magnetic Dirac operators with Coulomb-type perturbations

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Abstract

We carry out the spectral analysis of singular matrix valued perturbations of 3-dimensional Dirac operators with variable magnetic field of constant direction. Under suitable assumptions on the magnetic field and on the perturbations, we obtain a limiting absorption principle, we prove the absence of singular continuous spectrum in certain intervals and state properties of the point spectrum. Constant, periodic as well as diverging magnetic fields are covered, and Coulomb potentials up to the physical nuclear charge $Z < 137$ are allowed. The importance of an internal-type operator (a 2-dimensional Dirac operator) is also revealed in our study. The proofs rely on commutator methods.

Keywords: Dirac operator; Magnetic field; Coulomb potentials; Absolutely continuous spectrum; Limiting absorption principle; Commutators methods

1. Introduction and main results

In an earlier paper [16] we carried out the spectral analysis for matrix valued perturbations of three-dimensional Dirac operators with variable magnetic field of constant direction. Due to some technical difficulties, two restrictions on the perturbations were imposed: the perturbations

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had to be bounded, and the long-range part had to be of scalar-type. In the present paper both restrictions are removed. Coulomb potentials up to the physical nuclear charge $Z < 137$ are considered and matrix valued long-range perturbations are analysed.

When dealing with such a general Coulomb perturbation, one main difficulty has to be faced: The perturbation is not small with respect to the unperturbed operator. Therefore most of the usual techniques of perturbation theory are not available and some slightly more involved tools have to be employed. For instance, without magnetic field the problem of selfadjointness of Dirac operators with Coulomb potentials already has a long history. Distinguished selfadjoint extensions have to be considered, and it took time to treat the problem up to the coupling constant corresponding to $Z < 137$. We refer for example to the research papers [11–14] or to the book [17, Notes 4.3] for an account on this issue. More recently the study of Dirac operators with arbitrary Coulomb singularities was performed in [8] and [18].

On the other side the same situation with a magnetic field has been much less studied. Some results on the spectrum of Dirac operators with magnetic fields are available for example in [3, 6,9,10,19], but none of these papers deals with very general magnetic fields and with Coulomb-type singularities. Note however that some information on selfadjointness for these operators can be extracted from [4] and [5], but in these papers the nature of the spectrum is not considered. The purpose of the present article is to fill in this gap in a general situation that we shall now describe.

We consider a relativistic spin-$\frac{1}{2}$ particle evolving in $\mathbb{R}^3$ in presence of a variable magnetic field of constant direction. By virtue of the Maxwell equations, we may assume with no loss of generality that the magnetic field has the form $\vec{B}(x_1, x_2, x_3) = (0, 0, B(x_1, x_2))$. The unperturbed system is described in the Hilbert space $\mathsf{L}^2(\mathbb{R}^3; \mathbb{C}^4)$ by the Dirac operator

$$H_0 := \alpha_1 \Pi_1 + \alpha_2 \Pi_2 + \alpha_3 P_3 + \beta m,$$

where $\beta \equiv \alpha_0, \alpha_1, \alpha_2, \alpha_3$ are the usual Dirac–Pauli matrices, m is the strictly positive mass of the particle and $\Pi_j := -i\partial_j - a_j$ are the generators of the magnetic translations with a vector potential $\vec{a}(x_1, x_2, x_3) = (a_1(x_1, x_2), a_2(x_1, x_2), 0)$ that satisfies $B = \partial_1 a_2 - \partial_2 a_1$. Since $a_3 = 0$, we write $P_3 := -i\partial_3$ instead of Π_3.

In the sequel we study the stability of certain parts of the spectrum of H_0 under a matrix valued perturbation V. If V satisfies the natural hypotheses introduced below (which allow Coulomb singularities), and if H is the suitably defined selfadjoint operator associated with the formal sum $H_0 + V$, then we prove a limiting absorption principle and state properties of the point spectrum of H in intervals of $\mathbb{R}$ corresponding to gaps in the symmetrized spectrum of the operator $H^0 := \sigma_1 \Pi_1 + \sigma_2 \Pi_2 + \sigma_3 m$ in $\mathsf{L}^2(\mathbb{R}^2; \mathbb{C}^2)$. The matrices σ_j are the Pauli matrices and the symmetrized spectrum σ^0_{sym} of H^0 is the union of the spectra of H^0 and $-H^0$. We stress that our analysis does not require any restriction on the behaviour of the magnetic field at infinity. Nevertheless, the pertinence of our work depends on a certain property of the internal-type operator H^0; namely, the size and the number of gaps in σ^0_{sym}. For example, in the special but important case of a nonzero constant magnetic field B_0, σ^0_{sym} is equal to $\{\pm\sqrt{2nB_0 + m^2} \mid n = 0, 1, 2, \ldots\}$, which implies that there are plenty of gaps where our analysis gives results. We refer to [3,6,10] for various information on the spectrum of H^0, especially in the situations of physical interest, for example when B is constant, periodic or diverges at infinity. Let us also note that since Coulomb potentials are allowed in our approach, a more realistic study of Zeeman effect [9] is at hand.

In order to state precisely our results, let us introduce some notations. $\mathscr{B}_{\text{h}}(\mathbb{C}^4)$ stands for the set of 4×4 Hermitian matrices, and $\|\cdot\|$ denotes the norm of the Hilbert space $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^3; \mathbb{C}^4)$

as well as the norm of $\mathscr{B}(\mathcal{H})$, the set of bounded linear operators on $\mathcal{H}$. P_3 is considered as an operator in $\mathcal{H}$ or in $\mathsf{L}^2(\mathbb{R})$ depending on the context. $\mathbb{N} := \{0, 1, 2, \dots\}$ is the set of natural numbers. ϑ is an arbitrary $C^\infty([0,\infty))$-function such that $\vartheta = 0$ near 0 and $\vartheta = 1$ near infinity. Q_j is the multiplication operator by the coordinate x_j in $\mathcal{H}$, and $Q := (Q_1, Q_2, Q_3)$. The notation a.e. stands for "almost everywhere" and refers to the Lebesgue measure, and the expression $\langle \cdot \rangle$ corresponds to $\sqrt{1 + (\cdot)^2}$. We write $\mathcal{D}(S)$ for the domain of a selfadjoint operator (or a form) S. Finally, the limiting absorption principle for H is going to be expressed in terms of the Banach space $\mathcal{K} := (\mathcal{D}(\langle Q_3 \rangle), \mathcal{H})_{1/2,1}$ defined by real interpolation [1, Chapter 2]. For convenience, we recall that the weighted space $\mathcal{H}_s := \mathcal{D}(\langle Q_3 \rangle^s)$ is contained in $\mathcal{K}$ for each $s > 1/2$.

The perturbation V splits into two parts: a regular matrix valued function and a singular matrix valued function with compact support. The following definitions concern the former part.

Definition 1.1. Let V be a multiplication operator associated with an element of $\mathsf{L}^\infty(\mathbb{R}^3; \mathscr{B}_{\mathrm{h}}(\mathbb{C}^4))$.

(a) V is *small at infinity* if $\lim_{r\to\infty} \|\vartheta(|Q|/r)V\| = 0$,
(b) V is *short-range* if $\int_1^\infty \mathrm{d}r\, \|\vartheta(|Q_3|/r)V\| < \infty$,
(c) Assume that V is continuously differentiable with respect to x_3, and that the map $x \mapsto \langle x_3 \rangle (\partial_3 V)(x)$ belongs to $\mathsf{L}^\infty(\mathbb{R}^3; \mathscr{B}_{\mathrm{h}}(\mathbb{C}^4))$, then V is *long-range* if

$$\int_1^\infty \frac{\mathrm{d}r}{r} \big\| \vartheta\big(|Q_3|/r\big) \langle Q_3 \rangle (\partial_3 V) \big\| < \infty.$$

Note that Definitions 1.1(b) and 1.1(c) differ from the standard ones: the decay rate is imposed only in the x_3 direction. In the sequel we consider a magnetic field $B \in \mathsf{L}^\infty_{\mathrm{loc}}(\mathbb{R}^2; \mathbb{R})$ and always choose a vector potential $\vec{a} = (a_1, a_2, 0)$ in $\mathsf{L}^\infty_{\mathrm{loc}}(\mathbb{R}^2; \mathbb{R}^3)$, e.g. the one obtained by means of the transversal gauge [17, Section 8.4.2]. We are now in a position to state our main result. Let us already mention that Proposition 4.3 contains more information on the distinguished selfadjoint operator H.

