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On Relativistic Energy Band Corrections in the Presence of Periodic Potentials

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Abstract. A previously developed formalism to compute relativistic corrections of bound state energies for spin-$\frac{1}{2}$ particles is applied to relativistic corrections of energy bands of one-dimensional, periodic Hamiltonians. We explicitly describe Floquet theory for periodic Dirac operators on the line. Extensions including impurity potentials and/or $\nu \geqslant 2$ dimensions are straightforward and sketched at the end.

1. The Abstract Approach

For convenience, we summarize the main results obtained in [8, 9]. Let $\mathscr{H}_\pm$ be separable, complex Hilbert spaces and introduce self-adjoint operators α, β in $\mathscr{H} = \mathscr{H}_+ \oplus \mathscr{H}_-$ of the type

$$\alpha = \begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1.1}$$

where A is a densely defined, closed operator from $\mathscr{H}_+$ into $\mathscr{H}_-$. Next, we introduce the abstract free Dirac operator $H^0(c)$ by

$$H^0(c) = c\alpha + mc^2\beta, \qquad \mathscr{D}(H^0(c)) = \mathscr{D}(\alpha), \quad c \in \mathbb{R}\backslash\{0\}, \quad m > 0 \tag{1.2}$$

and the interaction V by

$$V = \begin{pmatrix} V_+ & 0 \\ 0 & V_- \end{pmatrix}, \tag{1.3}$$

where $V_\pm$ denotes self-adjoint operators in $\mathscr{H}_\pm$, respectively. Assuming V_+ (resp. V_-)

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to be bounded w.r. to A (resp. A^*), i.e.,

$$\mathscr{D}(V_+) \supseteq \mathscr{D}(A), \qquad \mathscr{D}(V_-) \supseteq \mathscr{D}(A^*), \tag{1.4}$$

the abstract Dirac operator $H(c)$ reads

$$H(c) = H^0(c) + V, \qquad \mathscr{D}(H(c)) = \mathscr{D}(\alpha). \tag{1.5}$$

Obviously $H(c)$ is self-adjoint for $|c|$ large enough. The corresponding self-adjoint (free) Pauli operators in $\mathscr{H}_\pm$ are then defined by

$$H_+^0 = (2m)^{-1}A^*A, \qquad H_-^0 = (2m)^{-1}AA^*, \tag{1.6}$$

$$\begin{aligned} H_+ &= H_+^0 + V_+, \qquad \mathscr{D}(H_+) = \mathscr{D}(A^*A), \\ H_- &= H_-^0 + V_-, \qquad \mathscr{D}(H_-) = \mathscr{D}(AA^*). \end{aligned} \tag{1.7}$$

Introducing in $\mathscr{H}$ the operator $B(c)$ [12]

$$B(c) = \begin{pmatrix} 1 & 0 \\ 0 & c \end{pmatrix}, \tag{1.8}$$

we recall [8, 9]

THEOREM 1.1. *Let* $H(c)$ *be defined as above and fix* $z \in \mathbb{C}\backslash\mathbb{R}$. *Then* (*a*) $(H(c) - mc^2 - z)^{-1}$ *is holomorphic w.r. to* c^{-1} *around* $c^{-1} = 0$

$$\begin{aligned} &(H(c) - mc^2 - z)^{-1} \\ &= \left\{1 + \begin{pmatrix} 0 & (2mc)^{-1}(H_+ - z)^{-1}A^*(V_- - z) \\ (2mc)^{-1}A(H_+^0 - z)^{-1}V_+ & (2mc^2)^{-1}z(H_-^0 - z)^{-1}(V_- - z) \end{pmatrix}\right\}^{-1} \times \\ &\times \begin{pmatrix} (H_+ - z)^{-1} & (2mc)^{-1}(H_+ - z)^{-1}A^* \\ (2mc)^{-1}A(H_+^0 - z)^{-1} & (2mc^2)^{-1}z(H_-^0 - z)^{-1} \end{pmatrix}. \end{aligned} \tag{1.9}$$

(b) $B(c)\,(H(c) - mc^2 - z)^{-1}B(c)^{-1}$ *is holomorphic w.r. to* c^{-2} *around* $c^{-2} = 0$

$$\begin{aligned} &B(c)\,(H(c) - mc^2 - z)^{-1}B(c)^{-1} \\ &= \left\{1 + \begin{pmatrix} 0 & (2mc^2)^{-1}(H_+ - z)^{-1}A^*(V_- - z) \\ 0 & (2mc^2)^{-1}[(2m)^{-1}A(H_+ - z)^{-1}A^* - 1]\,(V_- - z) \end{pmatrix}\right\}^{-1} \times \\ &\times \begin{pmatrix} (H_+ - z)^{-1} & (2mc^2)^{-1}(H_+ - z)^{-1}A^* \\ (2m)^{-1}A(H_+ - z)^{-1} & (2mc^2)^{-1}[(2m)^{-1}A(H_+ - z)^{-1}A^* - 1] \end{pmatrix}. \end{aligned} \tag{1.10}$$

