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Eigenvalues in gaps of perturbed periodic Dirac operators: numerical evidence

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Abstract

This paper presents a method for the numerical investigation of the distribution of the eigenvalues introduced into a spectral gap of a periodic Dirac system by a perturbation of the type of the angular momentum term. A number of examples illustrate the effectiveness of the method and show the remarkable accuracy of the strong coupling asymptotic formula even for small values of the perturbation coupling constant. Furthermore, the results shed some light on the spectrum in the exceptional gap of radially periodic three-dimensional Dirac operators.

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1. Introduction

It is well known from Floquet theory (see [3]) that the one-dimensional Schrödinger operator

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) \tag{1}$$

with periodic coefficient q has a spectrum with band structure, i.e., consisting of a sequence of intervals of purely absolutely continuous spectrum, separated in general by spectral gaps. Hempel et al. [4,5] discovered that the associated spherically symmetric Schrödinger operator $-\Delta + V$ with $V(x) = q(|x|)$ $(x \in \mathbb{R}^N)$ has intervals of pure dense point spectrum corresponding to the gaps of the one-dimensional operator.

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Recent efforts have very much clarified the mechanism leading to the filling of spectral gaps with eigenvalues. By a separation of variables in spherical polar coordinates, the Schrödinger operator is unitarily equivalent to a direct sum of one-dimensional partial-wave operators

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + q(r) + \frac{c_{l,N}}{r^2} \quad (r \in (0,\infty)),$$

where $c_{l,N} = l(l+N-2) + (N-1)(N-3)/4,\ l \in \mathbb{N}_0$.

Each of these half-line operators has the same essential spectrum as operator (1), with possibly additional discrete eigenvalues in the spectral gaps. For fixed angular momentum quantum number l, all but a finite number of spectral gaps contain only finitely many eigenvalues. Nevertheless, in each gap, for sufficiently large l, there are infinitely many eigenvalues accumulating at the lower end of the gap [6–9,14]. There are no eigenvalues below the essential spectrum except in the two-dimensional case $N=2$, $l=0$, when there are in fact infinitely many, accumulating at the infimum of the essential spectrum [13]. The eigenvalues are asymptotically exponentially close to their point of accumulation [14, Theorem 3], which accounts for the difficulty of observing even a few of them numerically (see [1]).

Furthermore, it is known that the number of eigenvalues in a fixed compact subinterval of a gap grows as $\sqrt{c_{l,N}} \sim l$ in the asymptotic limit $l \to \infty$, with a factor of proportionality given by a Weyl-type semiclassical integral in which the quasimomentum of the underlying periodic problem takes the role of the ordinary momentum [17]. A quantitative error bound for the asymptotic formula does not seem to be available; however, it has been observed in a numerical study [2] that it is surprisingly accurate even for small values of l. The rapid increase in the density of eigenvalues with growing angular momentum explains the appearance of dense point spectrum in the direct sum of the half-line operators.

The Dirac operator

$$H = -\mathrm{i}\alpha \cdot \nabla + \beta + V(x) \quad (x \in \mathbb{R}^3)$$

with symmetric 4×4 matrices $\alpha_1, \alpha_2, \alpha_3,\ \beta = \alpha_0$ satisfying

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 2\delta_{ij} \quad (i,j \in \{0,1,2,3\})$$

is the analogue of the Schrödinger operator in relativistic quantum mechanics, and one is therefore led to expect similar spectral behaviour if the potential V has the same structure.

Unlike the Schrödinger operator, however, the Dirac operator is always unbounded below, which means that only part of its spectrum compares to the spectrum of the former.

Nevertheless, the relationship between the spectrum of the one-dimensional periodic Dirac operator

$$h = -\mathrm{i}\sigma_2 \frac{\mathrm{d}}{\mathrm{d}x} + \sigma_3 + q(x),$$

with σ_2, σ_3 two of the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and that of the radially periodic operator H is widely analogous to the case of Schrödinger operators: the absolutely continuous spectral bands are preserved, and dense point spectrum appears in the gaps [10,12] (h has generically infinitely many gaps [11]). The mechanism producing the eigenvalues in gaps is also similar—H is unitarily equivalent to a direct sum of the partial-wave operators

$$h_c = -\mathrm{i}\sigma_2 \frac{\mathrm{d}}{\mathrm{d}r} + \sigma_3 + q(r) + \frac{c}{r}\sigma_1 \quad (r \in (0,\infty),\ c \in \mathbb{Z} \setminus \{0\}),$$

and the angular momentum term $(c/r)\sigma_1$ only introduces discrete eigenvalues in the gaps of the essential spectrum of h_c, which coincides with the essential spectrum of h [12]. There is, however, an essential difference in that the Dirac angular momentum term, as a matrix, does not have a fixed sign, and therefore the additional eigenvalues do not depend monotonically on c. Thus either end-point of a spectral gap of h can be an accumulation point of eigenvalues of h_c either for large $|c|$, or for c in some finite interval only, depending on the properties of the periodic operator h at that point (see the discussion at the end of Section 3).