Theorem 1.2. *Assume that B belongs to $\mathsf{L}^\infty_{\mathrm{loc}}(\mathbb{R}^2; \mathbb{R})$ and that $V(x)$ belongs to $\mathscr{B}_{\mathrm{h}}(\mathbb{C}^4)$ for a.e. $x \in \mathbb{R}^3$. Suppose that there exist $\chi \in C_0^\infty(\mathbb{R}^3; \mathbb{R})$, a finite set $\Gamma \subset \mathbb{R}^3$, and a positive number $\nu < 1$ such that*:

(i) *$V_{\mathrm{reg}} := (1 - \chi)V$ belongs to $\mathsf{L}^\infty(\mathbb{R}^3; \mathscr{B}_{\mathrm{h}}(\mathbb{C}^4))$, is small at infinity and can be written as the sum of a short-range and a long-range potential,*
(ii) *$V_{\mathrm{sing}} := \chi V$ can be written as the sum of two matrix-valued Borel functions $V_{\mathrm{loc}} \in \mathsf{L}^3_{\mathrm{loc}}(\mathbb{R}^3; \mathscr{B}_{\mathrm{h}}(\mathbb{C}^4))$ and V_{c} with*

$$\big\| V_{\mathrm{c}}(x) \big\|_{\mathscr{B}_{\mathrm{h}}(\mathbb{C}^4)} \leqslant \sum_{a \in \Gamma} \frac{\nu}{|x - a|} \quad \forall x \in \mathbb{R}^3.$$

Then there exists a unique selfadjoint operator H in $\mathcal{H}$, formally equal to $H_0 + V$, with domain $\mathcal{D}(H) \subset \mathcal{H}^{1/2}_{\mathrm{loc}}(\mathbb{R}^3; \mathbb{C}^4)$, such that:

(a) *$\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0)$,*

(b) *the point spectrum of the operator H in $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$ is composed of eigenvalues of finite multiplicity and with no accumulation point in $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$,*
(c) *the operator H has no singular continuous spectrum in $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$,*
(d) *the limits $\lim_{\varepsilon\searrow 0}\langle\psi,(H-\lambda\mp i\varepsilon)^{-1}\psi\rangle$ exist for each $\psi\in\mathcal{K}$, uniformly in λ on each compact subset of $\mathbb{R}\setminus\{\sigma^0_{\mathrm{sym}}\cup\sigma_{\mathrm{pp}}(H)\}$.*

As usual, the limiting absorption principle obtained in (d) leads to H-smooth operators, which imply for suitable short-range perturbations the existence of local wave operators. Since these constructions are rather standard, we shall not develop them here.

Let us finally give a description of the organisation of this paper and make a comment on its relation with the earlier work [16]. In Section 2 we study the operator H_0 and construct a suitable operator conjugated to H_0. The Mourre estimate is given at the end of Section 2.2. Regular perturbations are introduced in Section 3 and their properties with respect to the conjugate operator are then obtained. A version of Theorem 1.2 for regular perturbations is proved in Theorem 3.3. In Section 4 the singular part of the potential is added and a description of the selfadjoint operator H_0+V is given in Proposition 4.3. Last part of Section 4 is devoted to the proof of our main result in its full generality.

The major improvements contained in this paper are mainly due to (i) the use of a simple scalar conjugate operator (see Section 2.2), and (ii) the application of the new approach of [8] developed for dealing with singular perturbations (see Section 4). These two new technical tools allow us to treat Coulomb singularities and long-range matrix valued potentials. In the same time, we extend the class of magnetic fields that can be considered from continuous ones to locally bounded ones. Due to these various improvements, not a single result from [16] can be quoted without changing its statement or its proof. Therefore the present paper is self-contained and does not depend on any previous results from [16].

2. The unperturbed operator

2.1. Preliminaries

Let us start by recalling some known results. Since $\vec{a}$ belongs to $\mathsf{L}^\infty_{\mathrm{loc}}(\mathbb{R}^2;\mathbb{R}^3)$, it follows from [8, Lemma 4.3] and [4, Theorem 1.3] that H_0 is essentially selfadjoint on $\mathscr{D}:=C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$, with $\mathcal{D}(H_0)\subset\mathcal{H}^{1/2}_{\mathrm{loc}}\equiv\mathcal{H}^{1/2}_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{C}^4)$ (the local Sobolev space of order 1/2 of functions on $\mathbb{R}^3$ with values in $\mathbb{C}^4$). Moreover the spectrum of H_0 is symmetric with respect to 0 and does not contain the interval $(-m,m)$ [17, Section 5.5.2 and Corollary 5.14].

We now introduce a suitable representation of the Hilbert space $\mathcal{H}$. We consider the partial Fourier transformation

$$\mathscr{F}:\mathscr{D}\to\int_{\mathbb{R}}^{\oplus}\mathrm{d}\xi\,\mathcal{H}_{12},\quad (\mathscr{F}\psi)(\xi):=\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\mathrm{d}x_3\,\mathrm{e}^{-i\xi x_3}\psi(\cdot,x_3),\tag{2.1}$$

where $\mathcal{H}_{12} := \mathsf{L}^2(\mathbb{R}^2;\mathbb{C}^4)$. This map extends uniquely to a unitary operator from $\mathcal{H}$ onto $\int_{\mathbb{R}}^{\oplus} \mathrm{d}\xi\, \mathcal{H}_{12}$, which we denote by the same symbol $\mathscr{F}$. One obtains then the following direct integral decomposition of H_0:

$$\mathscr{F} H_0 \mathscr{F}^{-1} = \int_{\mathbb{R}}^{\oplus} \mathrm{d}\xi\, H_0(\xi),$$

where $H_0(\xi)$ is the selfadjoint operator in $\mathcal{H}_{12}$ acting as $\alpha_1\Pi_1 + \alpha_2\Pi_2 + \alpha_3\xi + \beta m$ on $C_0^\infty(\mathbb{R}^2;\mathbb{C}^4)$. In the following remark we draw the connection between the operators H_0, $H_0(0)$ and the internal-type operator H^0.

Remark 2.1. The operator $H_0(0)$ acting on $C_0^\infty(\mathbb{R}^2;\mathbb{C}^4)$ is unitarily equivalent to the direct sum

$$\begin{pmatrix} m & \Pi_- \\ \Pi_+ & -m \end{pmatrix} \oplus \begin{pmatrix} m & \Pi_+ \\ \Pi_- & -m \end{pmatrix}$$

acting on $C_0^\infty(\mathbb{R}^2;\mathbb{C}^2) \oplus C_0^\infty(\mathbb{R}^2;\mathbb{C}^2)$, where $\Pi_\pm := \Pi_1 \pm i\Pi_2$. These two matrix operators act in $\mathsf{L}^2(\mathbb{R}^2;\mathbb{C}^2)$ and are essentially selfadjoint on $C_0^\infty(\mathbb{R}^2;\mathbb{C}^2)$ [5, Theorem 2.1]. The first one is equal to H^0, while the second one is unitarily equivalent to $-H^0$ (this can be obtained with the abstract Foldy–Wouthuysen transformation [17, Theorem 5.13]). Therefore $H_0(0)$ is essentially selfadjoint on $C_0^\infty(\mathbb{R}^2;\mathbb{C}^4)$, and $H_0(\xi) = H_0(0) + \alpha_3\xi$ for each $\xi \in \mathbb{R}$. Since $\alpha_3 H_0(0) + H_0(0)\alpha_3 = 0$ it follows that $H_0(\xi)^2 = H_0(0)^2 + \xi^2$, and

$$\sigma\big[H_0(\xi)^2\big] = \sigma\big[H_0(0)^2 + \xi^2\big] = \big(\sigma_0^{\mathrm{sym}}\big)^2 + \xi^2. \tag{2.2}$$

Thus one has the identity

$$H_0^2 = H_0(0)^2 \otimes 1 + 1 \otimes P_3^2$$

with respect to the tensorial decomposition $\mathsf{L}^2(\mathbb{R}^2;\mathbb{C}^4) \otimes \mathsf{L}^2(\mathbb{R})$ of $\mathcal{H}$. In particular the spectrum of H_0^2 is purely absolutely continuous and equal to the interval $[\mu_0^2, \infty)$, where

$$\mu_0 := \inf\big|\sigma_{\mathrm{sym}}^0\big| \geqslant m.$$

Since the spectrum of H_0 is symmetric with respect to 0, it follows that

$$\sigma(H_0) = (-\infty, -\mu_0] \cup [\mu_0, +\infty).$$

We now state three technical lemmas that are constantly used in the sequel. Proofs can be found in Appendix A.