First-order expansions in (1.9) *and* (1.10) *yield*

$$\begin{aligned} &(H(c) - mc^2 - z)^{-1} \\ &= \begin{pmatrix} (H_+ - z)^{-1} & 0 \\ 0 & 0 \end{pmatrix} + c^{-1}\begin{pmatrix} 0 & (2m)^{-1}(H_+ - z)^{-1}A^* \\ (2m)^{-1}A(H_+ - z)^{-1} & 0 \end{pmatrix} + \\ &+ 0(c^{-2}) \end{aligned} \tag{1.11}$$

(clearly illustrating the nonrelativistic limit $|c|\to\infty$) and

$$B(c)(H(c)-mc^2-z)^{-1}B(c)^{-1}$$

$$=\begin{pmatrix}(H_+-z)^{-1} & 0\\ (2m)^{-1}A(H_+-z)^{-1} & 0\end{pmatrix}+c^{-2}\begin{pmatrix}R_{11} & R_{12}\\ R_{21} & R_{22}\end{pmatrix}+O(c^{-4})$$

$$\equiv R_0(z)+c^{-2}R_1(z)+O(c^{-4}), \tag{1.12}$$

$$R_{11}=(2m)^{-2}(H_+-z)^{-1}A^*(z-V_-)A(H_+-z)^{-1},$$

$$R_{12}=(2m)^{-1}(H_+-z)^{-1}A^*,$$

$$R_{21}=(2m)^{-2}[(2m)^{-1}A(H_+-z)^{-1}A^*-1](z-V_-)A(H_+-z)^{-1}, \tag{1.13}$$

$$R_{22}=(2m)^{-1}[(2m)^{-1}A(H_+-z)^{-1}A^*-1].$$

Analyzing the relationship between the spectrum of $(H_+-z)^{-1}$ and $R_0(z)$ (cf. Lemma 2.2 in [9]) one obtains the following result on relativistic eigenvalue corrections.

THEOREM 1.2. *Let $H(c)$ be defined as in (1.5) and assume $E_0\in\sigma_d(H_+)$ to be a discrete eigenvalue of H_+ of multiplicity $m_0\in\mathbb{N}$. Then, for c^{-2} small enough, $H(c)-mc^2$ has precisely m_0 eigenvalues (counting multiplicity) near E_0 which are all holomorphic w.r. to c^{-2}. More precisely, all eigenvalues $E_j(c^{-2})$ of $H(c)-mc^2$ near E_0 satisfy*

$$E_j(c^{-2})=E_0+\sum_{p=1}^{\infty}(c^{-2})^pE_{j,p},\quad j=1,\dots,j_0,\ j_0\leqslant m_0 \tag{1.14}$$

and if m_j denotes the multiplicity of $E_j(c^{-2})$ then $\Sigma_{j=1}^{j_0}m_j=m_0$.

In addition, there exist linearly independent vectors

$$f_{jl}(c^{-1})=\begin{pmatrix}f_{+jl}(c^{-2})\\ c^{-1}f_{-jl}(c^{-2})\end{pmatrix},\quad j=1,\dots,j_0,\ l=1,\dots,m_j \tag{1.15}$$

s.t. $f_{\pm jl}$ are holomorphic w.r. to c^{-2} near $c^{-2}=0$ and

$$H_+f_{+jl}(0)=E_0f_{+jl}(0),\qquad f_{-jl}(0)=(2m)^{-1}Af_{+jl}(0) \tag{1.16}$$

and

$$(H(c)-mc^2)f_{jl}(c^{-1})=E_j(c^{-2})f_{jl}(c^{-1}),\quad j=1,\dots,j_0,\ l=1,\dots,m_j. \tag{1.17}$$

The eigenvectors $f_{jl}(c^{-1})$ can be chosen to be orthonormal. Finally, the first-order corrections $E_{j,1}$ in (1.14) are explicitly given as the eigenvalues of the matrix

$$(2m)^{-2}(Af_r,(V_--E_0)Af_s),\quad r,s=1,\dots,m_0, \tag{1.18}$$

where $\{f_r\}_{r=1}^{m_0}$ is any orthonormal basis of the eigenspace of H_+ to the eigenvalue E_0.

Remark 1.3. (a) The main idea of [8, 9] behind Theorem 1.2 was to look for eigenvalues of the resolvent $(H(c)-mc^2-z)^{-1}$ and applying the strong spectral mapping theorem

[17] instead of looking directly for eigenvalues of the unbounded Hamiltonian $H(c) - mc^2$. For earlier results on the nonrelativistic limit we refer to [4, 12, 21, 22].