This lack of monotonicity lies at the root of an open question about the structure of the essential spectrum of H. The latter contains the set

$$\Pi(h) := \bigcup_{l_0 \in \mathbb{R}} \sigma_e(h + l_0\sigma_1),$$

which for relatively bounded q is known to be either all of $\mathbb{R}$ or the complement of a subinterval of a spectral gap of h [12, Theorem 1]. In the former case all spectral gaps are filled with eigenvalues, but in the latter there is an exceptional gap which may or may not be empty. It is not known whether H can have essential spectrum outside $\Pi(h)$. However, the relationship between $\Pi(h)$ and the spectrum of H is made quantitative by the asymptotic formula for the number of eigenvalues of h_c in a compact subinterval $[\lambda_1, \lambda_2]$ of a spectral gap of h,

$$\lim_{c\to\infty} \frac{N[\lambda_1,\lambda_2]}{c} = \frac{1}{\alpha\pi} \int_0^\infty (k(\lambda_2, 1/r) - k(\lambda_1, 1/r))\,\mathrm{d}r, \tag{2}$$

where $k(\lambda, l_0)$ denotes the quasimomentum of

$$-\mathrm{i}\sigma_2 u' + (m\sigma_1 + l_0\sigma_1 + q)u = \lambda u,$$

$\lambda, l_0 \in \mathbb{R}$ [16]. As the quasimomentum is constant in spectral gaps of $h + l_0\sigma_1$, this implies that the asymptotic eigenvalue density in the gap of $\Pi(h)$ is zero—which, however, does not rule out the existence of dense point spectrum there.

It is the aim of the present paper to present an approach to a numerical estimation of the distribution of eigenvalues of Dirac systems of the type of h_c. We focus on the specific perturbation $\sigma_1 c/r$ because of its significance for spherically symmetric Dirac operators, but our methods can easily be applied to more general perturbations decaying at ∞. We follow the fundamental idea of Brown et al. [2], with the additional complication of dealing with a matrix perturbation, and the fact that for a first-order ordinary differential equation system a careful study of the behaviour of Prüfer angles must replace the counting of zeros of solutions.

In its practical implementation, we then use this method to check for the presence of eigenvalues in the exceptional gap, and to see whether the asymptotic formula (2) gives a reasonably accurate prediction of the number of eigenvalues observed for finite values of c. The paper is organised as follows. In Section 2 the spectral problem for the Dirac system h_c inside a gap of h on the doubly singular interval $(0,\infty)$ is reduced to an analysis of the growth of the Prüfer angle of solutions on a finite interval, introducing a universally bounded error in the eigenvalue counts. In Section 3, we explain how to calculate the Prüfer angles based on a piecewise-constant approximation of the coefficients, which is again controlled by a precise error estimate. Section 4 contains the numerical results obtained for a couple of examples, and discusses their significance for the questions raised above.

2. Reduction to a regular problem

Consider the Dirac system on $(0,\infty)$

$$-\mathrm{i}\sigma_2 u'(r) + \left(m(r)\sigma_3 + l(r)\sigma_1 + q(r) + \frac{c}{r}\sigma_1\right)u(r) = \lambda u(r) \quad (r\in(0,\infty)), \tag{3}$$

where m, l, q are α-periodic and essentially bounded, and $c\in\mathbb{R}, |c| > \frac{1}{2}$. We wish to study the distribution of eigenvalues of (3) inside a spectral gap (Λ_1, Λ_2) of the periodic equation:

$$-\mathrm{i}\sigma_2 u'(x) + (m(x)\sigma_3 + l(x)\sigma_1 + q(x))u(x) = \lambda u(x) \quad (x\in\mathbb{R}). \tag{4}$$

To this end, we estimate the number of eigenvalues in the intervals $[\lambda_j, \lambda_{j+1})$, $j\in\{1,\dots,K-1\}$ obtained from a partitioning $\Lambda_1 < \lambda_1 < \lambda_2 < \cdots < \lambda_K < \Lambda_2$; as all subintervals of the resulting histogram are treated in the same way, we only consider the first of them $[\lambda_1, \lambda_2)$ in the following. As will be seen below, we do not actually need to calculate any eigenvalues, as by relative oscillation theory it will be sufficient to compare the growth of the Prüfer angles ϑ_1, ϑ_2 of $\mathbb{R}^2$-valued solutions of (3), defined by

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \varrho_j \begin{pmatrix} \cos\vartheta_j \\ \sin\vartheta_j \end{pmatrix},$$

with $\varrho_j > 0$, for $\lambda = \lambda_j$, $j\in\{1,2\}$.

