A polynomial approach to the spectrum of Dirac–Weyl polygonal Billiards

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Received 8 August 2020, revised 29 September 2020
Accepted for publication 5 October 2020
Published 19 October 2020

Abstract

The Schrödinger equation in a square or rectangle with hard walls is solved in every introductory quantum mechanics course. Solutions for other polygonal enclosures only exist in a very restricted class of polygons, and are all based on a result obtained by Lamé in 1852. Any enclosure can, of course, be addressed by finite element methods for partial differential equations. In this paper, we present a variational method to approximate the low-energy spectrum and wave-functions for arbitrary convex polygonal enclosures, developed initially for the study of vibrational modes of plates. In view of the recent interest in the spectrum of quantum dots of two dimensional materials, described by effective models with massless electrons, we extend the method to the Dirac–Weyl equation for a spin-1/2 fermion confined in a quantum billiard of polygonal shape, with different types of boundary conditions. We illustrate the method’s convergence in cases where the spectrum is known exactly, and apply it to cases where no exact solution exists.

Keywords: polynomial, spectrum, Schrödinger, Dirac–Weyl, eigenfunctions, confinement, continuum

(Some figures may appear in colour only in the online journal)

1. Introduction

One of the first problems solved in introductory quantum mechanics courses is that of particle enclosed in a square or rectangular box with hard walls—Dirichlet boundary conditions (BC), \( \psi(\mathbf{r}) = 0 \) at the boundary. Separation of variables easily turns the problem into two one-dimensional problems and the solutions are a finite sum of plane waves. The circle and the ellipse are also amenable to an exact treatment, again with separation of variables. But the vast majority of students are never led to consider the case of general polygonal enclosures.

The eigenvalue problem of the Schrödinger equation for an equilateral triangle with hard boundaries was solved, long before Schrödinger’s equation even came into existence, by Lamé [1] in 1852. This solution has been revisited often from different perspectives [2–6]. As in the case of a rectangle, Lamé’s solution is also a finite sum of plane waves, built to satisfy the boundary conditions, and remarkably, it has even been proven that the only shapes that share this feature are the square, the rectangle, the equilateral triangle, the half-square (right isosceles triangle) and the half equilateral triangle (30°–60° triangle) [7].

Following the pioneering work of Berry and Mondragon [8], and the discovery that two-dimensional (2D) materials, such as graphene, can be described by effective continuum models with the Dirac–Weyl equation [9, 10], there has been an upsurge of interest in the properties of confined relativistic particles (Dirac Billiards), either because low energy solutions have possible relevance for quantum dots of 2D materials [11–14], or to address fundamental questions concerning the classical-quantum relations and energy-level statistics in the semi-classical limit [8, 15–17].

Lacking exact analytical solutions, one usually has to resort to numerical methods, and finite element methods of integration of partial differential equations have universal application [13]. But such methods give little physical insight into the solutions. The aim of this article is to present an
essentially variational method that can yield the low energy spectrum of convex polygonal enclosures, both in the Schrödinger and Dirac equation cases, with the added benefit of providing approximate wave-functions which are polynomials. The method is well known in the Mechanical Engineering literature, in the context of the Helmholtz equation [18–20], where it was developed for the study of vibration of polygonal plates. The extension to the Schrödinger equation for free particle is trivial—the eigenvalue problem is the same as the Helmholtz problem, but, to our knowledge, its extension to the Dirac–Weyl equation has not been presented before.

This paper is structured as follows. In section 2, we present the polynomial method for the simple case of the Schrödinger equation, more specifically for the textbook problem of the free particle confined to a square well, and assess the convergence of the spectrum against the exact solution for this problem. We then apply the method to an hexagonal enclosure, a problem that has no analytical solution.

Section 3 reviews the different types of BC for the Dirac–Weyl equation, following closely reference [8]. We extend the polynomial method to 2-component spinors and the different types of BC, and illustrate it in exactly solvable one-dimensional enclosures. In sections 3.3–3.5 we study three different types of BC, and illustrate it in exactly solvable one-dimensional enclosures. We truncate the series at a finite $n$ and orthonormalize the functions, typically through Gram–Schmidt orthogonalization. The Hamiltonian matrix in this truncated basis is calculated and diagonalized. For regular polygons, one can take into account the symmetry group of the enclosure by replacing the monomials of equation (3) by increasing order polynomials that transform according to irreducible representations of the symmetry group [22]. The Hamiltonian matrix becomes block diagonal, and the resulting eigenstates end up classified according to their symmetry properties.