(b) Theorem 1.2 for $m_0 = 1$ is due to [8, 9]. In the general case $m_0 > 1$ only holomorphy of $E_j(c^{-1})$ w.r.t. to c^{-1} near $c^{-1} = 0$ and $E_j(c^{-1}) - mc^2 - E_0 =_{c\to\infty} 0(c^{-2})$ has been proven in [9]. The above result for $m > 1$ is due to [23]. The basic idea to prove holomorphy of E_j w.r. to c^{-2} is the following: Since $(H(c) - mc^2 - z)^{-1}$ is normal for $z \in \mathbb{C}\backslash\mathbb{R}$, (1.11) implies that the projection $P_j(c^{-1})$ onto the eigenspace of the eigenvalue $(E_j(c^{-1}) - z)^{-1}$ is holomorphic w.r. to c^{-1} near $c^{-1} = 0$. To prove that $E_j(c^{-1})$ is actually holomorphic w.r. to c^{-2} near $c^{-2} = 0$ one calculates

$$\begin{aligned} \tilde{P}_j(c^{-2}) \equiv B(c)P_j(c^{-1})B(c)^{-1} &= \begin{pmatrix} 1 & 0 \\ 0 & c \end{pmatrix} \begin{pmatrix} p_j & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1/c \end{pmatrix} \\ &\quad + [\text{terms holomorphic w.r. to } c^{-2}] \\ &= [\text{terms holomorphic w.r. to } c^{-2}] . \end{aligned} \tag{1.19}$$

Here $\tilde{P}_j(c^{-2})$ and p_j are the corresponding projections associated with $B(c)(H(c) - mc^2 - z)^{-1}B(c)^{-1}$ and $(H_+ - z)^{-1}$ of dimension m_j, respectively. Thus, $\| \tilde{P}_j(c^{-2}) \|$ is bounded as $c^{-2} \to 0$ and, hence, Butler's theorem ([13], p. 70) proves that $\tilde{P}_j(c^{-2})$ and $(E_j(c^{-1}) - z)^{-1}$ are actually holomorphic w.r. to c^{-2} near $c^{-2} = 0$.

2. Floquet Theory for One-Dimensional Dirac Operators

Let

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.1}$$

denote the Pauli matrices in $\mathbb{C}^2$ and define in $L^2(\mathbb{R}) \otimes \mathbb{C}^2$ the free Hamiltonian

$$\begin{aligned} H^0(c) &= c\, \frac{1}{i} \frac{\mathrm{d}}{\mathrm{d}x} \otimes \sigma_1 + mc^2 \otimes \sigma_3 , \\ \mathscr{D}(H^0(c)) &= H^{2,1}(\mathbb{R}) \otimes \mathbb{C}^2 , \quad c \in \mathbb{R}\backslash\{0\}, m \geqslant 0 . \end{aligned} \tag{2.2}$$

To avoid technicalities, we assume the interaction V to satisfy

$$V \in L^\infty(\mathbb{R}) \text{ real-valued, } V(x + a) = V(x) \text{ for some } a > 0 \tag{2.3}$$

and define the full Hamiltonian in $L^2(\mathbb{R}) \otimes \mathbb{C}^2$ by

$$\begin{aligned} H(c) &= H^0(c) + V \otimes \mathbf{1} = \begin{pmatrix} mc^2 + V & cp \\ cp & -mc^2 + V \end{pmatrix}, \\ \mathscr{D}(H(c)) &= H^{2,1}(\mathbb{R}) \otimes \mathbb{C}^2 , \end{aligned} \tag{2.4}$$

where

$$p = \frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x}, \qquad \mathscr{D}(p) = H^{2,1}(\mathbb{R}). \tag{2.5}$$

Since $H(c)$ is periodic with period $a > 0$, we get the direct integral decomposition [17]

$$\hat{U}H(c)\hat{U}^{-1} = \int_{[-\pi/a,\,\pi/a)}^{\oplus} \mathrm{d}\theta H(c, \theta), \tag{2.6}$$

where

$$L^2(\mathbb{R}) = \overline{U}^{-1}\frac{a}{2\pi}\int_{[-\pi/a,\,\pi/a)}^{\oplus} \mathrm{d}\theta L^2((-a/2, a/2)), \tag{2.7}$$

$$U: \mathscr{S}(\mathbb{R}) \to \frac{a}{2\pi}\int_{[-\pi/a,\,\pi/a)}^{\oplus} \mathrm{d}\theta L^2((-a/2, a/2)), \tag{2.8}$$

$$(Uf)(\theta, v) = \sum_{n=-\infty}^{\infty} \mathrm{e}^{+in\theta a} f(v + na),$$

$$v \in (-a/2, a/2),\ \theta \in [-\pi/a, \pi/a),\ f \in \mathscr{S}(\mathbb{R}),$$