We are facing the difficulty that both end-points in (3) are singular, as the perturbation has a nonintegrable singularity at the origin. However, as we shall show presently, the Prüfer angles need only be calculated on a compact subinterval of $(0,\infty)$, as the region close to 0 does not essentially contribute to the spectrum, and the solutions behave like those of the periodic problem for sufficiently large r.

Proposition 1. *Under the above hypotheses,* (3) *is in the limit point case at* 0. *Furthermore, if*

$$r_{\min} < \frac{|c| - 1/2}{\max\{\|q-\lambda_1\|_\infty, \|q-\lambda_2\|_\infty\} + \|m - m_0\|_\infty + \|l\|_\infty}$$

for some constant $m_0 \geqslant 0$, *then the self-adjoint operator* h_0 *realising*

$$-\mathrm{i}\sigma_2\frac{\mathrm{d}}{\mathrm{d}r} + m\sigma_3 + l\sigma_1 + q + \frac{c}{r}\sigma_1 \tag{5}$$

on the interval $(0, r_{\min})$ *with the boundary condition*

$$u_1(r_{\min}) + u_2(r_{\min}) = 0 \tag{6}$$

has no spectrum in $[\lambda_1, \lambda_2]$.

Remark. Eq. (3) is in the limit point case at ∞ as well [18, Theorem 6.8]. We introduce the constant m_0 in order to improve the bound for $r_{\min}$; obviously $m_0 = (\sup m + \inf m)/2$ (if nonnegative) is the best choice. For constant nonnegative m we then have $\|m - m_0\|_\infty = 0$.

Proof of Proposition 1. As $m\sigma_3 + l\sigma_1 + q$ is bounded, (3) is in the limit point case at 0 since

$$-\mathrm{i}\sigma_2 \frac{\mathrm{d}}{\mathrm{d}r} + \frac{c}{r}\,\sigma_1$$

is (even for $|c| \geqslant 1/2$) (see [12, Proof of Lemma 1]).

Therefore, h_0 is essentially self-adjoint on $D_0 = \{u \in D(h_0) \mid u \equiv 0 \text{ near } 0\}$. By contraposition, assume that there is $\lambda \in [\lambda_1, \lambda_2] \cap \sigma(h_0)$; then for $\varepsilon \in (0,1)$ there is $u \in D_0 \backslash \{0\}$ such that $\|(h_0 - \lambda)u\| < \varepsilon \|u\|$, which implies

$$\left\| \left(-\mathrm{i}\sigma_2 \frac{\mathrm{d}}{\mathrm{d}r} + m_0\sigma_3 + \frac{c}{r}\,\sigma_1 \right) u \right\| \leqslant (\|q - \lambda\|_\infty + \|m - m_0\|_\infty + \|l\|_\infty + \varepsilon)\|u\|.$$

On the other hand, an integration by parts using the boundary condition at $r_{\min}$ gives

$$\begin{aligned}
&\left\| -\mathrm{i}\sigma_2 u' + \left(m_0\sigma_3 + \frac{c}{r}\,\sigma_1 \right) u \right\|^2 \\
&= -\, m_0(\sigma_1 u)^{\mathrm{T}} \overline{u} \big|_0^{r_{\min}} + \int_0^{r_{\min}} \left(|u'|^2 + \left(m_0^2 + \frac{c^2}{r^2} \right) |u|^2 + \frac{c}{r^2}\,(\sigma_3 u)^{\mathrm{T}} \overline{u} \right) \\
&\geqslant m_0 |u(r_{\min})|^2 + \int_0^{r_{\min}} \left(\left(|u'|^2 - \frac{1}{4r^2}\,|u|^2 \right) + \frac{(|c| - 1/2)^2}{r^2}\,|u|^2 \right) \\
&\geqslant \frac{(|c| - 1/2)^2}{r_{\min}^2}\,\|u\|^2,
\end{aligned}$$

where we have used Hardy's inequality in the last step. For sufficiently small $r_{\min}$, this is a contradiction. □