The problem of the Schrödinger equation for a particle confined to a square well, provides a suitable example to assess convergence.

### 2. The polynomial method for convex polygonal enclosures

#### 2.1. The method: general idea

The essential idea of the polynomial method [18–20] is to generate orthonormal polynomials of increasing order that satisfy, from the start, the required BC. In the $Oxy$ plane a linear polynomial in $x$ and $y$, $P_1(x,y) = a_0 + a_1 x + a_2 y$ will be zero in a straight line, $a_0 + a_1 x + a_2 y = 0$. It follows that a product of $n$ such polynomials trivially satisfies the condition $P_n(x,y) = 0$ at the boundary of a polygonal convex region. After normalization, such a function is a zeroth order approximation to the ground state.

As an example, for a right triangle with vertexes $(0,0)$, $(1,0)$, $(0,1)$ we would choose

$$\psi_0(x,y) = N_0 xy(1-x-y)$$

with

$$N_0 = \left[ \int_0^1 dx \int_0^{1-x} dy [xy(1-x-y)]^2 \right]^{-1/2} = 12\sqrt{3}.5$$

If we multiply $\psi_0(x,y)$ by any polynomial, $\psi(x,y) = P(x,y) \psi_0(x,y)$, we end up with a function that still satisfies the BC. We therefore proceed to generate a set of linearly independent functions

$$\psi_n(x,y) = P_n(x,y) \psi_0(x,y)$$  

where $\{ P_n(x,y) : n = 0, 1, \ldots \}$ is a family of ascending-order monomials/polynomials. These can be generated by taking into account the symmetries of the enclosure in question, in a simple ordering of monomials, or as a generalization of Legendre polynomials discussed by Larcher [21]. In [20] the authors resort to the sorting

$$\{ 1, x, y, xy, x^2, y^2, x^2 y, y^2 x, x^2 y^2, x^3, \ldots \}.$$  

We truncate the series at a finite $n$ and orthonormalize the functions, typically through Gram–Schmidt orthogonalization. The Hamiltonian matrix in this truncated basis is calculated and diagonalized. For regular polygons, one can take into account the symmetry group of the enclosure by replacing the monomials of equation (3) by increasing order polynomials that transform according to irreducible representations of the symmetry group [22]. The Hamiltonian matrix becomes block diagonal, and the resulting eigenstates end up classified according to their symmetry properties.

The exact spectrum of the Schrödinger equation for a particle confined to a square well is

$$E_{n_1 n_2} = \frac{\hbar^2}{2m} \pi^2 \left( n_1^2 + n_2^2 \right),$$

where $L$ is the side length of the enclosure, and $n_1(2)$ positive integers.

Centering the enclosure at the origin, the starting wavefunction is

$$\psi_0(x,y) = N_0 \left[ \left( \frac{L}{2} \right)^2 - x^2 \right] \left[ \left( \frac{L}{2} \right)^2 - y^2 \right].$$

The higher order basis functions are generated as described previously, by multiplication by $x^{n_1}y^{n_2}$ monomials. Both the orthogonalization and the calculation of the matrix elements of the kinetic energy operator reduce to the calculation of integrals of $x^{n_1}y^{n_2}$ monomials in the domain of the enclosure; these are easily calculated symbolically and stored. Keeping the computation symbolic up until the diagonalization of the Hamiltonian avoids stability problems of the Gram–Schmidt procedure. We computed the Hamiltonian matrix for different basis sizes, and diagonalized it numerically using standard packages. The results are shown in figure 1, overlayed with the exact eigenvalues.

The method is seen to converge towards the exact eigenvalues as we increase the basis size. As the index of the eigenvalue increases, we require a larger basis, as expected. The numerical results indicate, roughly, that to get the lowest $n$ eigenvalues to within $1\%$ accuracy requires of the order of $3n$ basis functions.
2.3. The hexagonal enclosure

To apply this procedure to the Schrödinger equation for a particle confined to an hexagonal well of side length $L$, we define the initial normalized polynomial as

$$
\psi_0(x,y) = N_0 \left( \frac{3L^2}{4} - y^2 \right) \left[ L^2 - \left( x - \frac{y}{\sqrt{3}} \right)^2 \right] \left[ L^2 - \left( x + \frac{y}{\sqrt{3}} \right)^2 \right].
$$

(6)

We again calculated the Hamiltonian matrix elements for different basis sizes, and diagonalized it numerically using standard packages. The results are shown in figure 2, overlayed with the eigenvalues obtained via direct numerical integration of the partial differential equation (PDE), by finite elements method. The convergence is similar to the one found in the case of the square.