$$\hat{U} = \overline{U} \otimes \mathbf{1}. \tag{2.9}$$

(Here $\overline{U}$ denotes the (unitary) closure of U and $\mathscr{S}(\mathbb{R})$ the Schwartz space.) The fibers

$$H(c, \theta) = H^0(c, \theta) + V \otimes \mathbf{1} = \begin{pmatrix} mc^2 + V & cp_\theta \\ cp_\theta & -mc^2 + V \end{pmatrix},$$

$$\mathscr{D}(H(c, \theta)) = \mathscr{D}(p_\theta) \otimes \mathbb{C}^2, \tag{2.10}$$

respectively,

$$p_\theta = \frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}v},$$

$$\mathscr{D}(p_\theta) = \{g(\theta) \in H^{2,1}((-a/2, a/2)) \mid g(\theta, -a/2+) = \mathrm{e}^{i\theta a} g(\theta, a/2-)\} \tag{2.11}$$

are operators in $L^2((-a/2, a/2)) \otimes \mathbb{C}^2$ respectively in $L^2((-a/2, a/2))$.

In order to study the spectrum of $H(c, \theta)$ we first consider the discriminant associated with $H(c)$. Let

$$H(c)f = Ef, \quad E \in \mathbb{R} \tag{2.12}$$

in the distributional sense, or equivalently,

$$f'(x) = \begin{pmatrix} 0 & [V(x) - mc^2 - E]/ic \\ [V(x) + mc^2 - E]/ic & 0 \end{pmatrix} f(x). \tag{2.13}$$

Then f is of the type

$$f = c_1 \begin{pmatrix} u_1 \\ iu_2 \end{pmatrix} + c_2 \begin{pmatrix} iv_1 \\ v_2 \end{pmatrix}, \quad u_j,\ v_j \text{ real}, j = 1, 2 . \tag{2.14}$$

Assuming a fundamental system $\Phi(c)$ of the form

$$\Phi(c, x, E) = \begin{pmatrix} u_1 & iv_1 \\ iu_2 & v_2 \end{pmatrix} (c, x, E), \tag{2.15}$$

where

$$\Phi(c, -a/2, E) = \mathbf{1} \tag{2.16}$$

and, hence,

$$\operatorname{Det}[\Phi(c, x, E)] = 1, \quad c \in \mathbb{R}\backslash\{0\},\ x \in \mathbb{R},\ E \in \mathbb{R}, \tag{2.17}$$

the Floquet determinant (discriminant) [16] $D(c, E)$ is defined as

$$D(c, E) = \operatorname{Tr}[\Phi(c, a/2, E)] = u_1(c, a/2, E) + v_2(c, a/2, E), \quad E \in \mathbb{R} . \tag{2.18}$$

Suppressing the c-dependence of all quantities involved for a moment, we get (for fixed $c \in \mathbb{R}\backslash\{0\}$)

LEMMA 2.1. *$D(E)$, $E \in \mathbb{R}$ is a real-valued, analytic function on $\mathbb{R}$ with*
(i) *$D'(E) \neq 0$ for $|D(E)| < 2$ and*
(ii) *if $D(E_m) = \pm 2$ for some $E_m \in \mathbb{R}$, then $D'(E_m) = 0$ iff $u_2(a/2, E) = v_1(a/2, E) = 0$ (in this case one has $D''(E_m) \lesseqgtr 0$).*

Proof. Clearly $u_1(x, E)$, $v_2(x, E)$ are analytic w.r. to $E \in \mathbb{R}$. From (2.17) and (2.18) one infers

$$D(E)^2 = [u_1(a/2, E) - v_2(a/2, E)]^2 + 4[1 - u_2(a/2, E)v_1(a/2, E)] . \tag{2.19}$$

Differentiating (2.13) w.r. to E, taking

$$f = \begin{pmatrix} u_1 \\ iu_2 \end{pmatrix}, \text{ resp., } f = \begin{pmatrix} iv_1 \\ v_2 \end{pmatrix}$$

and solving the resulting inhomogeneous first-order system in the standard way yields

$$\begin{aligned} -cD'(E) = \int_{-a/2}^{a/2} ds \{ & [v_1(s, E)^2 + v_2(s, E)^2] u_2(a/2, E) + \\ & + [u_1(s, E)^2 + u_2(s, E)^2] v_1(a/2, E) + \\ & + [u_1(s, E)v_1(s, E) - u_2(s, E)v_2(s, E)] [v_2(a/2, E) - u_1(a/2, E)] \} . \end{aligned} \tag{2.20}$$