In order to treat the end-point at ∞, consider the behaviour of solutions of the unperturbed periodic equation (4) for $\lambda \in [\Lambda_1, \Lambda_2]$. Λ_1 and Λ_2 are the end-points of an instability interval of this equation, and thus there are α-periodic or α-semiperiodic solutions if $\lambda \in \{\Lambda_1, \Lambda_2\}$. Consequently, the corresponding Prüfer angles Θ_1, Θ_2 are α-periodic mod π, and mimicking the proof of Theorem 3.1.2 in [3] it is not difficult to verify that they satisfy

$$\Theta_j(x) = \frac{n\pi x}{\alpha} + \mathrm{O}(1) \quad (x \to \infty)$$

($j \in \{1,2\}$). Here $n \in \mathbb{Z}$ is the number of the instability interval. By Sturm comparison (cf [18, Theorem 16.1]) any Prüfer angle of a solution of the periodic equation with $\lambda \in [\Lambda_1, \Lambda_2]$ has the same asymptotics, even with a uniform O(1) term.

Thus

$$\Theta_1(x) = \frac{n\pi x}{\alpha} + \delta_1(x), \quad \Theta_2(x) = \frac{n\pi x}{\alpha} + \delta_2(x), \ (x \in \mathbb{R})$$

with α-periodic δ_1, δ_2. Note that unlike the situation of Sturm–Liouville operators, where the Prüfer angle has a preferred direction of growth and cannot go back across a certain threshold mod π, there is no such restriction on the Prüfer angles for Dirac systems, and in particular there is no a priori bound on δ_1, δ_2. Nevertheless, from the equation for the Prüfer angle,

$$\vartheta' = m \cos 2\vartheta - l \sin 2\vartheta + q - \lambda, \tag{7}$$

we see that Θ_1 cannot overtake Θ_2 in the sense that $\Theta_2 - \Theta_1 + m\pi$ cannot be negative to the right of a zero for any $m \in \mathbb{Z}$; it follows that if

$$\Theta_2 \in [\Theta_1 + m\pi, \Theta_1 + (m+1)\pi)$$

with $m \in \mathbb{Z}$ at some point, then this relation is preserved throughout. Assuming $m = 0$ without loss of generality, we have $\delta_1 \leqslant \delta_2 < \delta_1 + \pi$.

Turning now to the perturbed Eq. (3) with $\lambda \in (\Lambda_1, \Lambda_2)$, we observe that the perturbation satisfies the estimate

$$-\frac{|c|}{r} \leqslant \frac{c}{r}\sigma_1 \leqslant \frac{|c|}{r}$$

in the sense of quadratic forms, and hence, again using [18, Theorem 16.1] the Prüfer angle ϑ of a solution of the perturbed equation is caught between Θ_1 and $\Theta_2 \bmod \pi$ as soon as $|c|/r$ is no greater than the distance of λ to the ends of the gap. Therefore, choosing $r_{\max}(\lambda) > r_{\min}$ to be an integer multiple of the period α with

$$r_{\max}(\lambda) \geqslant \frac{|c|}{\min\{\lambda - \Lambda_1, \lambda - \Lambda_2\}},$$

we have

$$\vartheta(r) = \frac{n\pi r}{\alpha} + \delta(r) + m\pi \quad (r \geqslant r_{\max}(\lambda))$$

with some $m \in \mathbb{Z}$ and either $\delta_1 \leqslant \delta \leqslant \delta_2$ or $\delta_2 \leqslant \delta \leqslant \delta_1 + \pi$ throughout, depending on the initial value of ϑ. Consequently, δ is bounded on $[r_{\max}(\lambda), \infty)$ with a bound *uniform* in $\lambda \in (\Lambda_1, \Lambda_2)$. Furthermore, considering $\lambda = \lambda_j$, $j \in \{1, 2\}$, if $m \in \mathbb{Z}$ is such that the corresponding Prüfer angles ϑ_1, ϑ_2 satisfy $|\vartheta_2(r) - \vartheta_1(r) + m\pi| < \pi$ for one $r > \max(r_{\max}(\lambda_1), r_{\max}(\lambda_2))$, then the same holds true for all such r.