Lemma 2.2.

(a) *For each $n \in \mathbb{N}$, $H_0^{-n}\mathscr{D}$ and $|H_0|^{-n}\mathscr{D}$ are included in $\mathcal{D}(Q_3)$,*
(b) *$P_3|H_0|^{-1}$ is a bounded selfadjoint operator equal to $|H_0|^{-1}P_3$ on $\mathcal{D}(P_3)$. In particular, $|H_0|^{-1}\mathcal{H}$ is included in $\mathcal{D}(P_3)$.*

Lemma 2.3. *Let g be in $C^1(\mathbb{R})$ with g' bounded, and let $n \in \mathbb{N}$. Then $\mathcal{D}(Q_3)$ is included in $\mathcal{D}[g(Q_3)]$, and the following equality holds on $H_0^{-n}\mathscr{D}$:*

$$H_0^{-1} g(Q_3) - g(Q_3) H_0^{-1} = i H_0^{-1} \alpha_3 g'(Q_3) H_0^{-1}.$$

The last statement implies that the commutator of H_0^{-1} and $g(Q_3)$, defined on the core $\mathscr{D}$ of $g(Q_3)$, extends uniquely to a bounded operator. In the framework of [1, Definition 6.2.2], this means that the operator H_0 is of class $C^1(g(Q_3))$.

Given two appropriate functions f and g, we recall some properties of the commutator $[f(P_3), g(Q_3)]$ acting in the weighted space $\mathcal{H}_s$, $s \in \mathbb{R}$. We use the notation $\widehat{f}$ for the Fourier transform of f, and $S^m(\mathbb{R})$ for the vector space of symbols of degree m on $\mathbb{R}$.

Lemma 2.4. *Let $s \geqslant 0$ and $g \in S^1(\mathbb{R})$. Suppose that $f \in BC^\infty(\mathbb{R})$ is such that $x \mapsto \langle x \rangle^s \widehat{f'}(x)$ belongs to $\mathsf{L}^1(\mathbb{R})$. Then $f(P_3)$ leaves $\mathcal{D}(Q_3)$ invariant, and the operator $f(P_3)g(Q_3) - g(Q_3)f(P_3)$ defined on $\mathcal{D}(Q_3)$ extends uniquely to an operator in $\mathscr{B}(\mathcal{H})$, which is denoted by $[f(P_3), g(Q_3)]$. Furthermore, this operator restricts to an element of $\mathscr{B}(\mathcal{H}_s)$.*

2.2. *Strict Mourre estimate for the free Hamiltonian*

We now gather some results on the regularity of H_0 with respect to a conjugate operator. This operator is constructed with a function F satisfying the following hypotheses.

Assumption 2.5. *F is a non-decreasing element of $C^\infty(\mathbb{R}; \mathbb{R})$ with $F(x) = 0$ for $x \leqslant 0$ and $F(x) = 1$ for $x \geqslant 1$.*

A useful property of such a function is that $\widehat{F^{(k)}}$ belongs to the Schwartz space on $\mathbb{R}$, for any integer $k > 0$. In the sequel we always assume that F is a function satisfying Assumption 2.5. In particular, it follows that the formal expression

$$A := \frac{1}{2}\big[Q_3 F(P_3) + F(P_3) Q_3\big] \tag{2.3}$$

leads to a well-defined symmetric operator on $\mathscr{D}$.

Lemma 2.6. *The operator A is essentially selfadjoint on $\mathscr{D}$, and its closure is essentially selfadjoint on any core for $\langle Q_3 \rangle$.*

Proof. The claim is a consequence of Nelson's criterion of essential selfadjointness [15, Theorem X.37] applied to the triple $\{\langle Q_3 \rangle, A, \mathscr{D}\}$. So we simply verify the two hypotheses of that theorem. By using Lemma 2.4, one first obtains that for all $\psi \in \mathscr{D}$:

$$\|A\psi\| = \left\| \left(F(P_3) Q_3 - \frac{1}{2}\big[F(P_3), Q_3\big] \right) \psi \right\| \leqslant \mathrm{c} \big\| \langle Q_3 \rangle \psi \big\|$$

for some constant $\mathrm{c} > 0$ independent of ψ. Furthermore, one has for all $\psi \in \mathscr{D}$:

$$\big\langle A\psi, \langle Q_3 \rangle \psi \big\rangle - \big\langle \langle Q_3 \rangle \psi, A\psi \big\rangle = \tfrac{1}{2}\big\{ \big\langle Q_3 \psi, \big[F(P_3), \langle Q_3 \rangle\big]\psi \big\rangle - \big\langle \big[F(P_3), \langle Q_3 \rangle\big]\psi, Q_3 \psi \big\rangle \big\}.$$

Since $[F(P_3), \langle Q_3\rangle] \in \mathscr{B}(\mathcal{H}_{1/2})$ by Lemma 2.4 and since $Q_3 \in \mathscr{B}(\mathcal{H}_{1/2}, \mathcal{H}_{-1/2})$, one easily gets the estimate

$$\left|\left\langle A\psi, \langle Q_3\rangle\psi\right\rangle - \left\langle\langle Q_3\rangle\psi, A\psi\right\rangle\right| \leqslant \mathrm{D}\left\|\langle Q_3\rangle^{1/2}\psi\right\|^2$$

for all $\psi \in \mathscr{D}$ and a constant $\mathrm{D} > 0$ independent of ψ. □

From now on we set $\mathcal{G} := \mathcal{D}(H_0)$, and we write $\mathcal{G}^*$ for the adjoint space of $\mathcal{G}$. One has the continuous dense embeddings $\mathcal{G} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{G}^*$, where $\mathcal{H}$ is identified with its adjoint through the Riesz isomorphism. In the sequel we constantly use the fact that the bounded operators H_0^{-1} and $F(P_3)$ commute.

Proposition 2.7.

(a) *The quadratic form $\mathcal{D}(A) \ni \psi \mapsto \langle H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}\psi\rangle$ extends uniquely to the bounded form defined by the operator $-H_0^{-1}\alpha_3 F(P_3)H_0^{-1} \in \mathscr{B}(\mathcal{H})$.*
(b) *The group $\{e^{itA}\}_{t\in\mathbb{R}}$ leaves $\mathcal{G}$ invariant.*
(c) *The quadratic form*

$$\mathcal{D}(A) \ni \psi \mapsto \left\langle H_0^{-1}\alpha_3 F(P_3)H_0^{-1}\psi, iA\psi\right\rangle - \left\langle A\psi, iH_0^{-1}\alpha_3 F(P_3)H_0^{-1}\psi\right\rangle, \tag{2.4}$$

extends uniquely to a bounded form on $\mathcal{H}$.

In the framework of [1, Definition 6.2.2], statements (a) and (c) mean that H_0 is of class $C^1(A)$ and $C^2(A)$, respectively.

Proof. (a) For any $\psi \in \mathscr{D}$, one gets

$$\begin{aligned} 2\left[\left\langle H_0^{-1}\psi, iA\psi\right\rangle - \left\langle A\psi, iH_0^{-1}\psi\right\rangle\right] &= \left\langle i\left[H_0^{-1}, Q_3\right]\psi, F(P_3)\psi\right\rangle + \left\langle F(P_3)\psi, i\left[H_0^{-1}, Q_3\right]\psi\right\rangle \\ &= -2\left\langle\psi, H_0^{-1}\alpha_3 F(P_3)H_0^{-1}\psi\right\rangle, \end{aligned} \tag{2.5}$$

by using Lemma 2.3. Since $\mathscr{D}$ is a core for A, then the statement follows by density. We shall write $i[H_0^{-1}, A]$ for the bounded extension of the quadratic form $\mathcal{D}(A) \ni \psi \mapsto \langle H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}\psi\rangle$.

