Schnol's theorem and spectral properties of massless Dirac operators with scalar potentials.

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Abstract

The spectra of massless Dirac operators are of essential interest e.g. for the electronic properties of graphene, but fundamental questions such as the existence of spectral gaps remain open. We show that the eigenvalues of massless Dirac operators with suitable real-valued potentials lie inside small sets easily characterised in terms of properties of the potentials, and we prove a Schnol'-type theorem relating spectral points to polynomial boundedness of solutions of the Dirac equation. Moreover, we show that, under minimal hypotheses which leave the potential essentially unrestrained in large parts of space, the spectrum of the massless Dirac operator covers the whole real line; in particular, this will be the case if the potential is nearly constant in a sequence of regions.

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1 Introduction

The Dirac operators we shall consider in this paper are

$$H_2 = -i\,\sigma\cdot\nabla + q(x) \quad \text{in} \quad \mathsf{L}^2(\mathbb{R}^2;\mathbb{C}^2) \tag{1.1}$$

and

$$H_3 = -i\,\alpha\cdot\nabla + q(x) \quad \text{in} \quad \mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4), \tag{1.2}$$

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where $\sigma = (\sigma_1, \sigma_2)$ and $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ are given as follows:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

and

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \quad (j \in \{1, 2, 3\}) \quad \text{with} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The dot products are to be read as

$$\sigma \cdot \nabla = \sigma_1 \frac{\partial}{\partial x_1} + \sigma_2 \frac{\partial}{\partial x_2}$$

in (1.1) and

$$\alpha \cdot \nabla = \alpha_1 \frac{\partial}{\partial x_1} + \alpha_2 \frac{\partial}{\partial x_2} + \alpha_3 \frac{\partial}{\partial x_3}$$

in (1.2). The potential q is a real-valued function on $\mathbb{R}^d$, where $d = 2$ or $d = 3$, respectively. The operators H_2 and H_3 differ from the standard Dirac operator in that they lack a mass term, usually represented by an additional anti-commuting matrix: σ_3 for the two-dimensional case and

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

for the three-dimensional case, where I is a 2×2 identity matrix.

The purpose of the present paper is twofold. Firstly, we establish Schnol's theorem for H_d, $d = 2$ and 3, under minimal assumptions on q. Schnol's theorem for Schrödinger operators is well-known (cf. [6, p.21]); it asserts that an energy with polynomially bounded eigensolution belongs to the spectrum of the Schrödinger operator. In this context, we would like to mention some recent works on Schnol's theorem for generators of Dirichlet forms, cf. [4], [10] and [13]. To our knowledge, however, the present paper is the first to establish Schnol's theorem for Dirac operators. Secondly, we shall show that $\sigma(H_d) = \mathbb{R}$ under minimal assumptions on q as before. We shall not require any restriction on the growth or decay of the potential q at infinity.

The study of the spectrum of massless Dirac operators in the two- and three-dimensional case is intriguing, as the behaviour of these operators differs fundamentally from the more familiar cases of Schrödinger operators and Dirac operators with mass. The spectrum of the one-dimensional massless Dirac operator

$$H_1 = -i\sigma_2 \frac{d}{dx} + q(x) \quad \text{in} \quad \mathsf{L}^2(\mathbb{R}; \mathbb{C}^2) \tag{1.3}$$

covers the whole real axis and is purely absolutely continuous whenever $q \in \mathsf{L}^1_{loc}(\mathbb{R}, \mathbb{R})$. This surprising fact was first pointed out by one of the authors in [19]. By separation in spherical polar coordinates, this result also implies that $\sigma(H_d) = \mathbb{R}$ if q is rotationally symmetric. However, the situation is by no means clear in the more general higher-dimensional case. The two-dimensional massless Dirac operator is of particular interest because it governs electron transport in graphene, so its spectral properties will have a direct impact on the conductivity and potential use in electronic applications. It is known that total reflection of the quantum wave at a straight-edged potential step may occur [3], and initially there was some hope to capture bound states in localised quantum dots (see [3], Fig. 1(b)). However, this is impossible due to a result of [12] which, in particular, implies that a compactly supported potential cannot generate eigenvalues (see [12], Ex. 6.1). Furthermore, it is believed that the energy spectrum of graphene, irrespective of potential applied, has no bandgap (zero bandgap); see [3], [7], [15]. This question remains open, but from the results mentioned above it is clear that spectral phenomena such as gaps or eigenvalues will, if they occur at all, require potentials of a fairly complex global structure. Recently, the properties of disordered graphene have attracted much attention, and it is known [16] that the sources of disorder vary and can be described by various types of potentials. The dominant source of disorder is still under debate according to [26]. Under these circumstances, it is natural, from the mathematical point of view, to investigate spectral properties of H_d and, in particular, to make an attempt to show that $\sigma(H_d) = \mathbb{R}$, under minimal assumptions on the potential q.

An announcement of the present paper can be found in [21].

2 Embedded eigenvalues and the absolutely continuous spectrum

In contrast to the case of the one-dimensional Dirac operator H_1, the spectra of H_2 and H_3 are not always purely absolutely continuous regardless of q. Actually, in the three-dimensional case, we have an example of q which gives rise to a zero mode of H_3, *i.e.* an example of q for which H_3 has the embedded eigenvalue 0.

Example 2.1 *Let* $q(x) = -3/\langle x\rangle^2$, *where* $\langle x\rangle = \sqrt{1+|x|^2}$. *Then there exists a unique self-adjoint realization of* H_3 *in* $\mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4)$ *with* $\mathrm{Dom}(H_3) = \mathsf{H}^1(\mathbb{R}^3;\mathbb{C}^4)$, *the Sobolev space of order* 1. *If one puts*

$$f(x) = \langle x\rangle^{-3}(I_4 + i\alpha\cdot x)\phi_0$$

with ϕ_0 *a unit vector in* $\mathbb{C}^4$, *then a direct calculation shows that* $H_3 f = 0$. *Since* $f \in \mathsf{H}^1(\mathbb{R}^3;\mathbb{C}^4)$, *this implies that* $0 \in \sigma_{\mathrm{p}}(H_3)$. *Thus* H_3 *has a zero mode. As* $\lim_{|x|\to\infty} q(x) = 0$, *a simple singular sequence argument shows that* $\sigma(H_3) = \mathbb{R}$. *Hence the energy* 0 *is an embedded eigenvalue of* H_3.

We would like to mention that the potential q and the zero mode f in Example 2.1 were motivated by [14].

The analogous two-dimensional construction in Example 2.2 below gives a zero resonance of H_2, not a zero mode of H_2. We do not know if the potential q in Example 2.2 gives rise to a zero mode of H_2. However, zero modes of H_2 are known to occur with compactly supported rotationally symmetric potentials, see Theorem 3 of [20].

Example 2.2 *Let $q(x) = -2/\langle x\rangle^2$. Then there exists a unique self-adjoint realization of H_2 in $\mathsf{L}^2(\mathbb{R}^2;\mathbb{C}^2)$ with* $\mathrm{Dom}(H_2) = \mathsf{H}^1(\mathbb{R}^2;\mathbb{C}^2)$, *and $\sigma(H_2) = \mathbb{R}$. If*

$$\psi(x) = \langle x\rangle^{-2}(I_2 + i\sigma\cdot x)\phi_0,$$

ϕ_0 a unit vector in $\mathbb{C}^2$, then one sees that $H_2\psi = 0$. However, it is clear that $\psi \notin \mathsf{L}^2(\mathbb{R}^2;\mathbb{C}^2)$. Therefore, ψ is not a zero mode of H_2. On the other hand, one finds that $\psi \in \mathsf{L}^2_{-s}(\mathbb{R}^2;\mathbb{C}^2)$ for any $s > 0$, where

$$\mathsf{L}^2_{-s}(\mathbb{R}^2;\mathbb{C}^2) = \{\, \varphi \mid \|\langle x\rangle^{-s}\varphi\|_{L^2} < \infty \}.$$

This means that ψ is a zero resonance of H_2.