With these relations in mind, one can obtain an estimate for the number $N_\infty[\lambda_1, \lambda_2)$ of eigenvalues in $[\lambda_1, \lambda_2)$ of the self-adjoint realisation h_∞ of (5) on the interval $[r_{\min}, \infty)$ with the boundary condition (6) at $r_{\min}$, from a knowledge of the growth of the Prüfer angles ϑ_j on the compact intervals $[r_{\min}, r_{\max}(\lambda_j)]$, $j \in \{1, 2\}$. We fix the initial value such that $\vartheta_j(r_{\min}) = 3\pi/4$. Then [18, Theorem 16.4] gives the bounds

$$\limsup_{x\to\infty} \frac{1}{\pi}(\vartheta_2(x) - \vartheta_1(x)) - 2 \leqslant N_\infty[\lambda_1, \lambda_2) \leqslant \liminf_{x\to\infty} \frac{1}{\pi}(\vartheta_2(x) - \vartheta_1(x)) + 2.$$

To keep track of the global growth of the Prüfer angle ϑ_j, we introduce the half-plane number $H_j(x)$, defined to be the integer such that

$$\vartheta_j(x) \in [H_j(x)\pi, (H_j(x)+1)\pi).$$

In the following, we denote by floor(x) the largest integer not exceeding x, and by ceil(x) the smallest integer not less than x, for $x \in \mathbb{R}$. Thus, $H_j(x) = \mathrm{floor}(\vartheta_j(x)/\pi)$.

Since $\vartheta_{j(x)} - xn\pi/\alpha$ is caught mod π between the α-periodic δ_1, δ_2, we find

$$|H_j(r_{\max}(\lambda_j)) - H_j(r_{\max}(\lambda_j) + K\alpha) - Kn| \leqslant 1 \quad (K \in \mathbb{N}_0).$$

Hence for $K \in \mathbb{N}$ such that $K\alpha \geqslant \max\{r_{\max}(\lambda_1), r_{\max}(\lambda_2)\}$, we find

$$\mathrm{floor}\left(\frac{1}{\pi}(\vartheta_2(K\alpha) - \vartheta_1(K\alpha))\right) \leqslant H_2(r_{\max}(\lambda_2)) - H_1(r_{\max}(\lambda_1)) + \frac{n(r_{\max}(\lambda_1) - r_{\max}(\lambda_2))}{\alpha} + 2.$$

As observed above, this estimate continues to hold if $K\alpha$ is replaced by $r \geqslant \max(r_{\max}(\lambda_1), r_{\max}(\lambda_2))$. Similarly we have

$$\mathrm{ceil}\left(\frac{1}{\pi}(\vartheta_2(r) - \vartheta_1(r))\right) \geqslant H_2(r_{\max}(\lambda_2)) - H_1(r_{\max}(\lambda_1)) + \frac{n(r_{\max}(\lambda_1) - r_{\max}(\lambda_2))}{\alpha} - 2,$$

and hence

$$\left| N_\infty[\lambda_1, \lambda_2) - \left(H_2(r_{\max}(\lambda_2)) - H_1(r_{\max}(\lambda_1)) + \frac{n(r_{\max}(\lambda_1) - r_{\max}(\lambda_2))}{\alpha}\right)\right| \leqslant 4.$$

The self-adjoint operator h_c realising (5) on the whole interval $(0, \infty)$ is a two-dimensional extension of a two-dimensional restriction of the direct sum $h_0 \oplus h_\infty$, so the decomposition principle (cf. [12, Lemma 6]) yields the following estimate.

Proposition 2. *The number $N[\lambda_1, \lambda_2)$ of eigenvalues in $[\lambda_1, \lambda_2)$ of h_c satisfies*

$$\left| N[\lambda_1, \lambda_2) - \left(H_2(r_{\max}(\lambda_2)) - H_1(r_{\max}(\lambda_1)) + \frac{n(r_{\max}(\lambda_1) - r_{\max}(\lambda_2))}{\alpha}\right)\right| \leqslant 6.$$

Note that this error estimate is universal and does not depend on the position of λ_1, λ_2 in the gap. In particular, the error does not accumulate across several adjacent subintervals in the histogram.

3. The numerical procedure

The considerations of Section 2 have reduced the problem to calculating the half-plane number of the Prüfer angle of the solution of (3) on $[r_{\min}, r_{\max}(\lambda)]$ with initial condition $u(a) = \binom{1}{-1}$ for a given $\lambda \in (\Lambda_1, \Lambda_2)$. Instead of numerically solving the nonlinear differential equation for the Prüfer angle, we make use of the fact that the Dirac system

$$-\mathrm{i}\sigma_2 u' + (m_0\sigma_3 + l_0\sigma_1 + q_0)u = \lambda u \tag{8}$$

with *constant* $m_0, l_0, q_0 \in \mathbb{R}$ admits an explicit solution in the form of a transfer matrix for the interval $[x, x+L]$,