(b) Let $i[H_0, A]$ be the operator in $\mathscr{B}(\mathcal{G}, \mathcal{G}^*)$ associated with the unique extension to $\mathcal{G}$ of the quadratic form $\psi \mapsto \langle H_0\psi, iA\psi\rangle - \langle A\psi, iH_0\psi\rangle$ defined for all $\psi \in \mathcal{G} \cap \mathcal{D}(A)$. Then $\mathcal{G}$ is invariant under $\{e^{itA}\}_{t\in\mathbb{R}}$ if H_0 is of class $C^1(A)$ and if $i[H_0, A]\mathcal{G} \subset \mathcal{H}$ [7, Lemma 2]. From Eq. (2.5) and [1, Eq. (6.2.24)], one obtains the following equalities valid in form sense on $\mathcal{H}$:

$$-H_0^{-1}\alpha_3 F(P_3)H_0^{-1} = i\left[H_0^{-1}, A\right] = -H_0^{-1}i[H_0, A]H_0^{-1}.$$

Thus $i[H_0, A]$ and $\alpha_3 F(P_3)$ are equal as operators in $\mathscr{B}(\mathcal{G}, \mathcal{G}^*)$. But since the latter applies $\mathcal{G}$ into $\mathcal{H}$, $i[H_0, A]\mathcal{G}$ is included in $\mathcal{H}$.

(c) The boundedness on $\mathscr{D}$ of the quadratic form (2.4) follows by inserting (2.3) into the right-hand side term of (2.4), by applying repeatedly Lemma 2.3 with $g(Q_3) = Q_3$, and by taking Lemma 2.4 into account. Then one concludes by using the density of $\mathscr{D}$ in $\mathcal{D}(A)$. □

It will also be useful to show that $|H_0|$ is of class $C^1(A)$.

Lemma 2.8. *The quadratic form* $\mathcal{D}(A) \ni \psi \mapsto \langle |H_0|^{-1}\psi, iA\psi\rangle - \langle A\psi, i|H_0|^{-1}\psi\rangle$ *extends uniquely to the bounded form defined by* $-|H_0|^{-1}F(P_3)P_3|H_0|^{-2} \in \mathscr{B}(\mathcal{H})$.

Proof. A direct calculation using the transformation (2.1) and Lemma 2.2 gives for any $\psi \in \mathscr{D}$

$$i\big[|H_0|^{-1}, Q_3\big]\psi = -P_3|H_0|^{-3}\psi.$$

Thus one has the equalities

$$\begin{aligned} &2\big(\big\langle |H_0|^{-1}\psi, iA\psi\big\rangle - \big\langle A\psi, i|H_0|^{-1}\psi\big\rangle\big) \\ &\quad = \big\langle i\big[|H_0|^{-1}, Q_3\big]\psi, F(P_3)\psi\big\rangle + \big\langle F(P_3)\psi, i\big[|H_0|^{-1}, Q_3\big]\psi\big\rangle \\ &\quad = -2\big\langle \psi, |H_0|^{-1}F(P_3)P_3|H_0|^{-2}\psi\big\rangle. \end{aligned}$$

Since $\mathscr{D}$ is a core for A, then the statement follows by density. □

Due to Lemma 2.8 and [1, Eq. (6.2.24)] the operator $i[|H_0|, A]$ associated with the unique extension to $\mathcal{G}$ of the quadratic form $\mathcal{G} \cap \mathcal{D}(A) \ni \psi \mapsto \langle |H_0|\psi, iA\psi\rangle - \langle A\psi, i|H_0|\psi\rangle$ is equal to $F(P_3)P_3|H_0|^{-1} \in \mathscr{B}(\mathcal{H})$. From now on we simply write R for this operator and T for the operator $\alpha_3 F(P_3) \equiv i[H_0, A] \in \mathscr{B}(\mathcal{H})$.

In the following definition, we introduce two functions giving the optimal value to a Mourre-type inequality. Remark that a slight modification has been done with regard to the usual definition [1, Eq. (7.2.4)].

Definition 2.9. Let H be a selfadjoint operator in a Hilbert space $\mathcal{H}$ and assume that S is a symmetric operator in $\mathscr{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$. Let $E^H(\lambda;\varepsilon) := E^H((\lambda-\varepsilon, \lambda+\varepsilon))$ be the spectral projection of H for the interval $(\lambda-\varepsilon, \lambda+\varepsilon)$. Then, for all $\lambda \in \mathbb{R}$ and $\varepsilon > 0$, we set

$$\begin{aligned} \varrho_H^S(\lambda;\varepsilon) &:= \sup\big\{a \in \mathbb{R} \bigm| E^H(\lambda;\varepsilon) S E^H(\lambda;\varepsilon) \geqslant a E^H(\lambda;\varepsilon)\big\}, \\ \varrho_H^S(\lambda) &:= \sup_{\varepsilon>0} \varrho_H^S(\lambda;\varepsilon). \end{aligned}$$

Let us make three observations: the inequality $\varrho_H^S(\lambda;\varepsilon') \leqslant \varrho_H^S(\lambda;\varepsilon)$ holds whenever $\varepsilon' \geqslant \varepsilon$, $\varrho_H^S(\lambda) = +\infty$ if λ does not belong to the spectrum of H, and $\varrho_H^S(\lambda) \geqslant 0$ for all $\lambda \in \mathbb{R}$ if $S \geqslant 0$. We also mention that in the case of two selfadjoint operators H and A in $\mathcal{H}$, with H of class $C^1(A)$ and $S = i[H, A]$, the function $\varrho_H^S(\cdot)$ is equal to the function $\varrho_H^A(\cdot)$ defined in [1, Eq. (7.2.4)].

Lemma 2.10. *For* $\lambda > 0$ *and* $\varepsilon \in (0, \lambda)$*, one has* $\varrho_{H_0}^T(\lambda;\varepsilon) = \varrho_{H_0}^R(\lambda;\varepsilon)$. *Similarly, for* $\lambda < 0$ *and* $\varepsilon \in (0, |\lambda|)$*, one has* $\varrho_{H_0}^{-T}(\lambda;\varepsilon) = \varrho_{H_0}^R(\lambda;\varepsilon)$.

Proof. We give the proof of the first equality, the second one can be obtained in the same way.

Let $\varphi \in C_0^\infty(\mathbb{R};\mathbb{R})$ with $\operatorname{supp}(\varphi) \subset (0,\infty)$, and let $\psi \in \mathcal{D}(A)$. Since $\varphi(H_0) \in C^1(A)$ [1, Theorem 6.2.5], then $\varphi(H_0)\psi \in \mathcal{G} \cap \mathcal{D}(A)$. Thus by using the spectral theorem we get

$$\begin{aligned}
&\langle\psi, \varphi(H_0)T\varphi(H_0)\psi\rangle\\
&\quad=\langle H_0\varphi(H_0)\psi, iA\varphi(H_0)\psi\rangle-\langle A\varphi(H_0)\psi, iH_0\varphi(H_0)\psi\rangle\\
&\quad=\langle |H_0|\varphi(H_0)\psi, iA\varphi(H_0)\psi\rangle-\langle A\varphi(H_0)\psi, i|H_0|\varphi(H_0)\psi\rangle\\
&\quad=\langle\psi, \varphi(H_0)R\varphi(H_0)\psi\rangle.
\end{aligned}$$

Since $\mathcal{D}(A)$ is dense in $\mathcal{H}$ the identity

$$\langle\psi, \varphi(H_0)T\varphi(H_0)\psi\rangle=\langle\psi, \varphi(H_0)R\varphi(H_0)\psi\rangle$$

even holds for each $\psi\in\mathcal{H}$. Now, for $\lambda>0$ and $\varepsilon\in(0,\lambda)$ fixed one may choose $\eta\in C_0^\infty(\mathbb{R};\mathbb{R})$ with $\operatorname{supp}(\eta)\subset(0,\infty)$ satisfying $\eta(x)=1$ for all $x\in[\lambda-\varepsilon,\lambda+\varepsilon]$. Then

$$\begin{aligned}
E^{H_0}(\lambda;\varepsilon)TE^{H_0}(\lambda;\varepsilon)&=E^{H_0}(\lambda;\varepsilon)\eta(H_0)T\eta(H_0)E^{H_0}(\lambda;\varepsilon)\\
&=E^{H_0}(\lambda;\varepsilon)\eta(H_0)R\eta(H_0)E^{H_0}(\lambda;\varepsilon)\\
&=E^{H_0}(\lambda;\varepsilon)RE^{H_0}(\lambda;\varepsilon),
\end{aligned}$$

and the proof is complete. □

The operator $\mathscr{F}R\mathscr{F}^{-1}$ is decomposable, more precisely:

$$\mathscr{F}R\mathscr{F}^{-1}=\int_{\mathbb{R}}^{\oplus}\mathrm{d}\xi\,R(\xi)\quad\text{with } R(\xi)=F(\xi)\xi\left|H_0(\xi)\right|^{-1}\in\mathscr{B}(\mathcal{H}_{12}).$$

Taking advantage of this and of the direct integral decomposition of H_0, one obtains for each $\lambda\in\mathbb{R}$ and $\varepsilon>0$ the formula

$$\varrho_{H_0}^{R}(\lambda;\varepsilon)=\operatorname*{ess\,inf}_{\xi\in\mathbb{R}}\varrho_{H_0(\xi)}^{R(\xi)}(\lambda;\varepsilon).\tag{2.6}$$

Now we can deduce a lower bound for $\varrho_{H_0}^{T}(\cdot)$.