It is not an easy task to clarify whether H_d has embedded eigenvalues for general potentials. However, we have a good control of the embedded eigenvalues of H_d if $q(x)$ is rotationally symmetric. To formulate a result, we need to introduce the definition of the limit range $\mathcal{R}_\infty(q)$ of q:

$$\mathcal{R}_\infty(q) = \bigcap_{r>0} \overline{\{\, q(x) \mid |x| \geq r \}},$$

where $\overline{A}$ denotes the closure of a subset of $A \subset \mathbb{R}$.

Theorem 2.1 (Schmidt[20]) *Let $q(x) = \eta(|x|)$ and let $\eta \in \mathsf{L}^1_{loc}(0, \infty)$. Suppose that there exists a real number $\lambda \in \mathbb{R} \setminus \mathcal{R}_\infty(q)$ such that*

$$\frac{1}{r(\lambda - \eta(r)) - 1} \in BV(r_0, \infty) \tag{2.1}$$

for some $r_0 > 0$, where $BV(r_0, \infty)$ denotes the set of functions of bounded variations on the interval (r_0, ∞). Then $\sigma_p(H_d) \subset \mathcal{R}_\infty(q)$.

Theorem 2.1 is a direct consequence of [20, Corollary 1]. One should note that under the assumption that $\eta \in \mathsf{L}^1_{loc}(0, \infty)$ there exists a distinguished self-adjoint realization of H_d, see Propositions 2 and 3 of [20].

Note that the condition (2.1) just fails in the radially periodic case, i.e. if $\eta(r+p) = \eta(r)$ ($r \geq 0$) with period $p > 0$. Indeed, when we take $r, s \in [0, p]$ and $n \in \mathbb{N}$, then for λ not in the (limit) range of η,

$$\begin{aligned}
&\frac{1}{(r+np)(\lambda - \eta(r+np)) - 1} - \frac{1}{(s+np)(\lambda - \eta(s+np)) - 1}\\
&\sim \frac{1}{(r+np)(\lambda - \eta(r))} - \frac{1}{(s+np)(\lambda - \eta(s))}\\
&= \frac{sr}{(s+np)(r+np)} \left(\frac{1}{r\,(\lambda - \eta(r))} - \frac{1}{s\,(\lambda - \eta(s))} \right)\\
&\quad + \frac{np}{(s+np)(r+np)} \left(\frac{1}{\lambda - \eta(r)} - \frac{1}{\lambda - \eta(s)} \right)
\end{aligned}$$

as $n \to \infty$, so the total variation in the nth period interval is

$$\operatorname*{Var}_{r\in[np,\,(n+1)p]} \frac{1}{r(\lambda - \eta(r)) - 1)} \sim \frac{1}{np} \operatorname*{Var}_{[0,\,p]} \frac{1}{\lambda - \eta} \qquad (n \to \infty).$$

In fact, the limit range of the potential plays no role at all in the radially periodic case, as our following result shows.

Theorem 2.2 *Let $q(x) = \eta(|x|)$ and let $\eta \in L^1_{loc}(0, \infty)$ be p-periodic. Let $\hat{\eta} := \frac{1}{p}\int_0^p \eta$. Then H_d has purely absolutely continuous spectrum in $\mathbb{R} \setminus (\frac{\pi}{p}\mathbb{Z} + \hat{\eta})$.*

Proof. By a suitable shift of the spectral parameter, we may assume without loss of generality that $\hat{\eta} = 0$.

By separation of variables in polar coordinates (see e.g. [25], Appendix to Section 1),

$$H_d \cong \bigoplus_{k \in J_d} -i\sigma_2 \frac{d}{dr} + \eta(r) + \sigma_1 \frac{k}{r},$$

where the index set $J_d = \mathbb{Z} \setminus \{0\}$ if $d = 3$ and $J_d = \mathbb{Z} + \frac{1}{2}$ if $d = 2$. Hence it is sufficient to show that each of the half-line Dirac operators with the angular momentum term $\sigma_1 \frac{k}{r}$ has purely absolutely continuous spectrum in $\mathbb{R} \setminus \frac{\pi}{p}\mathbb{Z}$.

It follows from Gilbert-Pearson subordinacy theory ([8], [9]; see also [18]) that it is sufficient for this purpose to show that all solutions of the eigenvalue equation

$$-i\sigma_2 \frac{d}{dr}\, u(r) + \eta(r)\, u(r) + \sigma_1 \frac{k}{r}\, u(r) = \lambda\, u(r) \tag{2.2}$$

are bounded at infinity if $\lambda \notin \frac{\pi}{p}\mathbb{Z}$.

Let $\varepsilon > 0$; we shall prove the boundedness of all solutions of (2.2) for large r and for all $\lambda \in \Lambda := \mathbb{R} \setminus \bigcup_{n \in \mathbb{Z}} (\frac{n\pi}{p} - \varepsilon, \frac{n\pi}{p} + \varepsilon)$ by adapting an idea of Stolz [23]; see also [5, Theorem 5.2.1].

Let $Q(r) := \int_0^r \eta$ $(r \geq 0)$; then Q is p-periodic and $Q(0) = 0$. For $j \in \mathbb{N}$, the matrix-valued function $\Phi_j(r) := \exp\big[-i\sigma_2\{Q(r) - \lambda(r - (j-1)p)\}\big]$ $(r \geq 0)$ satisfies the unperturbed, periodic differential equation

$$-i\sigma_2 \frac{d}{dr}\, \Phi_j(r) + \eta(r)\, \Phi_j(r) = \lambda\, \Phi_j(r),$$

and $\Phi_j((j-1)p) = I$. $M(\lambda) := \Phi_j(jp) = I \cos \lambda p + i\sigma_2 \sin \lambda p$ is the monodromy matrix (cf. [5, p.5]) of the periodic equation and $D(\lambda) := \operatorname{tr} M(\lambda) = 2\cos \lambda p$ its discriminant (cf. [5, p.9]). Clearly there exists $\delta > 0$ such that $|D(\lambda)| \leq 2 - 2\delta$ $(\lambda \in \Lambda)$.