As an illustration of this method, we applied it to different polygons with increasing number of sides and plot the lowest eigenvalues against the inverse number of sides (squared) in figure 3, where the result for the circle, $\epsilon_i^\infty, i = 1, 2, 3$, is the analytical solution.

The dashed lines are fits of the form $\epsilon_i(n) = \epsilon_i^\infty + a_2 n^{-2} + a_4 n^{-4}$, where $n$ is the number of sides. A suitable fit could not be found for the third eigenvalue, and the point for $n = 3$ was excluded. The remaining data points are well fitted with $a_4 = 0$.

We now turn to the extension of these results to the Dirac–Weyl equation.

3. Confinement of Dirac–Weyl electrons

3.1. Boundary conditions in neutrino Billiards

Berry and Mondragon [8] were the first to address the issue of the boundary conditions of a two-component spinor solution of the Dirac–Weyl equation in a confining planar enclosure. The eigenvalue equation is

$$
- i \hbar v_F \sigma \cdot \nabla \Psi = E \Psi
$$

(7)

where $\sigma = (\sigma_x, \sigma_y)$. We assume a confining boundary at $y = 0$, excluding the region $y < 0$. The probability current is given by

$$
\mathbf{j} = \mathbf{v}_F \Psi^\dagger \sigma \Psi = \mathbf{v}_F \langle \sigma \rangle,
$$

(8)

which means that a necessary condition for confined states is

$$
\langle \sigma^\dagger \rangle_{\text{boundary}} = 0.
$$

(9)

This condition implies that the spinor at the boundary must be an eigenstate of $\sigma_u = \sigma \cdot \mathbf{u}$, where $\mathbf{u} = \cos \theta e_z + \sin \theta e_x$, i.e.,

$$
\begin{bmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{bmatrix} \begin{bmatrix} \psi_A \\ \psi_B \end{bmatrix} = \eta \begin{bmatrix} \psi_A \\ \psi_B \end{bmatrix}, \quad \eta = \pm 1,
$$

(10)
or simply
\[
\frac{\psi_B}{\psi_A} = \frac{\eta - \cos \theta}{\sin \theta}.
\]
(11)

Denoting \( t := \tan(\theta/2) \), simple trigonometric identities lead us to
\[
\frac{\psi_B}{\psi_A} = t,
\]
(12)
with a spinor, at the boundary, given by
\[
\begin{bmatrix}
\psi_A \\
\psi_B
\end{bmatrix}
= \frac{1}{\sqrt{1 + t^2}}
\begin{bmatrix}
1 \\
t
\end{bmatrix}
\]
(13)
for \( \eta = +1 \). The case for \( \eta = -1 \) is obtained by the substitution \( t \rightarrow -1/t \), or by changing \( \theta \rightarrow \pi - \theta \). As such, this is not a different solution, and we keep only \( \eta = +1 \).

Some special cases are:

\begin{itemize}
  \item \( t = 0 \) or \( r \rightarrow \infty \) (Dirichlet boundaries)
  \[
  \begin{cases}
  t = 0, & \psi_B = 0; \\
  t \rightarrow \infty, & \psi_A = 0,
  \end{cases}
  \]
  (14)
  so that, at the boundary, \( \langle \sigma^z \rangle = \pm 1 \).
  \item \( t = \pm 1 \)
  \[
  \psi_A = \pm \psi_B.
  \]
  (15)
\end{itemize}

In this case, the spin points along the x-direction.

The choice of the value of \( t \) depends on the physical nature of the confinement. Berry and Mondragon [8] considered adding a spatially dependent mass (gap) term,
\[
-\frac{\hbar v_F}{2} \sigma \cdot \nabla \psi + m(\mathbf{r}) \sigma_z \psi = E \psi.
\]
(16)
If \( m(\mathbf{r}) \) is non-zero outside a domain \( D \) and zero inside \( D \), energy states near zero energy have an exponential decay outside, because of the energy gap in the spectrum. If \( m(\mathbf{r}) \rightarrow \infty \) outside \( D \), with \( m(\mathbf{r}) = 0 \) inside, continuity of the spinor components at the boundary leads to a BC of the type of equation (15) [8]. We have asked whether a more general value of the parameter \( t \) can be obtained by a similar reasoning. One can show that a mass term with an extra scalar potential term of the form \([22]\)
\[
m(\mathbf{r}) (\sigma^2 - \cos \theta)
\]
leads to the more general BC of equation (12) with \( t = \tan(\theta/2) \) (see appendix A for details). The cases \( t = 0 \) or \( t \rightarrow \pm \infty \) correspond to Dirichlet boundaries in one of the spinor components, as in the case of zigzag boundaries in graphene.