Proposition 2.11. *For $\lambda\geqslant 0$ one has*

$$\varrho_{H_0}^{T}(\lambda)\geqslant\inf\left\{\frac{F(\sqrt{\lambda^2-\mu^2})\sqrt{\lambda^2-\mu^2}}{\lambda}\;\middle|\;\mu\in\sigma_{\mathrm{sym}}^0\cap[0,\lambda]\right\}\tag{2.7}$$

with the convention that the infimum over an empty set is $+\infty$.

Proof. (i) Recall from Remark 2.1 that $\mu_0=\inf|\sigma_{\mathrm{sym}}^0|=\inf\{\sigma(H_0)\cap[0,+\infty)\}$. Thus, for $\lambda\in[0,\mu_0)$ the left-hand side of (2.7) is equal to $+\infty$, since λ does not belong to the spectrum of H_0. Then, (2.7) is obviously satisfied on $[0,\mu_0)$.

(ii) If $\lambda\in\sigma_{\mathrm{sym}}^0$, then the right-hand side term of (2.7) is equal to 0. However, due to Lemma 2.10 and the positivity of R, we have $\varrho_{H_0}^{T}(\lambda)\geqslant 0$. Hence the relation (2.7) is again satisfied.

(iii) Let $0 < \varepsilon < \mu_0 < \lambda$. Direct computations using the explicit form of $R(\xi)$ and the spectral theorem for the operator $H_0(\xi)$ show that for ξ fixed, one has

$$\varrho_{H_0(\xi)}^{R(\xi)}(\lambda;\varepsilon) = \inf\left\{\frac{F(\xi)\xi}{|\rho|} \;\Big|\; \rho \in (\lambda-\varepsilon,\lambda+\varepsilon)\cap\sigma\big[H_0(\xi)\big]\right\} \geqslant \frac{F(\xi)\xi}{\lambda+\varepsilon}. \tag{2.8}$$

On the other hand one has $\varrho_{H_0(\xi)}^{R(\xi)}(\lambda;\varepsilon) = +\infty$ if $(\lambda-\varepsilon,\lambda+\varepsilon)\cap\sigma[H_0(\xi)] = \emptyset$, and a fortiori

$$\varrho_{H_0(\xi)}^{R(\xi)}(\lambda;\varepsilon) = +\infty \quad \text{if } \big((\lambda-\varepsilon)^2,(\lambda+\varepsilon)^2\big)\cap\sigma\big[H_0(\xi)^2\big] = \emptyset.$$

Thus, by taking into account Eqs. (2.6), (2.8), the previous observation and relation (2.2), one obtains that

$$\varrho_{H_0}^{R}(\lambda;\varepsilon) \geqslant \operatorname{ess\,inf}\left\{\frac{F(\xi)\xi}{\lambda+\varepsilon} \;\Big|\; \xi^2 \in \big((\lambda-\varepsilon)^2,(\lambda+\varepsilon)^2\big) - \big(\sigma_{\mathrm{sym}}^0\big)^2\right\}. \tag{2.9}$$

Suppose now that $\lambda \notin \sigma_{\mathrm{sym}}^0$, define $\mu := \sup\{\sigma_{\mathrm{sym}}^0 \cap [0,\lambda]\}$ and choose $\varepsilon > 0$ such that $\mu < \lambda - \varepsilon$. Then the inequality (2.9) implies that

$$\varrho_{H_0}^{R}(\lambda;\varepsilon) \geqslant \frac{F(\sqrt{(\lambda-\varepsilon)^2-\mu^2})\sqrt{(\lambda-\varepsilon)^2-\mu^2}}{\lambda+\varepsilon}.$$

Since $\varrho_{H_0}^{T}(\lambda;\varepsilon) = \varrho_{H_0}^{R}(\lambda;\varepsilon)$, the relation (2.7) follows from the above formula when $\varepsilon \searrow 0$. □

Remark 2.12. Using the conjugate operator $-A$ instead of A, and thus dealing with $-T$ instead of T, one can show as in Proposition 2.11 that $-A$ is strictly conjugate to H_0 on $(-\infty,0]\setminus\sigma_{\mathrm{sym}}^0$; more precisely, one has for each $\lambda \leqslant 0$

$$\varrho_{H_0}^{-T}(\lambda) \geqslant \inf\left\{\frac{F(\sqrt{\lambda^2-\mu^2})\sqrt{\lambda^2-\mu^2}}{|\lambda|} \;\Big|\; \mu \in \sigma_{\mathrm{sym}}^0 \cap \big[0,|\lambda|\big]\right\}, \tag{2.10}$$

with the convention that the infimum over an empty set is $+\infty$. In the rest of the paper, for the sake of brevity, we shall mostly concentrate on the positive part of the spectrum of H_0, and give few hints on the trivial adaptations for the negative part of the spectrum.

3. The bounded perturbation

In this section we consider the operator $H := H_0 + W$ with a potential W belonging to $\mathsf{L}^\infty(\mathbb{R}^3;\mathscr{B}_{\mathrm{h}}(\mathbb{C}^4))$. The operator H is selfadjoint and its domain is equal to the domain $\mathcal{G} \equiv \mathcal{D}(H_0)$ of H_0. We first give a result on the difference of the resolvents $(H-z)^{-1} - (H_0-z)^{-1}$ and, as a corollary, we obtain the localization of the essential spectrum of H. For that purpose we recall that a selfadjoint operator S in $\mathcal{H}$ is said to be locally compact if $\eta(Q)(S+i)^{-1}$ is a compact operator for each $\eta \in C_0(\mathbb{R}^3)$.

Lemma 3.1. *Assume that W is small at infinity. Then for all $z \in \mathbb{C}\setminus\{\sigma(H)\cup\sigma(H_0)\}$ the difference $(H-z)^{-1} - (H_0-z)^{-1}$ is a compact operator. In particular $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0)$.*

Proof. Since W is bounded and small at infinity, it is enough to check that H_0 is locally compact [17, Section 4.3.4]. However, as already mentioned in Section 2.1, one has $\mathcal{G} \subset \mathcal{H}^{1/2}_{\mathrm{loc}}$. Hence the statement follows by usual arguments. $\square$

In order to obtain a limiting absorption principle for H, we shall invoke some abstract results. For that purpose, we first prove an optimal regularity condition of H with respect to A. We refer to [1, Chapter 5] for the definitions of the classes $C^{1,1}(A)$ and $C^{1,1}(A;\mathcal{G},\mathcal{G}^*)$, and for more explanations on regularity conditions. The optimality of the regularity condition in the framework of commutator methods is shown in [1, Appendix 7.B].

Proposition 3.2. *Let W be the sum of a short-range and a long-range potential. Then $H = H_0 + W$ is of class $C^{1,1}(A)$.*

Proof. Since $\{e^{itA}\}_{t\in\mathbb{R}}$ leaves $\mathcal{D}(H) \equiv \mathcal{G}$ invariant, it is equivalent to prove that H belongs to $C^{1,1}(A;\mathcal{G},\mathcal{G}^*)$ [1, Theorem 6.3.4(b)]. But in Proposition 2.7(c), it has already been shown that H_0 is of class $C^2(A)$, so that H_0 belongs to $C^{1,1}(A;\mathcal{G},\mathcal{G}^*)$. Thus it is enough to prove that W belongs to $C^{1,1}(A;\mathcal{G},\mathcal{G}^*)$, which is readily satisfied if $W \in C^{1,1}(A)$. In the short-range case, we shall use [1, Theorem 7.5.8] for the couple $\mathcal{H}$ and $\langle Q_3\rangle$. The non-trivial conditions needed for that theorem are obtained in point (i) below. In the long-range case, the claim follows by [1, Theorem 7.5.7], which can be applied because of point (ii) below.