By the variation of constants method (cf. [5, p.3]), we can find an integral equation for the matrix-valued solution Ψ_j of (2.2) such that $\Psi_j((j-1)p) = I$,

$$\Psi_j(r) = \Phi_j(r) - \Phi_j(r) \int_{(j-1)p}^r \Phi_j(s)^{-1} \sigma_3 \frac{k}{s}\, \Psi_j(s)\, ds \qquad (r \geq (j-1)p). \tag{2.3}$$

Using the fact that Φ_j is always unitary, we hence obtain the estimate for the matrix operator norm

$$|\Psi_j(r)| \leq 1 + \int_{(j-1)p}^r \frac{|k|}{s}\, |\Psi_j(s)|\, ds \qquad (r \geq (j-1)p).$$

By Gronwall's inequality, it follows that

$$|\Psi_j(r)| \le \exp\left(|k| \log \frac{r}{(j-1)p}\right) = \frac{r^{|k|}}{(j-1)^{|k|}p^{|k|}},$$

and hence by (2.3), for $(j-1)p \le r \le jp$,

$$\begin{aligned}|\Psi_j(r) - \Phi_j(r)| &\le \int_{(j-1)p}^{r} \frac{|k|}{s} |\Psi_j(s)| \, ds \le \frac{r^{|k|} - (j-1)^{|k|}p^{|k|}}{(j-1)^{|k|}p^{|k|}} \\ &\le \frac{j^{|k|} - (j-1)^{|k|}}{(j-1)^{|k|}} = \big(1 + \frac{1}{j-1}\big)^{|k|} - 1 \to 0 \qquad (j \to \infty). \end{aligned} \tag{2.4}$$

In particular, the matrices $M_j(\lambda) := \Psi_j(jp)$ satisfy

$$\lim_{j\to\infty} |M_j(\lambda) - M(\lambda)| = 0 \tag{2.5}$$

uniformly in $\lambda \in \mathbb{R}$. This implies that $D_j(\lambda) := \operatorname{tr} M_j(\lambda) \to D(\lambda)$ uniformly in λ as $j \to \infty$. Thus there is $J \in \mathbb{N}$ such that $|D_j(\lambda)| \le 2 - \delta$ for all $j \ge J$ and $\lambda \in \Lambda$.

For such j and λ, the matrices $M_j(\lambda)$ have complex conjugate eigenvalues $\mu_j(\lambda), \overline{\mu_j(\lambda)}$, $|\mu_j(\lambda)| = 1$. (See [5, *Case 3* in p. 10] in conjunction with the fact that $\det\Psi_j(r) = 1$, which is obtained from [5, Liouville's formula in p.3]). A suitable matrix of eigenvectors can be written as

$$E_j(\lambda) := \begin{pmatrix} \mu_j(\lambda) - (M_j(\lambda))_{22} & \overline{\mu_j(\lambda)} - (M_j(\lambda))_{22} \\ (M_j(\lambda))_{21} & (M_j(\lambda))_{21} \end{pmatrix};$$

in the limit $j \to \infty$, this converges uniformly in $\lambda \in \Lambda$ to a corresponding matrix $E(\lambda)$ of eigenvectors of $M(\lambda)$ in view of (2.5).

Now consider the matrix-valued solution Ψ_J. For $n \ge J$ (omitting the variable λ for brevity),

$$\begin{aligned}\Psi_J(np) &= M_n M_{n-1} \cdots M_J \\ &= E_n \begin{pmatrix} \mu_n & 0 \\ 0 & \overline{\mu_n} \end{pmatrix} E_n^{-1} E_{n-1} \begin{pmatrix} \mu_{n-1} & 0 \\ 0 & \overline{\mu_{n-1}} \end{pmatrix} E_{n-1}^{-1} \cdots E_J \begin{pmatrix} \mu_J & 0 \\ 0 & \overline{\mu_J} \end{pmatrix} E_J^{-1}.\end{aligned}$$

Hence the matrix operator norm can be estimated as

$$|\Psi_J(np)| \le |E_n| \, |E_n^{-1} E_{n-1}| \, |E_{n-1}^{-1} E_{n-2}| \cdots |E_{J+1}^{-1} E_J| \, |E_J^{-1}|.$$

In order to estimate $|E_j^{-1} E_{j-1}|$, we again solve (2.2) on the interval $[(j-1)p, jp]$ by variation of constants, but this time using $\Psi_{j-1}(r-p)$ as a reference instead of $\Phi_j(r)$; this gives

$$\Psi_j(r) = \Psi_{j-1}(r-p) + \Psi_{j-1}(r-p) \int_{(j-1)p}^{r} \Psi_{j-1}(s-p)^{-1} \sigma_3 \, \frac{kp}{s(s-p)} \, \Psi_j(s) \, ds$$

$(r \ge (j-1)p)$. Consequently,

$$\begin{aligned}|M_j(\lambda) - M_{j-1}(\lambda)| &\le |M_{j-1}(\lambda)| \int_{(j-1)p}^{jp} |\Psi_{j-1}(s-p)^{-1}| \, \frac{|k|p}{s(s-p)} \, |\Psi_j(s)| \, ds \\ &\le C^3 |k| p \int_{(j-1)p}^{jp} \frac{ds}{s(s-p)}\end{aligned}$$

with a constant C which is independent of λ due to the uniform bound (2.4). This also implies such an estimate for $|D_j(\lambda) - D_{j-1}(\lambda)|$ and, since the D_j are Lipschitz continuous on Λ, for $|\mu_j(\lambda) - \mu_{j-1}(\lambda)|$ ($\lambda \in \Lambda$). Hence

$$|E_j(\lambda) - E_{j-1}(\lambda)| \leq C' \int_{(j-1)p}^{jp} \frac{ds}{s(s-p)}$$

with some other uniform constant C'. Now we can estimate

$$\begin{aligned} |\Psi_J(np)| &\leq |E_n|\,|E_J^{-1}| \prod_{j=J+1}^{n} |E_j^{-1}E_{j-1}| \leq C'' \prod_{j=J+1}^{n} (1 + |E_j^{-1}|\,|E_j - E_{j-1}|) \\ &\leq C'' \exp\left(\sum_{j=J+1}^{n} |E_j^{-1}|\,|E_j - E_{j-1}| \right) \leq C'' \exp\left(C''' \int_{Jp}^{np} \frac{ds}{s(s-p)} \right), \end{aligned}$$

with uniform constants C'', C'''; this is bounded as $n \to \infty$. Hence $\Psi_J(r)$ is bounded at infinity, since $\Psi_J(r) = \Psi_n(r)\Psi_J((n-1)p)$ and, by (2.4),

$$|\Psi_n(r)| \leq \big(1 + \frac{1}{n-1}\big)^{|k|} \leq 2^{|k|}$$

for $(n-1)p \leq r \leq np$ and $n > J$.

This concludes the proof of Theorem 2.2, since every solution of (2.2) is a linear combination of the columns of Ψ_J. ■

The above method of proof does not work at the points $\lambda \in \frac{\pi}{p}\mathbb{Z} + \hat{\eta}$; these points are potential candidates for embedded eigenvalues. However, it seems to be a rather delicate question to decide whether such embedded eigenvalues actually occur.

If q is not assumed to be rotationally symmetric, we can prove the following.

Theorem 2.3 *Let $q \in C^1(\mathbb{R}^d;\mathbb{R})$, and suppose that both q and $(x \cdot \nabla)q$ are bounded functions. Then $\sigma_p(H_d) \subset [m_q,\, M_q]$, where*

$$m_q = \inf_x \{q(x) + (x \cdot \nabla)q(x)\}, \quad M_q = \sup_x \{q(x) + (x \cdot \nabla)q(x)\}.$$

To prove Theorem 2.3, we shall apply the following simple abstract version of the virial theorem.