If the boundary is at an angle \( \phi \) with the x-axis, one must rotate the spinor in equation (13), resulting finally in
\[
\Psi = e^{-i\phi \sigma_z/2} \frac{1}{\sqrt{1 + t^2}}
\begin{bmatrix}
1 \\
t
\end{bmatrix}
 = \frac{1}{\sqrt{1 + t^2}}
\begin{bmatrix}
e^{-i\phi/2} \\
e^{i\phi/2} t
\end{bmatrix}.
\]
(18)

We will now show how to extend the polynomial method defined in section 2 to this new type of BC. As an illustration we begin with 1D cases, where one easily computes the exact spectrum.

3.2. One-dimensional Dirac–Weyl confinement

Consider the simple case where \( t = 1 \) and the confined region is the interval \( y \in [-L/2, L/2] \). The BC are \( \psi_B(-L/2)/\psi_A(-L/2) = 1 \) at one end, and \( \psi_B(L/2)/\psi_A(L/2) = -1 \) at the other \((\phi = \pi \text{ in equation (18)})\). This is a non-Dirichlet BC, thus requiring a non trivial extension of the polynomial method, and has already been used in [23].

Measuring energies in units of \( \hbar v_F/L, e = E / (\hbar v_F/L) \),
\[
-\partial_y \psi_B = \epsilon \psi_A,
\]
\[
\partial_y \psi_A = \epsilon \psi_B
\]
(19)

Squaring the Hamiltonian, one sees that the solutions have the form
\[
\psi_B = f_1 e^{iqy} + f_2 e^{-iqy},
\]
\[
\psi_A = f_1 e^{iqy} + f_4 e^{-iqy},
\]
(20)
with \( \epsilon = sq, s = \pm 1 \). With no loss of generality we assume \( q > 0 \).

The Dirac–Weyl equation implies
\[
f_4 = is f_2
\]
\[
f_3 = -is f_1.
\]
The BC then imply
\[
(1 - ist) f_1 + (1 + ist) f_2 e^{-iqL} = 0
\]
\[
(1 + ist) f_1 + (1 - ist) f_2 e^{iqL} = 0
\]
(21)

A non-zero solution to this homogeneous system of 2 equations, for \( t = 1 \), requires
\[
(1 - is)^2 e^{iqL} = (1 + is)^2 e^{-iqL}
\]
(22)
or
\[
q = \frac{\pi}{2L} (2n + 1)
\]
(23)
and the energies are [23]
\[
e_{n,s}(n) = \pm \frac{\pi}{2L} (2n + 1) \quad n \geq 0, s = \pm 1
\]
(24)

The Dirac–Weyl equation in free space has electron–hole symmetry; it is easily seen that for any solution \( \Psi = [\psi_A, \psi_B]^T \) of energy \( E \), the state \( \Psi = [\psi_A, -\psi_B]^T \) is a solution of energy \(-E\). But the BC we are choosing, \( \psi_B/\psi_A = \pm 1 \), breaks this symmetry, because \( \Psi \) and \( \overline{\Psi} \) cannot both obey these BC. This can be traced to the mass term we introduced outside the confining region to derive the BC: it explicitly breaks this particle–hole symmetry. Nevertheless, the spectrum of eigenvalues remains symmetrical (equation (24)), because it is still true for this complete 1D Hamiltonian, inside and outside the enclosure, that \( \sigma^z \) is a chiral symmetry operator, \( \sigma^z H \sigma^z = -H \).

To implement the polynomial method, we must first realize that the parities of \( \psi_A \) and \( \psi_B \) are opposite. We therefore choose
for the spinor components as the lowest order polynomials that satisfy the BC. For the conduction band ($s = 1$) we have,

$$
\Psi_0^{(1)} = N_0 \left[ \frac{1}{L/2} \right]
$$

(25)

where $N_0$ is a normalization constant. To obtain the valence band solution, $s = -1$, it is enough to swap $\psi_A \leftrightarrow \psi_B$. The basis is now generated by functions of the form $\Psi_n = \mathcal{P}_n(y)\Psi_0^{(s)}$, orthonormalized by the Gram–Schmidt process. One must take care, however, to orthogonalize states between the valence and conduction bands, as the states generated this way for $s = 1$ and $s = -1$ are not orthogonal to start with.