(i) The first condition is trivially satisfied since $\{e^{it\langle Q_3\rangle}\}_{t\in\mathbb{R}}$ is a unitary C_0-group in $\mathcal{H}$. For the second condition, one has to check that $\langle Q_3\rangle^{-2}A^2$ defined on $\mathcal{D}(A^2)$ extends to an operator in $\mathscr{B}(\mathcal{H})$. After some commutator calculations performed on $\mathscr{D}$, one obtains that $\langle Q_3\rangle^{-1}A$ and $\langle Q_3\rangle^{-2}A$ are respectively equal on $\mathscr{D}$ to some operators S_1 and $S_2\langle Q_3\rangle^{-1}$ in $\mathscr{B}(\mathcal{H})$, where S_1 and S_2 are linear combinations of products of operators $f(P_3)$, $g(G_3)$ and $[h(P_3),\langle Q_3\rangle]$ with $f,g,h \in BC^\infty(\mathbb{R};\mathbb{R})$ and $\widehat{h'} \in \mathsf{L}^1(\mathbb{R})$. Since $\mathscr{D}$ is a core for A, these equalities even hold on $\mathcal{D}(A)$. Hence one has on $\mathcal{D}(A^2)$:

$$\langle Q_3\rangle^{-2}A^2 = \big(\langle Q_3\rangle^{-2}A\big)A = S_2\langle Q_3\rangle^{-1}A = S_2S_1.$$

In consequence $\langle Q_3\rangle^{-2}A^2$ is equal on $\mathcal{D}(A^2)$ to an operator in $\mathscr{B}(\mathcal{H})$. The statement follows then by density.

(ii) It has been proved in Lemma 2.6 that the inclusion $\mathcal{D}(\langle Q_3\rangle) \subset \mathcal{D}(A)$ holds. Furthermore the inequality $r\|(\langle Q_3\rangle + ir)^{-1}\| \leqslant const$ for all $r > 0$ is trivially satisfied. Thus one is left in proving that the commutator $i[W,A]$, defined as a quadratic form on $\mathcal{D}(A)$, with W a long-range potential, is bounded and satisfies the estimate

$$\int_1^\infty \frac{\mathrm{d}r}{r}\big\|\vartheta\big(\langle Q_3\rangle/r\big)[W,A]\big\| < \infty$$

for an arbitrary function $\vartheta \in C^\infty([0,\infty))$ with $\vartheta = 0$ near 0 and $\vartheta = 1$ near infinity. However, such an estimate can be obtained by mimicking the proof given in [1, p. 345] and by taking into account the particular properties of F. $\square$

Theorem 3.3. *Assume that B belongs to $\mathsf{L}^\infty_{\mathrm{loc}}(\mathbb{R}^2;\mathbb{R})$, and that W belongs to $\mathsf{L}^\infty(\mathbb{R}^3;\mathscr{B}_{\mathrm{h}}(\mathbb{C}^4))$, is small at infinity and can be written as the sum of a short-range and a long-range potential. Then statements* (a)–(d) *of Theorem* 1.2 *hold for $H = H_0 + W$.*

Proof. Statement (a) has already been proved in Lemma 3.1. Proposition 3.2 implies that both H_0 and H are of class $C^{1,1}(A)$. Furthermore, the difference $(H+i)^{-1}-(H_0+i)^{-1}$ is compact by Lemma 3.1, and $\varrho^T_{H_0}>0$ on $[0,\infty)\setminus\sigma^0_{\mathrm{sym}}$ due to Proposition 2.11. Hence A is strictly conjugate to H on $[0,\infty)\setminus\{\sigma^0_{\mathrm{sym}}\cup\sigma_{\mathrm{pp}}(H)\}$ due to [1, Theorems 7.2.9 and 7.2.13]. Similar arguments taking Remark 2.12 into account show that $-A$ is strictly conjugate to H on $(-\infty,0]\setminus\{\sigma^0_{\mathrm{sym}}\cup\sigma_{\mathrm{pp}}(H)\}$. The assertions (b) and (c) then follow by the abstract conjugate operator method [1, Corollary 7.2.11 and Theorem 7.4.2].

The limiting absorption principle directly obtained via [1, Theorem 7.4.1] is expressed in terms of the interpolation space $(\mathcal{D}(A),\mathcal{H})_{1/2,1}$, and of its adjoint. Since both are not standard spaces, one may use [1, Corollary 2.6.3] to show that $\mathcal{K}\subset(\mathcal{D}(A),\mathcal{H})_{1/2,1}$ and to get the statement (d). The only non-trivial hypothesis one has to verify is the inclusion $\mathcal{D}(\langle Q_3\rangle)\subset\mathcal{D}(A)$, which has already been shown in Lemma 2.6. □

Note that these results imply that H has a spectral gap. We are now ready to add a singular part to the perturbation W.

4. Locally singular perturbations

In this section we deal with perturbations which are locally singular. A particular attention is paid to Coulomb-type interactions. Our approach is deeply inspired from [8, Section 3]. In Lemma 3.4 of this reference, the authors show that if H and $\widetilde{H}$ are two selfadjoint operators in $\mathcal{H}$ that coincide in some neighbourhood of infinity and if one of them has a certain regularity property with respect to the operator Q, then the difference of their resolvents is short-range in the usual sense. This result is the key ingredient for what follows.

Let us first recall some notations. If $\Lambda\subset\mathbb{R}^3$ is an open set, then H_Λ is defined as the restriction of the selfadjoint operator H to the subset $\mathcal{D}(H_\Lambda):=\{\psi\in\mathcal{D}(H)\mid \mathrm{supp}(\psi)\subset\Lambda\}$. We write $H_\Lambda\subset\widetilde{H}$ if for each $\psi\in\mathcal{D}(H_\Lambda)$ one has $\psi\in\mathcal{D}(\widetilde{H})$ and $\widetilde{H}\psi=H\psi$. Next lemma is an application of the abstract result mentioned above that takes [1, Remark 7.6.9] and the observation following [8, Definition 2.16] into account.

Lemma 4.1. *Let H be as in Theorem 3.3, and let $\widetilde{H}$ be a selfadjoint operator in $\mathcal{H}$ such that $H_\Lambda\subset\widetilde{H}$ for some neighbourhood $\Lambda\subset\mathbb{R}^3$ of infinity. Then for each $z\in\mathbb{C}\setminus\{\sigma(H)\cup\sigma(\widetilde{H})\}$ and for each $\vartheta\in C^\infty([0,\infty))$ with $\vartheta=0$ near 0 and $\vartheta=1$ near infinity one has*:

$$\int_1^\infty \mathrm{d}r\,\big\|\vartheta\big(|Q|/r\big)\big[(\widetilde{H}-z)^{-1}-(H-z)^{-1}\big]\big\|<\infty. \tag{4.1}$$

Proof. Since the statement is an application of [8, Lemma 3.4] one only has to check its non-trivial hypotheses, i.e. (i) $\theta(Q)\mathcal{D}(H)\subset\mathcal{D}(H)$ for all $\theta\in C_0^\infty(\mathbb{R}^3)$, and (ii) for all $\theta\in C_0^\infty(\mathbb{R}^3\setminus\{0\})$ one has

$$\int_1^\infty \mathrm{d}r\big\{\big\|\big[\theta(Q/r),H\big]\big\|^2_{\mathcal{D}(H)\to\mathcal{H}}+\big\|\big[\theta(Q/r),\big[\theta(Q/r),H\big]\big]\big\|_{\mathcal{D}(H)\to\mathcal{H}}\big\}<\infty.$$

Condition (i) follows from the identity

$$\theta(Q)(H+i)^{-1} = (H+i)^{-1}\theta(Q) - i(H+i)^{-1}\alpha\cdot(\nabla\theta)(Q)(H+i)^{-1}$$

valid on $\mathcal{H}$ (the proof of this relation is similar to that of Lemma 2.3 but simpler since θ is a bounded function). For (ii) one observes that $[\theta(Q/r), H] = ir^{-1}\alpha\cdot(\nabla\theta)(Q/r)$ and that $[\theta(Q/r),[\theta(Q/r),H]] = 0$. Since $\|\alpha\cdot(\nabla\theta)(Q/r)\|$ is bounded uniformly in r and since $r\mapsto r^{-1}$ belongs to $\mathsf{L}^2([1,\infty),\mathrm{d}r)$, one readily finishes the proof. □

Taking last lemma into account, we can prove that H and $\widetilde{H}$ have several similar properties.