$$u(x+L) = \begin{pmatrix} \cos(C,L) - l_0\sin(C,L) & (m_0 - q_0 + \lambda)\sin(C,L) \\ (m_0 + q_0 - \lambda)\sin(C,L) & \cos(C,L) + l_0\sin(C,L) \end{pmatrix} u(x),$$

where $C = l_0^2 + m_0^2 - (q_0 - \lambda)^2$, and

$$\cos(C,L) = \begin{cases} \cos\sqrt{-C}L & \text{if } C < 0, \\ 1 & \text{if } C = 0, \\ \cosh\sqrt{C}L & \text{if } C > 0, \end{cases}$$

$$\sin(C,L) = \begin{cases} \dfrac{\sin\sqrt{-C}L}{\sqrt{-C}} & \text{if } C < 0, \\ L & \text{if } C = 0, \\ \dfrac{\sinh\sqrt{C}L}{\sqrt{C}} & \text{if } C > 0. \end{cases}$$

At face value, this only gives the value of $u(x+L)$ in terms of $u(x)$, and hence just the Prüfer angle mod π. However, because of the simple structure of the solutions of (8), one can also infer the change of the global half-plane number from these data. In the elliptic case $C < 0$ the half-plane number changes either by the even number

$$\operatorname{sgn}(q_0 - \lambda) 2 \operatorname{floor}\left(\frac{L\sqrt{-C}}{2\pi} + \frac{1}{2}\right)$$

or by the odd number

$$\operatorname{sgn}(q_0 - \lambda)\left(1 + 2\operatorname{floor}\left(\frac{L\sqrt{-C}}{2\pi}\right)\right)$$

across the interval $(x, x+L]$; and which of the two cases applies is clear from whether $u(x)$ and $u(x+L)$ lie in the same or opposite (upper or lower) half-planes of $\mathbb{R}^2$.

In the hyperbolic-parabolic case $C \geqslant 0$ the equation for the Prüfer angle (7) shows that it can only change by less than π, as the right-hand side changes sign as ϑ varies, thus introducing critical points where $\vartheta' = 0$. Consequently, the half-plane number changes by at most ± 1; if $u(x)$ and $u(x+L)$ are in opposite half-planes, it increases if

$$u_1(x)u_2(x+L) - u_2(x)u_1(x+L) > 0$$

and decreases otherwise.

Taking these observations together and using the continuity of solutions, we can thus calculate the solution and half-plane number for a Dirac system with piecewise constant coefficients. Given $\varepsilon > 0$, we approximate the angular momentum term $\sigma_1 c/r$ by a piecewise constant function $\sigma_1 \tilde{l}(r)$ such that

$$\sup_{r \in [r_{\min}, r_{\max}(\lambda)]} \left| \frac{c}{r} - \tilde{l}(r) \right| \leqslant \varepsilon.$$

As a result, we actually estimate the number of eigenvalues of the perturbed operator $\tilde{h}_c = h_c + \sigma_1(\tilde{l}(r) - c/r)$. However, these are just the eigenvalues of h_c shifted by at most ε; indeed, by operator perturbation theory (cf [12, Lemma 6]) the total spectral multiplicities of h_c and $\tilde{h}_c$ satisfy the estimate

$$N_{h_c}[\lambda_1 + \varepsilon, \lambda_2 - \varepsilon) \leqslant N_{\tilde{h}_c}[\lambda_1, \lambda_2) \leqslant N_{h_c}[\lambda_1 - \varepsilon, \lambda_2 + \varepsilon).$$

In particular, in the histogram of eigenvalue counts an eigenvalue shifted out of one interval will reappear in a neighbouring interval. Thus, in conjunction with the universality of the first error estimate (Proposition 2), we can expect that the histogram will give a reliable picture of the eigenvalue distribution inside the gap.

If the periodic coefficients m, l, q are piecewise constant, we can perform the calculation as outlined above; otherwise we replace them by piecewise constant functions invoking the same perturbation argument.

This numerical procedure was implemented in a C++ programme which accepts piecewise constant periodic coefficients m, l, q.