Lemma 2.1 (Balinsky and Evans[1], [2]) *Let $U(a)$, $a > 0$, be a one-parameter family of unitary operators on a Hilbert space $\mathcal{H}$, which converges strongly to the identity as $a \to 1$. Let T be a self-adjoint operator in $\mathcal{H}$ and $T_a := aU(a)TU(a)^{-1}$. If f belongs to* $\mathrm{Dom}(T) \cap \mathrm{Dom}(T_a)$ *and is an eigenvector of T corresponding to an eigenvalue λ, then*

$$\lim_{a \to 1} \Big(f_a, \Big[\frac{T_a - T}{a-1}\Big] f \Big)_{\mathcal{H}} = \lambda\, \|f\|_{\mathcal{H}}^2,$$

where $f_a = U(a)f$.

Proof of Theorem 2.3. We only give the proof for H_3, because the proof for H_2 is exactly the same.

Let $\lambda \in \sigma_p(H_3)$, and let f be a corresponding eigenfunction with $\|f\| = 1$. In particular, $f \in \mathrm{Dom}(H_3) = \mathsf{H}^1(\mathbb{R}^3;\mathbb{C}^4)$ and $H_3 f = \lambda f$. With the dilation group $\{U(a)\}_{a>0}$, defined by $U(a)g(x) := a^{3/2}g(ax)$, $g \in \mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4)$, we introduce a family of self-adjoint operators $\{H(a)\}_{a>0}$ by $H(a) := a\,U(a)HU(a)^{-1}$. We then see that

$$\big(U(a)f,\, H(a)f\big) = \big(H(a)U(a)f,\, f\big) = \big(aU(a)Hf,\, f\big) = \lambda a\big(U(a)f,\, f\big),$$

which implies that

$$\big(U(a)f,\, H(a)f - Hf\big) = \lambda(a-1)\big(U(a)f,\, f\big). \tag{2.6}$$

On the other hand, we find that

$$[H(a)g](x) = -i\alpha\cdot\nabla g(x) + a\,q(ax)g(x), \quad \forall g \in \mathsf{H}^1(\mathbb{R}^3;\mathbb{C}^4),$$

hence we have

$$[H(a)f](x) - [Hf](x) = \{a\,q(ax) - q(x)\}f(x). \tag{2.7}$$

Combining (2.6) with (2.7) yields

$$\Big(U(a)f,\, \frac{a\,q(a\,\cdot) - q(\,\cdot\,)}{a-1}f\,\Big) = \lambda\big(U(a)f,\, f\,\big). \tag{2.8}$$

Since $\operatorname{s-lim}_{a\to 1} U(a) = I$, (2.8) implies, by the Lebesgue dominated convergence theorem, that

$$\int_{\mathbb{R}^3} \big(q(x) + (x\cdot\nabla q)(x)\big)|f(x)|^2\,dx = \lambda. \tag{2.9}$$

The conclusion of the theorem follows from (2.9). ■

3 Schnol's theorem

In this section, we state and prove Schnol's theorem for H_d. The idea of our proof is based on that of [6, p. 21, Theorem 2.9], where Schnol's theorem for Schrödinger operators is established. In the three-dimensional case, our Schnol's theorem can be stated as follows:

Theorem 3.1 *Let $q \in \mathsf{L}^2_{loc}(\mathbb{R}^3,\mathbb{R})$, and let λ be a real number. Suppose f is a polynomially bounded measurable function on $\mathbb{R}^3$, not identically* 0, *and satisfies the equation*

$$(-i\alpha\cdot\nabla + q)f = \lambda f \tag{3.1}$$

in the distribution sense. Then $\lambda \in \sigma(H_3)$ for any self-adjoint realization H_3 such that $\mathrm{Dom}(H_3) \supset \mathsf{H}^1(\mathbb{R}^3;\mathbb{C}^4) \cap \mathrm{Dom}(q)$.

Proof. It is sufficient to prove the assertion for $\lambda = 0$, because any $\lambda \neq 0$ can be absorbed in q. The proof will be devided into two steps.
Step 1. The case of $f \in \mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4)$.

Let $\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C})$. Then it follows that

$$\begin{aligned}(-i\alpha\cdot\nabla)(\varphi f) &= (-i\alpha\cdot\nabla\varphi)f + \varphi(-i\alpha\cdot\nabla)f \\ &= (-i\alpha\cdot\nabla\varphi)f - \varphi\, q f,\end{aligned} \tag{3.2}$$

where we have used (3.1) in the second equality. Since $\varphi q \in \mathsf{L}^2(\mathbb{R}^3;\mathbb{C})$ and f is locally bounded, we see that $\varphi\, q f \in \mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4)$, hence by (3.2) that $(-i\alpha\cdot\nabla)(\varphi f) \in \mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4)$. This implies that $(-i\alpha\cdot\nabla)^2(\varphi f) \in \mathsf{H}^{-1}(\mathbb{R}^3;\mathbb{C}^4)$, the Sobolev space of order -1. On the other hand, $(-i\alpha\cdot\nabla)^2(\varphi f) = -\Delta(\varphi f)$. Hence we find that $\varphi f \in \mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4) \subset \mathsf{H}^{-1}(\mathbb{R}^3;\mathbb{C}^4)$ and $-\Delta(\varphi f) \in \mathsf{H}^{-1}(\mathbb{R}^3;\mathbb{C}^4)$. We now apply the ellipticity argument, and we get

$$\varphi f \in \mathsf{H}^1(\mathbb{R}^3;\mathbb{C}^4) \quad \text{for} \ \ \forall\varphi \in C_0^\infty(\mathbb{R}^3;\mathbb{C}). \tag{3.3}$$

By the ellipticity argument, we mean the following: "$u \in \mathsf{H}^\ell(\mathbb{R}^3;\mathbb{C})$ and $\Delta u \in \mathsf{H}^\ell(\mathbb{R}^3;\mathbb{C})$ for some $\ell \in \mathbb{R} \Longrightarrow u \in \mathsf{H}^{\ell+2}(\mathbb{R}^3;\mathbb{C})$."

We now choose $\chi \in C_0^\infty(\mathbb{R}^3;\mathbb{C})$ so that $\chi(x) = 1$ ($|x| \le 1$) and $= 0$ ($|x| \ge 2$), and we set

$$\chi_n(x) = \chi(x/n) \quad (n = 1,\, 2,\, 3,\, \cdots). \tag{3.4}$$

It follows from (3.3) that $\chi_n f \in \mathsf{H}^1(\mathbb{R}^3;\mathbb{C}^4)$. It is evident that $\chi_n f \in \mathrm{Dom}(Q)$. Hence $\chi_n f \in \mathrm{Dom}(H_3)$ for $n = 1,\, 2,\, 3,\, \cdots$. To construct a singular sequence, we define

$$f_n = \frac{1}{\|\chi_n f\|_{\mathsf{L}^2}}\, \chi_n f. \tag{3.5}$$

It is obvious that $f_n \in \mathrm{Dom}(H_3)$ and $\|f_n\|_{\mathsf{L}^2} = 1$. We now only have to show that $\|H f_n\|_{\mathsf{L}^2} \to 0$ as $n \to \infty$. In fact, we see that

$$\begin{aligned} H f_n &= \frac{1}{\|\chi_n f\|_{\mathsf{L}^2}} \big[\{(-i\alpha\cdot\nabla)\chi_n\} f + \chi_n(-i\alpha\cdot\nabla + q) f\big] \\ &= \frac{1}{\|\chi_n f\|_{\mathsf{L}^2}} \Big[\frac{1}{n}\Big\{(-i\alpha\cdot\nabla\chi)\big(\frac{x}{n}\big)\Big\} f\Big], \end{aligned} \tag{3.6}$$

where we have used the hypothesis that $(-i\alpha\cdot\nabla + q)f = 0$. Noting the fact that $\lim_{n\to\infty}\|\chi_n f\|_{\mathsf{L}^2} = \|f\|_{\mathsf{L}^2} \ne 0$, we can deduce from (3.6) that $\|H f_n\|_{\mathsf{L}^2} \to 0$. Hence we can conclude that $0 \in \sigma(H_3)$.