Having generated the basis, one easily computes and diagonalizes the Hamiltonian matrix. We obtained the approximate spectrum visible in figure 4; the inset shows the convergence analysis of the first three eigenvalues of the conduction band. An almost exact match is also present in the first eigenfunction of the conduction band, as shown in figure 5.

Having checked the validity of this method against a simple solution of the Dirac–Weyl equation, we will now proceed to consider planar enclosures.

### 3.3. 2D enclosures

To generalize this procedure to 2D enclosures, we must be aware of a difference between Dirichlet boundaries and boundaries with finite $t$. If one has a Dirichlet BC, one can square the Dirac–Weyl Hamiltonian and easily prove that each spinor component obeys a Schrödinger equation inside the enclosure where the mass term is zero. As such, one can use the method we presented before for this equation to calculate the square of the eigenvalues and the spinor component that is zero at the boundary. Since the Dirac–Weyl equation has particle–hole symmetry—if one changes the sign of one of the spinor components in a state with energy $E$, one obtains a state of energy $-E$, which still preserves the Dirichlet BC—, one effectively obtains all the eigenvalues. Applying the Dirac operator to the

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**Figure 4.** Exact solution vs polynomial approximation for a 1D strip with $t = 1$. Convergence of the first three eigenvalues in the inset.

**Figure 5.** Comparison between the exact solution (full lines) and the lowest-energy polynomial eigenfunction (dots) for the 1D strip with boundary condition parameter $t = 1$, with 16 polynomials.
component which is zero at the Boundary, one generates the other component of the spinor and completes the solution [14].

3.3.1. Non-Dirichlet BC. The same procedure cannot be used for finite \( t \), when the BC only fixes the ratio between the spinor components, \( \psi_B/\psi_A = \tau^{(0)} \). The circle is the only 2D enclosure where an exact solution is known for the infinite-mass BC we are using [22]. The solution is given by [24]

\[
\Psi_{s,m}(r, \theta) = \left[ e^{i\theta}J_m(qr) \right] \frac{e^{i\phi}}{i\alpha e^{i(n+1)\phi}J_{n+1}(qr)}
\]

where \( s = \pm 1 \) is the band index, \( J_m \) is the Bessel function of the first kind of order \( m \) and \( \epsilon = s/\sqrt{\epsilon^2} \), is the energy of the state. Imposing the boundary condition, the allowed energy levels are those in which

\[
\frac{J_{n+1}(qR)}{J_n(qR)} = s.
\]

To apply the polynomial method to this enclosure, we must build the initial functions carefully. The rotation symmetry is non-orthogonal basis is

\[
\psi_A(r, \theta - \phi) = e^{-i\theta} \psi_A(r, \theta - \phi)
\]

we get

\[
\hat{U}\psi = e^{-i\phi} \psi,
\]

with \( k = m + 1/2 \). The only functions which are invariant under this symmetry are linear combinations of \( z^{2n} = r^{2n} \), for \( n \geq 0 \). For each \( m \), the initial states that respect the symmetries and the BC, \( \psi_B/\psi_A = i\tau^{(0)} \) are (with \( \zeta = x + iy \) and \( \bar{\zeta} \) the complex conjugate of \( \zeta) \)

\[
\psi_0^{(m \geq 0)}(z, \bar{\zeta}) = z^m \left[ -i \frac{\bar{\zeta}}{\zeta} \right],
\]

\[
\psi_0^{(m < 0)}(z, \bar{\zeta}) = (\bar{\zeta})^{-m+1} \left[ \frac{\zeta}{\bar{\zeta}} \right].
\]

With no loss of generality, we discuss the states with \( m = 0 \). The procedure is analogous for the remaining representations. A polynomial state can have the form

\[
|P(r), Q(r)\rangle = \left[ -iP(r) \right] zQ(r).
\]

if \( P \) and \( Q \) are even polynomials in \( r \) such that \( P(1) = Q(1) = 1 \), thus respecting both the BC and the symmetries in question. Simple monomials \( P_n(r) = r^{2n} \) satisfy both conditions and a non-orthogonal basis is

\[
\{ P_0, P_0 \}, \{ P_1, P_0 \}, \{ P_0, P_1 \}, \{ P_2, P_0 \}, \{ P_0, P_2 \}, \ldots \}
\]

After applying the G–S process, the Hamiltonian is straightforwardly computed and diagonalized for different basis sizes.