The location of the nth instability interval is determined based on its characterization as the interval in which the discriminant D of the periodic equation has absolute value larger than 2 and the half-plane number after one period of the Prüfer angle with $\vartheta(0) = 0$ (corresponding to the solution with $u(0) = \binom{1}{0}$) is either n or $n - 1$. Furthermore, in the case of constant $m > 0$, the partial derivatives $(\partial/\partial m)D$, $(\partial/\partial q)D$ of the discriminant with respect to (constant) perturbations of the coefficients m and q are calculated at the end-points of the instability interval. According to the relative oscillation–nonoscillation criterion [15], a gap end-point is [not] an accumulation point of eigenvalues if

$$m\alpha^2 + 2\left(c^2 \frac{\partial D}{\partial m} + c \frac{\partial D}{\partial q} \right) < 0 \; [\, > 0]; \tag{9}$$

depending on the sign of $(\partial/\partial m)D$, this is the case either for sufficiently large c, or only on some bounded c interval.

With a chosen $\varepsilon > 0$ for the piecewise-constant approximation of the perturbation, the interval $[\Lambda_1 + \varepsilon, \Lambda_2 - \varepsilon]$ is divided into subintervals of equal length for the histogram. In the case $l \equiv 0$ we calculate an approximation of the integral on the right-hand side of the asymptotic formula (2) for each subinterval, in order to compare the actual number of eigenvalues from our numerical estimate to the value given by the asymptotic formula.

4. Examples

1. *The Dirac–Meissner operator*

Consider (3) with $m \equiv 1$, $l \equiv 0$ and the 2-periodic potential

$$q(r) = \begin{cases} a, & r \in [0,1) \bmod 2, \\ -a, & r \in [1,2) \bmod 2. \end{cases}$$

For $a = 1$, the corresponding set $\Pi(h)$ has a gap coinciding with the 0th gap $(-0.845502, 0.845502)$ of the periodic operator h (cf. [10, Section 3]); hence the asymptotic density (2) vanishes identically in the 0th gap. Both end-points of this gap are not accumulation points of eigenvalues by criterion (9). Eigenvalue histograms were computed by the method of Section 3 for coupling constants $c = 10^j$ ($j \in \{1, \ldots, 7\}$) and accuracy $\varepsilon = 0.01$. In all cases one single eigenvalue was reported in the subinterval $[0.50131, 0.668402]$, which, however, may well be spurious in view of Proposition 2. In any case, no significant number of eigenvalues could be found in the first gap, suggesting that indeed $\sigma_e = \Pi(h)$ in this case.

Table 1 shows the results for the 1st gap $(1.491123, 2.126314)$ and the 2nd gap $(3.214706, 3.400224)$, both with $\varepsilon = 0.01$. For each λ-subinterval, the eigenvalue counts for different values of the coupling constant c are shown; the last column gives the value of the right-hand side of the asymptotic formula (2).

In both gaps and for all values of c considered, the lower end-point is an accumulation point of eigenvalues while the upper end-point is not. The calculated eigenvalue counts are remarkably close

Table 1

λ	$c = 10$	100	1000	10,000	100,000	1,000,000	10,000,000	asympt. int.
1.501123								
	2	13	123	1230	12298	122973	1229729	0.122972857
1.562642								
	0	5	47	476	4757	47570	475698	0.047569849
1.624161								
	1	3	32	319	3191	31907	319074	0.031907389
1.685681								
	0	2	25	243	2431	24315	243150	0.024314956
1.747200								
	0	2	19	197	1969	19685	196849	0.019684913
1.808719								
	0	2	17	166	1652	16520	165200	0.016519992
1.870238								
	0	1	14	142	1420	14202	142024	0.014202451
1.931757								
	1	2	13	124	1242	12426	124252	0.012425210
1.993276								
	0	1	11	110	1102	11016	110163	0.011016249
2.054795								
	0	1	10	99	987	9871	98708	0.009870801
2.116314								
3.224706								
	1	4	31	319	3188	31872	318731	0.318730898
3.241258								
	0	1	19	182	1826	18263	182624	0.182623858
3.257810								
	0	2	13	135	1354	13542	135420	0.135419253
3.274362								
	0	1	12	110	1103	11034	110345	0.110344657
3.290913								
	0	1	8	95	945	9444	94441	0.094440861
3.307465								
	0	0	9	83	833	8330	83292	0.083292828
3.324017								
	0	1	8	75	749	7495	74958	0.074957672
3.340569								
	0	2	7	68	685	6844	68438	0.068438203
3.357121								
	0	0	6	65	631	6317	63166	0.063166480
3.373673								
	0	1	6	58	588	5880	58794	0.058793558
3.390224								