Step 2. The case of $f \notin \mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4)$.

We may assume that f satisfies the estimate

$$|f(x)| \le C(1 + |x|)^N \tag{3.7}$$

for some $N \in \mathbb{N}$. Let f_n be defined in the same way as (3.5). As was shown in Step 1, it follows that $f_n \in \mathrm{Dom}(H_3)$ and that (3.6) is still valid. Then we have

$$\|H f_n\|_{\mathsf{L}^2}^2 \le \frac{1}{n^2\|\chi_n f\|_{\mathsf{L}^2}^2}\Big[\sup_{1\le|x|\le 2}|\nabla\chi(x)|\Big]^2 \int_{n\le|x|\le 2n}|f(x)|^2\,dx. \tag{3.8}$$

We now introduce a sequence $(M(n))_{n\in\mathbb{N}}$ by

$$M(n) := \int_{|x|\le n}|f(x)|^2\,dx \quad (n \in \mathbb{N}), \tag{3.9}$$

which is diverging and monotonically increasing. It follows from (3.8) and (3.9) that

$$\|Hf_n\|_{\mathsf{L}^2}^2 \le C\frac{M(2n)-M(n)}{n^2M(n)}, \tag{3.10}$$

where C is a positive constant, independent of n.

For the sake of contradiction, suppose that

$$\liminf_{n\to\infty} \frac{M(2n)-M(n)}{n^2M(n)} > 0. \tag{3.11}$$

Then there would be a large integer ν_0 and a positive constant α_0 such that

$$\frac{M(2n)-M(n)}{n^2M(n)} \ge \alpha_0 \quad \text{for } \forall n \ge \nu_0. \tag{3.12}$$

This implies that

$$M(2n) \ge (1+\alpha_0 n^2)M(n) \quad \text{for } \forall n \ge \nu_0. \tag{3.13}$$

By repeated use of (3.13), we obtain

$$M(2^n\nu_0) \ge \Big\{\prod_{j=0}^{n-1}(1+\alpha_0\nu_0^2 2^{2j})\Big\}M(\nu_0) \quad (n\in\mathbb{N}). \tag{3.14}$$

We now write $n = 2\ell$. It follows from (3.14) that

$$\begin{aligned} M(4^\ell\nu_0) &\ge \Big\{\prod_{j=0}^{2\ell-1}(1+\alpha_0\nu_0^2 4^{j})\Big\}M(\nu_0) \\ &\ge \Big\{\prod_{j=\ell}^{2\ell-1}(1+\alpha_0\nu_0^2 4^{j})\Big\}M(\nu_0) \\ &\ge \alpha_0^\ell \nu_0^{2\ell} 4^{\ell^2} M(\nu_0). \end{aligned} \tag{3.15}$$

On the other hand, it follows from (3.7) and (3.9) that

$$\begin{aligned} M(4^\ell\nu_0) &\le C\int_{|x|\le 4^\ell\nu_0}(1+|x|)^{2N}\,dx \\ &= C'\int_0^{4^\ell\nu_0}(1+r)^{2N}r^2\,dr \\ &\le C''_{\nu_0}4^{(2N+3)\ell}. \end{aligned} \tag{3.16}$$

It follows from (3.15) and (3.16) that

$$C''_{\nu_0}4^{(2N+3)\ell} \ge \alpha_0^\ell \nu_0^{2\ell} 4^{\ell^2} M(\nu_0) \quad (\ell\in\mathbb{N}). \tag{3.17}$$

Taking the logarithm of both sides of (3.17), one gets

$$\begin{aligned} &\log C''_{\nu_0} + (2N+3)\ell\,\log 4 \ge \\ &\qquad \ell\,\log(\alpha_0\nu_0^2) + \ell^2\,\log 4 + \log M(\nu_0) \qquad (\ell\in\mathbb{N}). \end{aligned} \tag{3.18}$$

Since the right hand side of (3.18) grows faster than the left hand side of (3.18) as ℓ goes to infinity, the inequality (3.18) is a contradiction. Hence we can deduce that

$$\liminf_{n\to\infty} \frac{M(2n) - M(n)}{n^2 M(n)} = 0, \tag{3.19}$$

which yields that there is a subsequence $\{M(n_k)\}$ such that

$$\lim_{k\to\infty} \frac{M(2n_k) - M(n_k)}{n_k^2 M(n_k)} = 0. \tag{3.20}$$

This fact, together with (3.10), implies that $\|Hf_{n_k}\|_{\mathsf{L}^2} \to 0$ as $k \to \infty$. Thus we can conclude that $0 \in \sigma(H_3)$. ■

In the two dimensional case, Schnol's theorem is as follows:

Theorem 3.2 *Let $q \in \mathsf{L}^2_{loc}(\mathbb{R}^2, \mathbb{R})$ and λ be a real number. Suppose ψ is a polynomially bounded measurable function on $\mathbb{R}^2$, not identically 0, and satisfies the equation*

$$(-i\sigma \cdot \nabla + q)\psi = \lambda\psi$$

in the distribution sense. Then $\lambda \in \sigma(H_2)$ for any self-adjoint realization H_2 such that $\mathrm{Dom}(H_2) \supset \mathsf{H}^1(\mathbb{R}^2; \mathbb{C}^2) \cap \mathrm{Dom}(q)$.

The proof of Theorem 3.2 is similar to that of Thorem 3.1, and is omitted.

When applying either of Theorems 3.1 and 3.2, one needs to construct a polynomially bounded eigensolution for a given energy of the Dirac operator H_d with q being locally square integrable. However, it is not easy to construct such an eigensolution unless q decays at infinity in an appropriate sense. If q decays rapidly, it is well-known that one can construct bounded eigensolutions (generalized eigenfunctions) of H_d by exploiting the limiting absorption principle. In Example 3.1 below, we shall construct a bounded eigensolution (cf. (3.21)) for a given energy of H_d with potential q of a specific form. We would like to stress that we do not require any decay assumption of q at infinity.