Multiplying (2.20) with $4v_1(a/2, E)$, observing (2.19), results in

$$\begin{aligned} & -c4v_1(a/2, E)D'(E) \\ & = \int_{-a/2}^{a/2} \mathrm{d}s\{[4 - D(E)^2]\,[v_1(s,E)^2 + v_2(s,E)^2] + \\ & + [2u_1(s,E)v_1(a/2,E) - u_1(a/2,E)v_1(s,E) + v_1(s,E)v_1(a/2,E)]^2 + \\ & + [2u_2(s,E)v_1(a/2,E) + u_1(a/2,E)v_2(s,E) - v_2(a/2,E)v_2(s,E)]^2\}\,. \qquad (2.21) \end{aligned}$$

Thus (2.19) implies $v_1(a/2, E) \neq 0$ for $|D(E)| < 2$ and, hence, (2.21) proves (i). Next we assume that $D(E_m) = 2$ for some $E_m \in \mathbb{R}$. If $u_2(a/2, E_m) = v_1(a/2, E_m) = 0$, then (2.18) and (2.19) imply $u_1(a/2, E_m) = v_2(a/2, E_m) = 1$. Thus $D'(E_m) = 0$ by (2.20). Conversely, if $D'(E_m) = 0$, then (2.21) implies

$$2u_j(s,E)v_1(a/2,E) - [u_1(a/2,E) - v_2(a/2,E)]\,v_j(s,E) = 0\,, \quad j = 1, 2\,.$$

Since u_j and v_j are linearly independent, we get

$$v_1(a/2, E) = 0\,, \qquad u_1(a/2, E) = v_2(a/2, E) = 1$$

and (2.20) then yields $u_2(a/2, E) = 0$. If $D'(E_m) = 0$, then differentiating (2.20) w.r. to E finally yields

$$\begin{aligned} & -(c^2/2)D''(E_m) \\ & = \int_{-a/2}^{a/2} \mathrm{d}s[u_1(s,E_m)^2 + u_2(s,E_m)^2] \int_{-a/2}^{a/2} \mathrm{d}t[v_1(t,E_m)^2 + v_2(t,E_m)^2] - \\ & - \left\{\int_{-a/2}^{a/2} \mathrm{d}s[u_1(s,E_m)v_1(s,E_m) - u_2(s,E_m)v_2(s,E_m)]\right\}^2 > 0 \qquad (2.22) \end{aligned}$$

by Schwarz′ inequality. (The inequality is a strict one since

$$\begin{pmatrix} u_1 \\ iu_2 \end{pmatrix}, \quad \begin{pmatrix} iv_1 \\ v_2 \end{pmatrix}$$

and linearly independent.) Similarly one discusses the case $D(E_m) = -2$. □

Concerning the spectrum of $H(c, \theta)$ we have

THEOREM 2.2. *Let* $\theta \in [-\pi/a, \pi/a)$ *and fix* $c \in \mathbb{R}\backslash\{0\}$. *Then*

(i) $\sigma_{\mathrm{ess}}(H(c, \theta)) = \emptyset$, i.e., $H(c, \theta)$ *has purely discrete spectrum.*

(ii) *Define the time reversal operator* K *by*

$$K\begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} \overline{f_1} \\ -\overline{f_2} \end{pmatrix}, \qquad \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \in L^2((-a/2, a/2)) \otimes \mathbb{C}^2 \qquad (2.23)$$

(*where the bar denotes complex conjugation*) *then*

$$KH(c, \theta)K^{-1} = H(c, -\theta)\,, \quad \theta \in (-\pi/a, 0)\,. \qquad (2.24)$$

(iii) *For* $\theta \in (-\pi/a, 0) \cup (0, \pi/a)$, $H(c, \theta)$ *has simple spectrum. The multiplicity of degenerate eigenvalues of* $H(c, \theta)$, $\theta \in \{\pm \pi/a, 0\}$ *equals two. By choosing an appropriate enumeration of the eigenvalues* $E_n(c, \theta)$, $n \in \mathbb{Z}$ *of* $H(c, \theta)$ *one may assume that* $E_{\pm(2m+1)}(c, \theta)$ *(resp.* $E_{\pm 2m}(c, \theta)$*),* $m \in \mathbb{N}_0$, *are strictly monotonously decreasing (resp. increasing) w.r. to* $\theta \in [-\pi/a, 0]$, *i.e.,*

$$\begin{aligned} \ldots &\leqslant E_{-1}(c, 0) < E_{-1}(c, -\pi/a) \leqslant E_0(c, -\pi/a) < E_0(c, 0) \leqslant E_1(c, 0) < \\ &< E_1(c, -\pi/a) \leqslant \cdots \leqslant E_{2m-1}(c, 0) < E_{2m-1}(c, -\pi/a) \leqslant \\ &\leqslant E_{2m}(c, -\pi/a) < \cdots \end{aligned} \tag{2.25}$$

(iv) $H(c, \theta)$ *is an analytic family for* θ *in a neighbourhood of* $(-\pi/a, \pi/a)$. $E_n(c, \theta)$, $n \in \mathbb{Z}$ *are real analytic in* $(-\pi/a, 0) \cup (0, \pi/a)$ *and continuous at* $\pm \pi/a, 0$. *Similarly, the corresponding eigenfunctions* $f_n(c, \theta)$, $n \in \mathbb{Z}$ *can be chosen to be analytic in* $(-\pi/a, 0) \cup (0, \pi/a)$ *and continuous in* $\pm \pi/a, 0$ *s.t.* $f_n(c, -\pi/a) = f_n(c, \pi/a)$.