Table 2

λ	$c=10$	100	1000	10,000	100,000	1,000,000	10,000,000	asympt. int.
−0.048900								
	0	0	1	7	64	639	6408	0.00064080
−0.039120								
	0	0	0	4	45	460	4587	0.00045864
−0.029340								
	0	1	0	2	31	311	3109	0.00031080
−0.019560								
	0	0	0	2	19	180	1806	0.00018061
−0.009780								
	0	0	0	0	4	58	591	0.00005928
0.000000								
	0	1	3	3	7	61	594	0.00005928
0.009780								
	0	0	0	2	19	180	1806	0.00018061
0.019560								
	0	0	0	2	31	311	3109	0.00031080
0.029340								
	0	0	0	4	45	459	4587	0.00045864
0.039120								
	1	1	2	8	65	641	6409	0.00064080
0.048900								
1.475555								
	0	0	2	9	97	967	9668	0.00096687
1.493040								
	0	0	1	10	102	1020	10210	0.00102089
1.510526								
	1	1	2	12	108	1083	10809	0.00108083
1.528011								
	0	0	1	12	115	1150	11499	0.00115000
1.545497								
	0	0	1	12	124	1236	12361	0.00123604
1.562982								
	0	0	1	14	137	1367	13668	0.00136681
1.580468								
	0	0	1	16	160	1593	15929	0.00159298
1.597953								
	0	0	2	14	140	1411	14125	0.00141240
1.615439								
	1	1	2	13	137	1367	13658	0.00136587
1.632925								
	0	0	2	14	137	1360	13595	0.00135944
1.650410								

to the value obtained by multiplying the asymptotic integral by c in the whole range of coupling constants.

Qualitatively similar results were obtained for the 0th, 1st and 2nd gaps for the operator with $a=\frac{1}{2}$.

In the case $a=10$, $\Pi(h)$ covers the whole real line (cf. [10]). The results of the histogram calculation with ε=0.001 for the 0th gap $(-0.049900, 0.049900)$ and the 1st gap (1.474555, 1.651410) are collected in Table 2. For all values of c studied, the end-points for both gaps are not accumulation points of eigenvalues, with the single exception of the lower end-point of the 0th gap for $c=10$. Note that none of the infinitely many gap eigenvalues appear in the histogram; even when the calculation was pushed much closer to the gap edge ($\varepsilon=0.0000001$) no more eigenvalues were observed. Thus, interesting spectral effects may actually occur extremely close to the essential spectrum, which escape the attention of numerical calculation; the observed essential absence of eigenvalues in the 0th gap for $a=1$, $a=\frac{1}{2}$ must therefore be taken with some caution.

Table 2 again shows excellent agreement with the asymptotic formula throughout the c region. In the 0th gap 3 possibly spurious eigenvalues appear near 0 for $c=10^j$, $j\in\{3,4,5,6,7\}$; though not for $c\in\{10,100\}$.

2. As a second example with less symmetry, we consider (3) with $m\equiv 1$, $l\equiv 0$ and the 1-periodic potential with

$$q(r)=r^2 \quad (r\in[0,1)).$$

In practice, this function q is replaced by a piecewise-constant function $\tilde{q}$ with $\|\tilde{q}-q\|_\infty<\frac{1}{200}$.

Table 3

λ	$c=10$	100	1000	10,000	100,000	1,000,000	asympt. int.
−3.003616							
	0	1	6	59	591	5908	0.00590793
−2.991922							
	0	0	7	65	651	6511	0.00651145
−2.980227							
	1	2	8	74	731	7306	0.00730433
−2.968533							
	0	1	8	84	842	8419	0.00841929
−2.956838							
	0	1	10	101	1012	10123	0.01012350
−2.945143							
	0	1	14	132	1316	13153	0.01315301
−2.933449							
	1	2	20	206	2059	20596	0.02059485
−2.921754							
3.589501							
	1	2	20	202	2028	20276	0.02027550
3.601004							
	0	1	13	130	1300	13005	0.01300498
3.612506							
	0	1	10	101	1003	10023	0.01002348
3.624008							
	0	1	9	83	834	8342	0.00834195
3.635510							
	0	1	7	73	724	7241	0.00724133
3.647012							
	1	2	7	65	647	6456	0.00645487
3.658514							
	0	0	6	59	586	5860	0.00585994
3.670016							

The asymptotic density in the 0th gap $(-0.663414, 1.330506)$ vanishes identically, and both end-points are not accumulation points of eigenvalues. No eigenvalues were observed in the calculated histograms.

The results for the -1st gap $(-3.013616, -2.911754)$ and the 1st gap $(3.579501, 3.680016)$, with $\varepsilon = 0.01$, are shown in Table 3; note again the excellent agreement with the asymptotic formula throughout, in spite of the fact that ε is almost as large as the length of each subinterval.

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