Example 3.1 *Let η be a real-valued continuous function on $\mathbb{R}$ and define $q(x) := \eta(x \cdot k)$ on $\mathbb{R}^d$, $d \in \{2, 3\}$, where $k \in \mathbb{R}^d$ is a unit vector. One can show, by the standard technique (cf. [17, p.257, Corollary], [24, p.113, Theorem 4.3]) , that H_d is essentially self-adjoint on $H^1(\mathbb{R}^d; \mathbb{C}^{2^{d-1}}) \cap \mathrm{Dom}(q)$. Let H_d be the unique self-adjoint realization. Then $\sigma(H_d) = \mathbb{R}$.*

For $d = 3$, this fact is proved in the following manner: Put

$$\xi(t) = \int_0^t \eta(\tau)\, d\tau.$$

As the eigenvalues of the matrix $\alpha \cdot k$ are ± 1 (each with geometric multiplicity 2) we can choose a spinor $\phi_0 \in \mathbb{C}^4$ so that $|\phi_0| = 1$, $(\alpha \cdot k)\phi_0 = \phi_0$. For a given $\lambda \in \mathbb{R}$, define

$$f(x) = e^{-i(\alpha\cdot k)\,\xi(x\cdot k)} e^{i\lambda x\cdot k}\phi_0. \tag{3.21}$$

Then f is in $C^1(\mathbb{R}^3; \mathbb{C}^4)$, and satisfies the equation (3.1). In fact, one can see that

$$-i\alpha_j \frac{\partial f}{\partial x_j} = -i\alpha_j k_j\, (-i\alpha \cdot k)\, q(x) f + \lambda \alpha_j k_j f \qquad (j \in \{1, 2, 3\}),$$

hence that

$$
\begin{aligned}
(-i\alpha\cdot\nabla)f &= (-i\alpha\cdot k)^2\, q(x)f + \lambda(\alpha\cdot k)f \\
&= -q(x)f + \lambda\, e^{-i(\alpha\cdot k)\,\xi(x\cdot k)} e^{i\lambda x\cdot k}(\alpha\cdot k)\phi_0 \\
&= -q(x)f + \lambda f,
\end{aligned}
\tag{3.22}
$$

where we have used the fact that $(\alpha\cdot k)\phi_0 = \phi_0$ *and the facts that* $(\alpha\cdot k)^2 = I_4$ *and that* $\alpha\cdot k$ *commutes with the exponential* $e^{-i(\alpha\cdot k)\,\xi(x\cdot k)}$. *It is obvious that* $|f(x)|_{\mathbb{C}^4} = 1$ *for all* $x\in\mathbb{R}^3$. *Hence, it follows from Theorem 3.1 that* $\lambda\in\sigma(H_3)$. *Since* λ *is an arbitrary real number, one can conclude that* $\sigma(H_3) = \mathbb{R}$.

For $d = 2$, *the proof is similar to that for* $d = 3$ *and is omitted.*

4 Spectra of H_d

In this section, we shall prove that $\sigma(H_3) = \mathbb{R}$ under minimal assumptions on the potential q. As mentioned in the introduction, the one-dimensional Dirac operator H_1 in (1.3) has (purely absolutely continuous) spectrum $\sigma(H_1) = \mathbb{R}$ for all potentials $q\in \mathsf{L}^1_{loc}(\mathbb{R};\mathbb{R})$. In view of this fact, the question naturally arises whether the spectrum of H_d, $d\in\{2,\,3\}$, also covers the whole real line for all potentials $q\in\mathsf{L}^2_{loc}(\mathbb{R}^d;\mathbb{R})$? (Here we assume local square-integrability of the potential to ensure that the Dirac operator will be well-defined on $C_0^\infty(\mathbb{R}^d;\mathbb{R})$.)

While attempting to give an answer to this question in greatest possible generality, we shall, however, need to impose some hypotheses on the potential q. The reason for this restriction is technical. Compared to the number of tools available to study the spectrum of the one-dimensional Dirac operator (an ordinary differential operator), the techniques for showing that a real number belongs to $\sigma(H_d)$ are relatively limited. The main tool available for addressing the general question above is Weyl's criterion in some form, *i.e.* the construction of a Weyl singular sequence, as we have done in the previous section; and we shall use this method again here. However, we emphasize that the conditions we shall impose are fairly mild in that they restrict the potential q only on some sequence of balls of increasing radius, which can be arbitrarily positioned and far apart. In the remaining space, there is no constraint at all beyond the general assumption of local square-integrability. More specifically, in Theorem 4.1, we need the potential q to be sufficiently close, in an L^2 sense, to a function which varies only in one direction, and hence is constant on the planes perpendicular to this direction in each ball. Theorem 4.2 is a generalization of Theorem 4.1, where the planes of constancy are replaced with more general curved manifolds. In Theorem 4.3, we need the mean oscillations of q on the sequence of balls to go to zero. This condition will be satisfied whenever the potential is close to constant on wide stretches, even if these lie in e.g. a narrow sector or cone. This indicates that a spectral gap could, if at all, only occur in the case of a potential which changes in a complicated multidimensional way essentially everywhere; an arrangement which would seem difficult to realise in practice.

Note that we don't need any growth or decay property of the potential q at infinity.

Theorem 4.1 *Let* $q \in \mathsf{L}^2_{loc}(\mathbb{R}^3;\mathbb{R})$. *Suppose that there is a sequence* $(k_n)_{n\in\mathbb{N}}$ *of unit vectors in* $\mathbb{R}^3$, *a sequence* $(B_{r_n}(a_n))_{n\in\mathbb{N}}$ *of disjoint balls with centre* $a_n \in \mathbb{R}^3$ *and radius* $r_n \to \infty$ $(n \to \infty)$, *and a sequence of square-integrable functions* $\eta_n : (-r_n, r_n) \to \mathbb{R}$ $(n \in \mathbb{N})$ *such that*

$$r_n^{-3} \int_{B_{r_n}(a_n)} \big|q(x) - \eta_n\big((x-a_n)\cdot k_n\big)\big|^2\, dx \to 0$$

as $n \to \infty$. *Then* $\sigma(H_3) = \mathbb{R}$ *for any self-adjoint extension* H_3 *of*

$$(-i\alpha\cdot\nabla + q)\big|_{C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)}.$$

Remark 4.1 *The two dimensional analogue of Theorem 4.1 holds true.*

Proof of Theorem 4.1. Let $\lambda \in \mathbb{R}$; we shall show that λ belongs to the spectrum of H_3 by constructing a Weyl singular sequence.

In a similar way to Example 3.1, we can choose a sequence of spinors $(\phi_n)_{n\in\mathbb{N}}$ in $\mathbb{C}^4$ such that

$$|\phi_n| = 1, \quad (\alpha\cdot k_n)\phi_n = \phi_n. \tag{4.1}$$

Since $C^\infty(-r_n, r_n)$ is dense in $\mathsf{L}^2(-r_n, r_n)$, there are functions $\tilde\eta_n \in C^\infty(-r_n, r_n)$ such that

$$\frac{1}{2r_n}\int_{-r_n}^{r_n} |\eta_n(\tau) - \tilde\eta_n(\tau)|^2 d\tau \to 0 \tag{4.2}$$

as $n \to \infty$. Let $\xi_n(t) := \int_0^t \tilde\eta_n(\tau)d\tau$ $\;(t \in (-r_n, r_n); n \in \mathbb{N})$, and define

$$F_n(x) := e^{-i(\alpha\cdot k_n)\xi_n((x-a_n)\cdot k_n)} e^{i\lambda x\cdot k_n}\phi_n \;:\; B_{r_n}(a_n) \to \mathbb{C}^4. \tag{4.3}$$

Since $e^{-i(\alpha\cdot k_n)\xi_n((x-a_n)\cdot k_n)}$ is a unitary matrix, it follows from (4.1) that $|F_n(x)|_{\mathbb{C}^4} = 1$ for all $n \in \mathbb{N}$ and all $x \in B_{r_n}(a_n)$. Furthermore, we see that $F_n \in C^\infty(B_{r_n}(a_n))^4$, and we make the same computation as in (3.22) to get

$$(-i\alpha\cdot\nabla)F_n(x) = \big\{-\tilde\eta_n\big((x-a_n)\cdot k_n\big) + \lambda\big\}\, F_n(x). \tag{4.4}$$

Here we have used (4.1) and the facts that $(\alpha\cdot k_n)^2 = I_4$ and that $\alpha\cdot k_n$ commutes with the exponentials in (4.3).