Lemma 4.2. *Let H and $\widetilde{H}$ be as in Lemma* 4.1, *and assume that $\widetilde{H}$ is locally compact. Then $\sigma_{\mathrm{ess}}(\widetilde{H}) = \sigma_{\mathrm{ess}}(H)$, $\widetilde{H}$ is of class $C^{1,1}(A)$, the operator A is strictly conjugate to $\widetilde{H}$ on* $[0,\infty)\setminus\{\sigma^0_{\mathrm{sym}}\cup\sigma_{\mathrm{pp}}(\widetilde{H})\}$ *and the operator $-A$ is strictly conjugate to $\widetilde{H}$ on* $(-\infty,0]\setminus\{\sigma^0_{\mathrm{sym}}\cup\sigma_{\mathrm{pp}}(\widetilde{H})\}$.

Proof. The difference $(\widetilde{H}+i)^{-1} - (H+i)^{-1}$ is a compact operator due to [8, Lemma 3.8] (the proof of this result is based on the fact that both H and $\widetilde{H}$ are locally compact and that H has some regularity properties with respect to the operator Q). This fact implies the first claim.

Since H and $\widetilde{H}$ have the same essential spectrum and H has a spectral gap, these operators have a common spectral gap, and thus there exists $z\in\mathbb{R}\setminus\{\sigma(H)\cup\sigma(\widetilde{H})\}$. Let $R := (H-z)^{-1}$ and $\widetilde{R} := (\widetilde{H}-z)^{-1}$, then $\widetilde{R}-R$ is compact. Furthermore, for each $\vartheta\in C^\infty([0,\infty))$ with $\vartheta = 0$ near 0 and $\vartheta = 1$ near infinity, it follows from Lemma 4.1 that $\|\vartheta(|Q|/r)(\widetilde{R}-R)\|\in\mathsf{L}^1([1,\infty),\mathrm{d}r)$. Then an easy calculation shows that one also has

$$\int_1^\infty \mathrm{d}r\,\big\|\vartheta\big(|Q_3|/r\big)(\widetilde{R}-R)\big\| < \infty.$$

By applying [1, Theorem 7.5.8] as in the proof of Proposition 3.2, it follows that $\widetilde{R}-R$ belongs to $C^{1,1}(A)$. Now R also belongs to $C^{1,1}(A)$ due to Proposition 3.2. Thus $\widetilde{R}$ belongs to $C^{1,1}(A)$ and the second claim is proved.

The last claim is obtained from what precedes as in the proof of Theorem 3.3. □

Thus one only has to put into evidence non-trivial perturbations $\widetilde{H}$ of H such that the hypotheses of the previous lemma are satisfied. For Coulomb perturbations of the free Dirac operator without magnetic field, we recall that some care has to be taken when choosing the selfadjoint extension to be considered (see for example [2,4,11,13] and references therein). Such a difficulty also occurs when a magnetic field is present. The treatment of this problem requires the introduction of some notations. $\mathcal{H}^s := \mathcal{H}^s(\mathbb{R}^3;\mathbb{C}^4)$, $s\in\mathbb{R}$, is the usual Sobolev space of functions on $\mathbb{R}^3$ with values in $\mathbb{C}^4$, $\mathscr{E}'(\mathbb{R}^3;\mathbb{C}^4)$ the set of compactly supported distributions on $\mathbb{R}^3$ with values in $\mathbb{C}^4$, $\mathcal{H}^s_{\mathrm{c}}(\mathbb{R}^3;\mathbb{C}^4) := \mathcal{H}^s\cap\mathscr{E}'(\mathbb{R}^3;\mathbb{C}^4)$, and H_m is the free Dirac operator $\alpha\cdot P+\beta m$ with domain $\mathcal{H}^1$ and form domain $\mathcal{H}^{1/2}$. Finally, if S is a selfadjoint operator in $\mathcal{H}$, we recall that there exist a unitary operator U and a positive selfadjoint operator $|S|$ such that $S = U|S| = |S|U$. The form associated with S is then defined by

$$h_S(\varphi,\psi) := \big\langle |S|^{1/2}\varphi, U|S|^{1/2}\psi\big\rangle,\quad \varphi,\psi\in\mathcal{D}(h_S) := \mathcal{D}\big(|S|^{1/2}\big).$$

Next statement is a corollary of the main result of [4] on selfadjoint extensions for the perturbed Dirac operators. The behaviour of the potential at infinity is prescribed by assumption (i) of Theorem 1.2, and the local regularity conditions of the potential are prescribed in assumption (ii) of that theorem. In order to be consistent with the notations of the introduction, we shall now write H for the "fully" perturbed operator (which was previously denoted by $\widetilde{H}$) and H_{reg} for the operator $H_0 + V_{\mathrm{reg}} \equiv H_0 + W$ (which was previously denoted by H for simplicity).

Proposition 4.3. *Assume that the hypotheses on B and V of Theorem* 1.2 *hold. Then there exists a unique selfadjoint operator H in $\mathcal{H}$, formally equal to $H_0 + V$, such that*:

(a) $\mathcal{D}(H) \subset \mathcal{H}^{1/2}_{\mathrm{loc}}$,
(b) $\forall \varphi \in \mathcal{D}(H)$ *and* $\psi \in \mathcal{H}^{1/2}_{\mathrm{c}}(\mathbb{R}^3; \mathbb{C}^4)$*, one has*

$$\langle H\varphi, \psi\rangle = h_{H_m}(\varphi, \psi) + h_{-\alpha\cdot a+V}(\varphi, \psi).$$

Proof. In order to apply [4, Theorem 1.3] one has to verify the first two hypotheses of that theorem. The first one consists in showing that for any $\phi \in C_0^\infty(\mathbb{R}^3, [0,1])$ one has $\phi(Q)(-\alpha \cdot a + V) \in \mathscr{B}(\mathcal{H}^{1/2}, \mathcal{H}^{-1/2})$. Fortunately, it is known that $\phi(Q)V_{\mathrm{loc}}$ is H_m-bounded with relative bound 0 and that $\phi(Q)V_{\mathrm{c}}$ is H_m-bounded with relative bound 2ν. Moreover V_{reg} belongs to $\mathscr{B}(\mathcal{H})$ and the vector potential a is in $\mathsf{L}^\infty_{\mathrm{loc}}(\mathbb{R}^2; \mathbb{R}^3)$. Thus the hypothesis $\phi(Q)(-\alpha \cdot a + V) \in \mathscr{B}(\mathcal{H}^{1/2}, \mathcal{H}^{-1/2})$ is clearly fulfilled. It follows that $H_m + \phi(Q)(-\alpha \cdot a + V)$ can be defined as an operator sum in $\mathscr{B}(\mathcal{H}^{1/2}, \mathcal{H}^{-1/2})$.

The second hypothesis requires that for any $\phi \in C_0^\infty(\mathbb{R}^3, [0,1])$ the operator $H_\phi := H_m + \phi(Q)(-\alpha \cdot a + V)$ defined on

$$\mathcal{D}_\phi := \bigl\{\varphi \in \mathcal{H}^{1/2} \bigm| \bigl[H_m + \phi(Q)(-\alpha \cdot a + V)\bigr]\varphi \in \mathcal{H}\bigr\}$$

is a selfadjoint operator. Now, such a statement follows from the main result of [13] and [14] (see also [11]), which we recall in our setting: under our assumptions on V, there exists a unique selfadjoint operator H^ϕ such that $\mathcal{D}(H^\phi) \subset \mathcal{H}^{1/2}$ and

$$\bigl\langle H^\phi\varphi, \psi\bigr\rangle = h_{H_m}(\varphi, \psi) + h_{\phi(Q)(-\alpha\cdot a+V)}(\varphi, \psi), \quad \forall \varphi \in \mathcal{D}\bigl(H^\phi\bigr),\ \psi \in \mathcal{H}^{1/2}.$$

Since H_ϕ has the same properties, then H_ϕ is equal to H^ϕ by unicity, and the second hypothesis of [4, Theorem 1.3] is thus fulfilled. □

We can finally prove our main result.