Proof. Assertions (i), (ii), and (iv) follow in complete analogy to the Schrödinger case as discussed in [6] and [17] (e.g. in connection with (i) one uses $\sigma(p_\theta) = \{-\theta + (2\pi/a)m \mid m \in \mathbb{Z}\}$) while (iii) follows from Lemma 2.1 and the fact that the eigenvalues $E_n(c, \theta)$, $n \in \mathbb{Z}$ *of* $H(c, \theta)$ are precisely the solutions of

$$2 \cos(\theta) = D(c, E). \tag{2.26}$$ □

Remark 2.3. In contrast to the Schrödinger situation the spectrum of $H(c, \theta)$ is now unbounded from below and above, i.e.

$$E_n(c, \theta) \underset{n \to \pm\infty}{\longrightarrow} \pm\infty .$$

We also remark that all eigenvalues $E_n(c, -\pi/a)$, $E_n(c, 0)$, $n \in \mathbb{Z}$ might be twice degenerate as the example $m = V = 0$ shows.

THEOREM 2.4. *The spectrum* $\sigma(H(c))$ *is purely absolutely continuous*

$$\begin{aligned} &\sigma(H(c)) = \sigma_{ac}(H(c)) = \bigcup_{n \in \mathbb{Z}} [A_n(c), B_n(c)], \\ &\sigma_p(H(c)) = \sigma_{sc}(H(c)) = \emptyset, \end{aligned} \tag{2.27}$$

where

$$A_n(c) = \begin{cases} E_n(c, 0), & n \text{ odd}, \\ E_n(c, -\pi/a), & n \text{ even}, \end{cases}$$

$$B_n(c) = \begin{cases} E_n(c, -\pi/a), & n \text{ odd}, \\ E_n(c, 0), & n \text{ even}, \end{cases} \qquad n \in \mathbb{Z}. \tag{2.28}$$

Proof. Given Theorem 2.2, one can follow the proof of Theorem XIII.90 in [17] step by step. □

3. Relativistic Energy Band Corrections for One-Dimensional Systems

Let V satisfy conditions (2.3) and define the Schrödinger operator h_∞ in $L^2(\mathbb{R})$ by

$$h_\infty = -(2m)^{-1} \frac{\mathrm{d}^2}{\mathrm{d}x^2} + V, \qquad \mathscr{D}(h_\infty) = H^{2,2}(\mathbb{R}), \tag{3.1}$$

i.e., $h_\infty = H_\pm$ in the terminology of Section 1 and

$$A = \frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x}, \qquad \mathscr{D}(A) = H^{2,1}(\mathbb{R}), \qquad V_\pm = V. \tag{3.2}$$

Standard Floquet theory for h_∞ then yields [6, 17]

$$\overline{U}h_\infty\overline{U}^{-1} = \int_{[-\pi/a,\,\pi/a)}^{\oplus} \mathrm{d}\theta h_\infty(\theta) \tag{3.3}$$

(cf. (2.7) and (2.9)), where

$$h_\infty(\theta) = -(2m)^{-1} \frac{\mathrm{d}^2}{\mathrm{d}v^2} + V,$$

$$\mathscr{D}(h_\infty(\theta)) = \{g(\theta) \in H^{2,2}((-a/2, a/2)) \mid g(\theta, -a/2+) = \mathrm{e}^{i\theta a}g(\theta, a/2-),$$
$$g'(\theta, -a/2+) = \mathrm{e}^{i\theta a}g'(\theta, a/2-)\}, \quad \theta \in [-\pi/a, \pi/a)$$

is the corresponding fiber of h_∞ in $L^2((-a/2, a/2))$.