We now choose $\chi \in C_0^\infty(\mathbb{R}^3;\mathbb{R})$ so that $\mathrm{supp}(\chi) \subset B_1(0)$ and $\|\chi\|_{\mathsf{L}^2} = 1$, and define

$$\chi_n(x) := r_n^{-3/2}\,\chi\big(r_n^{-1}(x-a_n)\big). \tag{4.5}$$

We shall show that the sequence $(f_n)_{n\in\mathbb{N}}$ defined by $f_n := \chi_n F_n$ $(n \in \mathbb{N})$ is a Weyl singular sequence for $H_3 - \lambda$. First, we note that $\|f_n\|_{\mathsf{L}^2} = 1$ and $f_n \in C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$. Next, we see that

$$\begin{aligned}(-i\alpha\cdot\nabla)f_n(x) &= \big\{(-i\alpha\cdot\nabla)\chi_n(x)\big\}\,F_n(x) + \chi_n(x)(-i\alpha\cdot\nabla)F_n(x)\\ &= r_n^{-5/2}\,\big[(-i\alpha\cdot\nabla)\chi\big]\big(r_n^{-1}(x-a_n)\big)F_n(x)\\ &\quad - \tilde\eta_n\big((x-a_n)\cdot k_n\big)\,f_n(x) + \lambda f_n(x),\end{aligned} \tag{4.6}$$

where we have used (4.4) and (4.5). Finally, it follows from (4.6) that

$$
\begin{aligned}
(H_3-\lambda)f_n(x) &= r_n^{-5/2}\left[(-i\alpha\cdot\nabla)\chi\right]\big(r_n^{-1}(x-a_n)\big)\,F_n(x) \\
&\quad + \big\{q(x)-\tilde{\eta}_n\big((x-a_n)\cdot k_n\big)\big\}\,r_n^{-3/2}\,\chi\big(r_n^{-1}(x-a_n)\big)\,F_n(x),
\end{aligned}
\tag{4.7}
$$

which — adding and subtracting $\eta_n\big((x-a_n)\cdot k_n\big)$ — implies that

$$
\begin{aligned}
\|(H_3-\lambda)f_n\| &\le r_n^{-1}\left(\int_{|x|\le 1}\big|(\alpha\cdot\nabla)\chi(x)\big|^2\,dx\right)^{1/2} \\
&\quad + \|\chi\|_\infty\left(r_n^{-3}\int_{B_{r_n}(a_n)}\big|q(x)-\eta_n\big((x-a_n)\cdot k_n\big)\big|^2\,dx\right)^{1/2} \\
&\quad + \|\chi\|_\infty\left(\frac{\pi}{r_n}\int_{-r_n}^{r_n}\big|\eta_n(\tau)-\tilde{\eta}_n(\tau)\big|^2 d\tau\right)^{1/2} \\
&\quad \to 0 \quad \text{as} \quad n\to\infty.
\end{aligned}
\tag{4.8}
$$

Hence we can conclude that $\lambda\in\sigma(H_3)$. ■

In the following theorem, we shall show that the result of Theorem 4.1 extends to potentials which are close to constants on a local foliation of curved surfaces, which could be fattened to sets of positive measure, provided that their curvature becomes asymptotically small. We assume that the potential is approximated by C^∞ smooth functions, which in the light of the proof of the preceding theorem is no serious restriction of generality.

Theorem 4.2 *Let $q\in \mathsf{L}^2_{loc}(\mathbb{R}^3;\mathbb{R})$. Suppose that there is a sequence $(k_n)_{n\in\mathbb{N}}$ of unit vectors in $\mathbb{R}^3$, a sequence $(B_{r_n}(a_n))_{n\in\mathbb{N}}$ of disjoint balls with centre $a_n\in\mathbb{R}^3$ and radius $r_n\to\infty$ $(n\to\infty)$, and sequences of functions $\varphi_n\in C^\infty(B_{r_n}(a_n);\mathbb{R})$ and $\eta_n\in C^\infty(\mathbb{R};\mathbb{R})$ $(n\in\mathbb{N})$ such that*

$$
r_n^{-3}\int_{B_{r_n}(a_n)}\big|q(x)-\eta_n\big(x\cdot k_n+\varphi_n(x)\big)\big|^2\,dx\to 0\quad (n\to\infty)
\tag{4.9}
$$

and

$$
r_n^{-3}\int_{B_{r_n}(a_n)}\big|\nabla\phi_n(x)\big|^2\big|\eta_n\big(x\cdot k_n+\varphi_n(x)\big)\big|^2\,dx\to 0\quad (n\to\infty).
\tag{4.10}
$$

Then $\sigma(H_3)=\mathbb{R}$ for any self-adjoint extension H_3 of

$$
(-i\alpha\cdot\nabla+q)\big|_{C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)}
\tag{4.11}
$$

Remark 4.2 *The two dimensional analogue of Theorem 4.2 holds true.*

Proof of Theorem 4.2. We follow the general line of the proof of Theorem 4.1. Let $\lambda\in\mathbb{R}$ be arbitrary, and ϕ_n as in (4.1). Define $\xi_n(t):=\int_0^t\eta_n(\tau)\,d\tau$ $(t\in\mathbb{R})$ and

$$
F_n(x):=e^{-i(\alpha\cdot k_n)\xi_n(x\cdot k_n+\varphi_n(x))}e^{i\lambda\,x\cdot k_n}\phi_n \qquad (x\in B_{r_n}(a_n));
\tag{4.12}
$$

Then $F_n \in C^\infty(B_{r_n}(a_n), \mathbb{C}^4)$ and $|F_n(x)|_{\mathbb{C}^4} = 1$ ($n \in \mathbb{N}, x \in B_{r_n}(a_n)$). Moreover, abbreviating $q_n(x) := \eta_n(x \cdot k_n + \varphi_n(x))$ we get

$$\begin{aligned} -i\alpha \cdot \nabla F_n(x) &= -i\alpha \cdot \big(-i(\alpha \cdot k_n)\, q_n(x)\, \{k_n + \nabla\varphi_n(x)\} + i\lambda\, k_n \big)\, F_n(x) \\ &= -q_n(x)\, F_n(x) - \big(\alpha \cdot \nabla\varphi_n(x)\big)\, (\alpha \cdot k_n)\, q_n(x)\, F_n(x) + \lambda\, F_n(x) \end{aligned} \tag{4.13}$$

($x \in B_{r_n}(a_n)$). To construct a singular sequence, let χ_n be as in (4.5), and define $f_n := \chi_n F_n$. Then $\|f_n\|_{\mathsf{L}^2} = 1$ and $f_n \in C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$. Furthermore, we have

$$\begin{aligned} -i\alpha \cdot \nabla f_n(x) &= \big(-i\alpha \cdot \nabla\chi_n(x)\big) F_n(x) + \chi_n(x)\big(-i\alpha \cdot \nabla F_n(x)\big) \\ &= r_n^{-5/2} \big[(-i\alpha \cdot \nabla)\chi\big] \big(r_n^{-1}(x - a_n)\big)\, F_n(x) \\ &\quad - \chi_n(x)\, q_n(x)\, F_n(x) \\ &\quad - \chi_n(x)\big(\alpha \cdot \nabla\varphi_n(x)\big)(\alpha \cdot k_n) q_n(x)\, F_n(x) + \lambda f_n(x), \end{aligned} \tag{4.14}$$

from which we obtain

$$\begin{aligned} (H_3 - \lambda) f_n(x) &= r_n^{-5/2} \big[(-i\alpha \cdot \nabla)\chi\big] \big(r_n^{-1}(x - a_n)\big)\, F_n(x) \\ &\quad + \chi_n(x)\big(q(x) - q_n(x)\big)\, F_n(x) \\ &\quad - \chi_n(x)\big(\alpha \cdot \nabla\varphi_n(x)\big)(\alpha \cdot k_n)\, q_n(x) F_n(x). \end{aligned} \tag{4.15}$$