Proof of Theorem 1.2. Clearly the operator $H_{\mathrm{reg}} = H_0 + V_{\mathrm{reg}}$ is selfadjoint and satisfies the hypotheses of Theorem 3.3. Let $\Lambda \subset \mathbb{R}^3$ be a neighbourhood of infinity such that

$$\Lambda \cap \operatorname{supp}(\chi) = \emptyset.$$

Then, using the definitions of $\mathcal{D}[(H_{\mathrm{reg}})_\Lambda]$, $\mathcal{D}(H)$ and V_{reg}, we get

$$\begin{aligned}\mathcal{D}\big[(H_{\mathrm{reg}})_\Lambda\big] &= \big\{\varphi \in \mathcal{H}^{1/2}_{\mathrm{loc}} \mid H_m\varphi + (-\alpha\cdot a + V_{\mathrm{reg}})\varphi \in \mathcal{H}, \operatorname{supp}(\varphi) \subset \Lambda\big\}\\ &= \big\{\varphi \in \mathcal{H}^{1/2}_{\mathrm{loc}} \mid H_m\varphi + (-\alpha\cdot a + V)\varphi \in \mathcal{H}, \operatorname{supp}(\varphi) \subset \Lambda\big\}\\ &\subset \big\{\varphi \in \mathcal{H}^{1/2}_{\mathrm{loc}} \mid H_m\varphi + (-\alpha\cdot a + V)\varphi \in \mathcal{H}\big\}\\ &= \mathcal{D}(H).\end{aligned}$$

Thus, the property $(H_{\mathrm{reg}})_\Lambda \subset H$ holds. Furthermore the operator H is locally compact due to the inclusion $\mathcal{D}(H) \subset \mathcal{H}^{1/2}_{\mathrm{loc}}$ (Proposition 4.3(a)). Thus the couple (H_{reg}, H) satisfies both hypotheses of Lemma 4.2. Then, statement (a) follows from Lemma 3.1 and from the first assertion of Lemma 4.2. Statements (b) and (c) follow from the other assertions of Lemma 4.2 and from the abstract conjugate operator method [1, Corollary 7.2.11 and Theorem 7.4.2]. Statement (d) is obtained as in Theorem 3.3. □

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Appendix A

Proof of Lemma 2.2. (a) Let φ, ψ be in $\mathscr{D}$. Using the transformation (2.1), one gets

$$\big\langle H_0^{-n}\varphi, Q_3\psi\big\rangle = \int_{\mathbb{R}} \mathrm{d}\xi \big\langle H_0(\xi)^{-n}(\mathscr{F}\varphi)(\xi), (i\partial_\xi \mathscr{F}\psi)(\xi)\big\rangle_{\mathcal{H}_{12}}.$$

Now the map $\mathbb{R} \ni \xi \mapsto H_0(\xi)^{-n} \in \mathscr{B}(\mathcal{H}_{12})$ is norm differentiable, with its derivative given by

$$-\sum_{j=1}^{n} H_0(\xi)^{-j}\alpha_3 H_0(\xi)^{j-n-1}.$$

Hence the collection $\{\partial_\xi[H_0(\xi)^{-n}(\mathscr{F}\varphi)(\xi)]\}_{\xi\in\mathbb{R}}$ belongs to $\int_{\mathbb{R}}^{\oplus} \mathrm{d}\xi\, \mathcal{H}_{12}$. Thus one can perform an integration by parts (with vanishing boundary contributions) and obtain

$$\big\langle H_0^{-n}\varphi, Q_3\psi\big\rangle = \int_{\mathbb{R}} \mathrm{d}\xi \big\langle i\partial_\xi\big[H_0(\xi)^{-n}(\mathscr{F}\varphi)(\xi)\big], (\mathscr{F}\psi)(\xi)\big\rangle_{\mathcal{H}_{12}}.$$

It follows that $|\langle H_0^{-n}\varphi, Q_3\psi\rangle| \leqslant const\|\psi\|$ for all $\psi \in \mathscr{D}$. Since Q_3 is essentially selfadjoint on $\mathscr{D}$, this implies that $H_0^{-n}\varphi$ belongs to $\mathcal{D}(Q_3)$. The second statement can be proved using a similar argument.

(b) The boundedness of $P_3|H_0|^{-1}$ is a consequence of the estimate

$$\operatorname{ess\,sup}_{\xi\in\mathbb{R}}\big\|\xi\,|H_0(\xi)|^{-1}\big\|_{\mathscr{B}(\mathcal{H}_{12})}=\operatorname{ess\,sup}_{\xi\in\mathbb{R}}\big\|\xi\,[H_0(0)^2+\xi^2]^{-1/2}\big\|_{\mathscr{B}(\mathcal{H}_{12})}<\infty$$

and of the direct integral formalism. The remaining assertions follow by standard arguments. □

Proof of Lemma 2.3. The first statement is easily obtained by using the equality $g(x)=g(0)+\int_0^x \mathrm{d}y\, g'(y)$. For the second one, let us observe that the following equality holds on $\mathscr{D}$:

$$H_0^{-1}g(Q_3)H_0=g(Q_3)+iH_0^{-1}\alpha_3 g'(Q_3). \tag{A.1}$$

Now, for $\varphi,\psi\in\mathscr{D}$ and $\eta\in H_0^{-n}\mathscr{D}$, one has

$$\begin{aligned}
&\langle\varphi,H_0^{-1}g(Q_3)\eta\rangle-\langle\varphi,g(Q_3)H_0^{-1}\eta\rangle\\
&\quad=\langle\varphi,H_0^{-1}g(Q_3)H_0\psi\rangle+\langle\varphi,H_0^{-1}g(Q_3)(\eta-H_0\psi)\rangle-\langle\bar g(Q_3)\varphi,H_0^{-1}\eta\rangle\\
&\quad=\langle\varphi,g(Q_3)\psi\rangle+\langle\varphi,iH_0^{-1}\alpha_3g'(Q_3)\psi\rangle+\langle\bar g(Q_3)H_0^{-1}\varphi,(\eta-H_0\psi)\rangle\\
&\qquad-\langle\bar g(Q_3)\varphi,H_0^{-1}\eta\rangle\\
&\quad=\langle\bar g(Q_3)\varphi,H_0^{-1}(H_0\psi-\eta)\rangle+\langle\varphi,iH_0^{-1}\alpha_3g'(Q_3)H_0^{-1}\eta\rangle\\
&\qquad+\langle\varphi,iH_0^{-1}\alpha_3g'(Q_3)H_0^{-1}(H_0\psi-\eta)\rangle+\langle\bar g(Q_3)H_0^{-1}\varphi,(\eta-H_0\psi)\rangle,
\end{aligned}$$

where we have used (A.1) in the second equality. Hence there exists a constant $\mathrm{c}>0$ (depending on φ) such that

$$\big|\langle\varphi,H_0^{-1}g(Q_3)\eta\rangle-\langle\varphi,g(Q_3)H_0^{-1}\eta\rangle-\langle\varphi,iH_0^{-1}\alpha_3g'(Q_3)H_0^{-1}\eta\rangle\big|\leqslant\mathrm{c}\|\eta-H_0\psi\|.$$

Then the statement is a direct consequence of the density of $H_0\mathscr{D}$ and $\mathscr{D}$ in $\mathcal{H}$. □

Proof of Lemma 2.4. The invariance of the domain of Q_3 follows from the fact that $f(P_3)\in C^1(Q_3)$. Thus the expression $f(P_3)g(Q_3)-g(Q_3)f(P_3)$ is well defined on $\mathcal{D}(Q_3)$. Moreover, by using the commutator expansions given in [1, Theorem 5.5.3], one gets the following equality in form sense on $\mathscr{D}$:

$$f(P_3)g(Q_3)-g(Q_3)f(P_3)=-i\int_0^1\mathrm{d}\tau\int_{\mathbb{R}}\mathrm{d}x\,\mathrm{e}^{iP_3\tau x}g'(Q_3)\mathrm{e}^{iP_3(1-\tau)x}\widehat{f'}(x). \tag{A.2}$$

Since the right-hand side extends to a bounded operator, and since $\mathscr{D}\subset\mathcal{D}(Q_3)$ is a core for $g(Q_3)$, the second statement follows.

The last statement is obtained by proving that the operator $\langle Q_3\rangle^s[f(P_3),g(Q_3)]\langle Q_3\rangle^{-s}$, defined in form sense on $\mathscr{D}$, extends to a bounded operator. Again, by using the explicit formula (A.2), the submultiplicative property of the function $\langle\cdot\rangle$ and the hypothesis on the map $x\mapsto\langle x\rangle^s\widehat{f'}(x)$, this result is easily obtained. □

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