Then, changing $H(c, \theta)$ into $h_\infty(\theta)$, $E_n(c, \theta)$ into $e_n(\theta)$, $n \in \mathbb{N}$ (the eigenvalues of $h_\infty(\theta)$) and K into $k(kf = \overline{f}, f \in L^2((-a/2, a/2)))$, Theorems 2.2 and 2.4 hold for $h_\infty(\theta)$. (Obviously, one ignores the statements on $E_n(c, \theta)$, $-n \in \mathbb{N}_0$ since now $h_\infty(\theta)$ is bounded from below.) In particular,

$$e_1(0) < e_1(-\pi/a) \leqslant e_2(-\pi/a) < e_2(0) \leqslant \cdots$$
$$\leqslant e_{2m-1}(0) \leqslant e_{2m-1}(-\pi/a) \leqslant e_{2m}(-\pi/a) < e_{2m}(0) \leqslant \cdots \tag{3.5}$$

and

$$\sigma(h_\infty(\theta)) = \sigma_{ac}(h_\infty(\theta)) = \bigcup_{n\in\mathbb{N}} [a_n, b_n], \tag{3.6}$$

where

$$a_n = \begin{cases} e_n(0), & n \text{ odd}, \\ e_n(-\pi/a), & n \text{ even}, \end{cases} \qquad b_n = \begin{cases} e_n(-\pi/a), & n \text{ odd}, \\ e_n(0), & n \text{ even} \end{cases}, \quad n \in \mathbb{N}. \tag{3.7}$$

Moreover, $e_1(0)$ is a simple eigenvalue of $h_\infty(0)$. Theorem 1.2 then yields

THEOREM 3.1. *Let $\theta \in [-\pi/a, 0]$ and assume $e_0(\theta) \in \sigma_d(h_\infty(\theta))$ to be a discrete eigenvalue of $h_\infty(\theta)$ of multiplicity $m_0(\theta) = 1$ or 2. Then, for c^{-2} small enough, $H(\theta, c) - mc^2$ has precisely $m_0(\theta)$ eigenvalues (counting multiplicity) near $e_0(\theta)$. More* *precisely, all eigenvalues* $E_j(\theta, c^{-2})$ *of* $H(\theta, c) - mc^2$ *near* $e_0(\theta)$ *satisfy*

$$E_j(\theta, c^{-2}) = e_0(\theta) + \sum_{p=1}^{\infty} (c^{-2})^p e_{j,p}(\theta), \quad j = 1, \ldots, j_0; \, j_0 \leqslant m_0(\theta) \leqslant 2. \tag{3.8}$$

The first-order corrections $e_{j,1}(\theta)$ *are given as the eigenvalues of the matrix*

$$(2m)^{-2}(A(\theta)f_r(\theta), [V - e_0(\theta)]A(\theta)f_s(\theta)), \quad r, s = 1, \ldots, m_0(\theta), m_0(\theta) \leqslant 2, \tag{3.9}$$

where $A(\theta) = p_\theta$ *and* $\{f_r(\theta)\}_{r=1}^{m_0(\theta)}$ *is an orthonormal basis of the eigenspace of* $h_\infty(\theta)$ *to the eigenvalue* $e_0(\theta)$. *We omit the corresponding assertions on holomorphic eigenvectors* (cf. Theorem 1.2).

Remark 3.2. Obviously $m_0(\theta) = 1$ for $\theta \in (-\pi/a, 0)$ (cf. Theorem 2.2 (iii)). But also for $\theta \in \{-\pi/a, 0\}$, the band edges $e_0(-\pi/a)$, $e_0(0)$ are generically nondegenerate [19].

Remark 3.3. Let $n = 2m + 1$, $m \in \mathbb{N}_0$, $0 < \delta < \pi/2a$ and assume $e_0(\theta)$ in Theorem 3.1 equals $e_n(\theta)$. Then there exist constants $M_1, M_2 > 0$ s.t.

$$c^{-2} < \min_{1 \leqslant j \leqslant j_0} \min \left\{ \frac{M_1 \cdot |(e_0(-\pi/a) - e_0(-\pi/a + \delta))|}{\theta \in \max_{[-(\pi/a)+\delta, 0]} |e_{j,1}(\theta) - e_{j,1}(-\pi/a)|}, M_2 \frac{|e_0'(-\pi/a)|}{|e'_{j,1}(-\pi/a)|} \right\}$$

implies

$$\begin{aligned} &e_0(-\pi/a) + c^{-2}e_{j,1}(-\pi/a) > e_0(\theta) + c^{-2}e_{j,1}(\theta), \\ &\theta \in (-\pi/a, 0], \; j = 1, \ldots, j_0 \end{aligned} \tag{3.10}$$

if both denominators do not vanish. Otherwise take the $e_{j,k}(.)$ with the lowest k giving a nonvanishing denominator in the first term, or from the nonvanishing $e'_{j,k}(-\pi/a)$'s that with the lowest k in the second term, correspondingly.

The opposite inequality holds for $n \in \mathbb{N}$ even. Consequently, for c large enough, the band edges of the nth band are determined by $e_0(\theta) + c^{-2}e_{j,1}(\theta)$ at $\theta = -\pi/a, 0$ to first order w.r. to c^{-2}.