Hence

$$\begin{aligned} \|(H_3 - \lambda) f_n\|_{\mathsf{L}^2} &\le r_n^{-1} \Big(\int_{|x| \le 1} \big|(\alpha \cdot \nabla)\chi(x)\big|^2\, dx \Big)^{1/2} \\ &\quad + \|\chi\|_{\mathsf{L}^\infty} \Big(r_n^{-3} \int_{B_{r_n}(a_n)} \big|q(x) - \eta_n\big((x - a_n) \cdot k_n\big)\big|^2\, dx \Big)^{1/2} \\ &\quad + \|\chi\|_{\mathsf{L}^\infty} \Big(r_n^{-3} \int_{B_{r_n}(a_n)} \big|\nabla\varphi_n(x)\big|^2\, \big|\eta_n\big((x - a_n) \cdot k_n\big)\big|^2\, dx \Big)^{1/2} \\ &\quad \to 0 \quad \text{as} \quad n \to \infty, \end{aligned} \tag{4.16}$$

by (4.9) and (4.10). Here we twice used the fact that $|(\alpha \cdot v)u| = |v||u|$ for any $v \in \mathbb{R}^3$ and $u \in \mathbb{C}^4$. Thus we can conclude that $\lambda \in \sigma(H_3)$. ■

The following theorem can be obtained as a special case of Theorem 4.1, when the functions η_n are taken to be constants with value q_n defined in (4.18). However, it has a quick and simple separate proof which we include below.

Theorem 4.3 *Let $q \in \mathsf{L}^2_{loc}(\mathbb{R}^3; \mathbb{R})$. Suppose that there is a sequence $(B_{r_n}(a_n))_{n \in \mathbb{N}}$ of disjoint balls with centre $a_n \in \mathbb{R}^3$ and radius $r_n \to \infty$ ($n \to \infty$) such that*

$$r_n^{-3} \int_{B_{r_n}(a_n)} \big|q(x) - q_n\big|^2\, dx \to 0 \quad (n \to \infty), \tag{4.17}$$

where q_n is the mean value of q over the ball $B_{r_n}(a_n)$:

$$q_n = \frac{3}{4\pi r_n^3} \int_{B_{r_n}(a_n)} q(x)\, dx. \tag{4.18}$$

Then $\sigma(H_3) = \mathbb{R}$ for any self-adjoint extension H_3 of

$$(-i\alpha \cdot \nabla + q)\big|_{C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)}$$

Proof. Let $\lambda \in \mathbb{R}$ be arbitrary. As in Theorems 4.1 and 4.2, we shall show that λ belongs to the spectrum of H_3 by constructing a Weyl singular sequence.

We first choose a sequence $(k_n)_{n\in\mathbb{N}}$ in $\mathbb{R}^3$ so that $|k_n| = |q_n - \lambda|$ for each n. Note that $k_n = 0$ if $q_n = \lambda$. Since the eigenvalues of the matrix $\alpha \cdot k_n$ are $\pm|k_n|$, we can choose a sequence of spinors $(\phi_n)_{n\in\mathbb{N}}$ in $\mathbb{C}^4$ so that

$$|\phi_n| = 1, \quad (\alpha \cdot k_n)\phi_n = \begin{cases} -|k_n|\phi_n & \text{if } q_n - \lambda > 0 \\ \ \ |k_n|\phi_n & \text{if } q_n - \lambda < 0 \\ \ \ 0 & \text{if } q_n - \lambda = 0, \end{cases} \tag{4.19}$$

which readily implies that

$$(\alpha \cdot k_n + q_n - \lambda)\phi_n = 0. \tag{4.20}$$

With χ_n introduced in (4.5), we shall show that the sequence $(f_n)_{n\in\mathbb{N}}$ defined by $f_n := \chi_n\, e^{ix\cdot k_n}\phi_n$ is a Weyl singular sequence for $H_3-\lambda$. To this end, we first note that $\|f_n\|_{\mathsf{L}^2} = 1$ and $f_n \in C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$. We next see that

$$\begin{aligned} (-i\alpha \cdot \nabla)f_n(x) = r_n^{-5/2}\left[(-i\alpha\cdot\nabla)\chi\right]\bigl(r_n^{-1}(x-a_n)\bigr)\ e^{ix\cdot k_n}\phi_n \\ + \chi_n(x)\, e^{ix\cdot k_n}(\alpha\cdot k_n)\phi_n \end{aligned} \tag{4.21}$$

Combining (4.20) and (4.21), we get

$$\begin{aligned} \bigl(-i\alpha\cdot\nabla + q(x) - \lambda\bigr)f_n(x) = r_n^{-5/2}\left[(-i\alpha\cdot\nabla)\chi\right]\bigl(r_n^{-1}(x-a_n)\bigr)\ e^{ix\cdot k_n}\phi_n \\ + \chi_n(x)\, e^{ix\cdot k_n}\bigl(q(x) - q_n\bigr)\phi_n, \end{aligned} \tag{4.22}$$

which implies

$$\begin{aligned} \|(H_3-\lambda)f_n\|_{\mathsf{L}^2} \le r_n^{-1}\Bigl(\int_{|x|\le 1}\bigl|(\alpha\cdot\nabla)\chi(x)\bigr|^2\,dx\Bigr)^{1/2} \\ + \|\chi\|_{\mathsf{L}^\infty}\Bigl(r_n^{-3}\int_{B_{r_n}(a_n)}\bigl|q(x)-q_n\bigr|^2\,dx\Bigr)^{1/2} \to 0 \end{aligned} \tag{4.23}$$

as $n\to\infty$, by assumption (4.17). ■

Remark 4.3 *In (4.17), the mean oscillation is taken in L^2 sense. The mean oscillation in the usual sense is, however, taken in L^1 sense; see e.g. [22]. One can see that (4.17) implies the mean oscillation in the usual sense tends to zero as follows:*

$$\begin{aligned} &\frac{1}{|B_{r_n}(a_n)|}\int_{B_{r_n}(a_n)}\bigl|q(x)-q_n\bigr|\,dx \\ &\le \frac{1}{|B_{r_n}(a_n)|}\Bigl\{\int_{B_{r_n}(a_n)}\bigl|q(x)-q_n\bigr|^2\,dx\Bigr\}^{1/2}\Bigl\{\int_{B_{r_n}(a_n)}dx\Bigr\}^{1/2} \\ &= \Bigl\{\frac{3}{4\pi}r_n^{-3}\int_{B_{r_n}(a_n)}\bigl|q(x)-q_n\bigr|^2\,dx\Bigr\}^{1/2}dx \to 0 \quad (n\to\infty), \end{aligned}$$

where $|\cdot|$ denotes the Lebesgue measure: $|B_{r_n}(a_n)| = 4\pi r_n^3/3$.

Remark 4.4 *The two dimensional analogue of Theorem 4.3 holds true.*

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