Proof. By Theorem 2.2 (iii) we have

$$E_n(c, -\pi/a) - mc^2 > E_n(c, \theta) - mc^2, \quad c^{-2} \geqslant 0, \, \theta \in (-\pi/a, 0].$$

Equation (3.10) then follows by a Taylor expansion w.r. to (c^{-2}, θ) near $(0, -\pi/a)$. □

4. Generalizations

We briefly sketch generalizations including impurities and higher-dimensional systems. We start with a short discussion of impurities in one dimension. In order to avoid the use of quadratic form techniques [13, 17] we assume the impurity potential U to be essentially bounded, $U \in L^\infty(\mathbb{R})$. The full Dirac Hamiltonian $H_U(c)$ in $L^2(\mathbb{R}) \otimes \mathbb{C}^2$, respectively the corresponding Schrödinger operator $h_{\infty, U}$ in $L^2(\mathbb{R})$ then read

$$H_U(c) = H(c) + U \otimes \mathbf{1}, \qquad \mathscr{D}(H_U(c) = H^{2,1}(\mathbb{R}) \otimes \mathbb{C}^2, \quad c \in \mathbb{R} \backslash \{0\}, \tag{4.1}$$

$$h_{\infty, U} = h_\infty + U, \qquad \mathscr{D}(h_{\infty, U}) = H^{2,2}(\mathbb{R}), \tag{4.2}$$

with $H(c)$ (resp. h_∞) given by (2.4) (resp. (3.1)). For a short-range impurity one assumes

$$U \in L^1(\mathbb{R}, (1 + |x|)\,\mathrm{d}x)\,. \tag{4.3}$$

Because of (4.3), $h_{\infty, U}$ has only finitely many eigenvalues in each gap of its essential spectrum [18] (here, by definition, each gap is an open interval and the band edges are never eigenvalues of $h_{\infty, U}$). Moreover, if

$$\int_{\mathbb{R}} \mathrm{d}x\, U(x) \neq 0\,, \tag{4.4}$$

it is known that $h_{\infty, U}$ has precisely one eigenvalue in each gap sufficiently far out (see [25, 7] and the references therein). However, if $\int_{\mathbb{R}} \mathrm{d}x\, U(x) = 0$, $U \in L^1(\mathbb{R}, (1 + |x|^2)\,\mathrm{d}x)$ and U is reflectionless, then $h_{\infty, U}$ has no eigenvalues in the distant gaps of the spectrum [7]. The coupling constant threshold behaviour of periodic Hamiltonians subject to short-range impurities is discussed in [15].

The case of long-range impurity potentials

$$c_1(1 + |x|)^{-\alpha} \leqslant |U(x)| \leqslant c_2(1 + |x|)^{-\alpha}, \quad 0 < \alpha < 2\,, \tag{4.5}$$

where the eigenvalues accumulate at the ends of each gap in $\sigma_{\mathrm{ess}}(h_{\infty, U})$ is considered in [14, 24]. In either case, Theorem 1.2 applies to any eigenvalue (impurity level) $e_{0, U}$ of $h_{\infty, U}$ in a gap of $\sigma_{\mathrm{ess}}(h_{\infty, U})$. In particular, for c^{-2} small enough,

$$E_{j, U}(c^{-2}) = e_{0, U} + \sum_{p=1}^{\infty} (c^{-2})^p e_{j, p, U}\,, \quad j = 1, \ldots, j_0,\ j_0 \leqslant m_{0, U} \leqslant 2 \tag{4.6}$$

are the only eigenvalues of $H_U(c)$ near $e_{0, U}$ and the first-order relativistic corrections $e_{j, 1, U}$ are given by the eigenvalues of the matrix

$$(2m)^{-2}(Af_{r, U}, (V + U - e_{0, U})Af_{s, U})\,, \quad r, s = 1, \ldots, m_{0, U}\,. \tag{4.7}$$

Here $\{f_{r, U}\}_{r=1}^{m_{0, U}}$ is any orthonormal basis of the $m_{0, U}$-dimensional eigenspace of $h_{\infty, U}$ to the eigenvalue $e_{0, U}$.

All the above results now extend in a straightforward manner to higher-dimensional systems. In fact, the direct integral decomposition (cf. Section 2) for ν-dimensional Schrödinger operators has been developed in [1–3, 6, 17]. Since the corresponding fibers have compact resolvent, the approach of Section 3 immediately extends to $\nu \geqslant 2$ dimensions. The main difference to the one-dimensional situation concerns the fact that due to eigenvalue denegeracy, bands might overlap and according to the Bethe–Sommerfeld conjecture (see, e.g., [20] and the references therein) only finitely many gaps in the spectrum may exist (cf. also [11]). Finally, one can add an impurity potential (and external magnetic fields [10]) and consider relativistic corrections to impurity bound states in analogy to (4.6). The existence of such eigenvalues has been discussed in [5].

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