Table 1. Convergence of polynomial method for the circular enclosure.

| Basis Size | \( \epsilon_0 \) | \( \epsilon_1 \) | \( \epsilon_2 \) | \( \epsilon_3 \) |
|------------|----------------|----------------|----------------|----------------|
| 2          | 1.4415         | -2.77485       | 4.17305        |
| 3          | 1.4344         | -3.20749       | 4.61325        |
| 5          | 1.4347         | -3.11371       | -7.05342       |
| 7          | 1.4347         | -3.11287       | 4.67908        |
| Exact      | 1.4347         | -3.11286       | 4.6801         |

The comparison with the exact results is presented in table 1. As the method quickly converges towards the exact results, we will now apply it to the square enclosure with the same BC.

3.4. Non-Dirichlet square enclosure

The case of square with edges at \( x, y = \pm L/2 \) and \( t = 1 \) has no known analytic solution. As these boundary conditions correspond to an uniform gap outside the enclosure, the Hamiltonian will be invariant under \( \pi/2 \) rotations.

\[
\hat{U} = e^{-i\pi/2}e^{i\pi/2}R_{\pi/2}
\]

The one-dimensional representations of this symmetry are given by

\[
\hat{U}\psi = e^{i\alpha}\psi
\]

where

\[
\alpha = \frac{\pi}{4} + m\frac{\pi}{2} \in [-\pi, \pi]
\]

Each time we multiply one of these states by \( e^{i\phi} \), \( \alpha \) changes as

\[
\alpha \rightarrow \alpha + (n - m)\frac{\pi}{2}
\]

We stay in the same irreducible representation, provided \( \alpha \) is unchanged modulo \( 2\pi \), i.e.,

\[
n - m = 0 \mod 4
\]

Invariant monomials of \( z \) and \( \bar{z} \) are \( |z|^2, z^4, (\bar{z})^4 \) and their products. There are two issues that need to be addressed at this point:

(a) the states of equation (33) do not satisfy the BC, and are therefore not suitable as starting states upon which to build a basis. Taking the \( \alpha = -\pi/4 \) as an example, we
require states of the form

\[ \Phi_0 = \begin{bmatrix} P_0 \left( |z|^2, z^4, (\bar{z})^4 \right) \\ zQ_0 \left( |z|^2, z^4, (\bar{z})^4 \right) \end{bmatrix} \]  

where the invariant polynomials, satisfy \( P_0 - Q_0 z = 1 \) for \( y = -1/2 \). If this is verified at this edge, the symmetry will ensure the BC are also verified at the other edges. The choice

\[ P_0 = -\frac{i}{5} - iz^4 + \frac{i}{5} \bar{z}^4, \]

\[ Q_0 = 1 + \frac{z^4}{5} - 2|z|^2 - \frac{1}{5} \bar{z}^4 \]  

proved convenient in the sense that the behavior of the ket \( \Phi_0(x, y) \) near the origin resembles that of the lowest eigenvalue of the circular enclosure,

(b) the basis must be built by multiplying each component of the spinor by increasing order invariant polynomials which are required to be unity at the edges of the enclosure so that the BC are preserved. Such polynomials can be generated order by order, by imposing

\[ P_n \left( |z|^2, z^4, (\bar{z})^4 \right) = 1 \]  

for \( y = -1/2 \). Once these steps are performed, the calculation proceeds as for the circle, by orthogonalizing the basis and calculating of the Hamiltonian matrix, separately for each of the 4 symmetry representations. The necessary work is halved.
because the transformation $\sigma_xK$ ($K$ is the complex conjugation operator) changes the sign of the Hamiltonian and preserves the BC; the states of the representations with $\alpha = 1/4, 3\pi/4$ can be obtained from those of $\alpha = -1/4, -3\pi/4$ by this transformation; the eigenvalue spectrum remains symmetrical.

The spectrum is displayed in figure 6, with the low-energy regime in the inset. The number of polynomials in the legend refers to the basis size in each irreducible representation.

This method again converges, as it did in case of the circular enclosure.

As stated before, the method also provides the eigenstates as polynomials. The valence band state with energy closest to zero is plotted in figure 7. At the centre of the square, the behavior of the two spinor components is not unlike that of the corresponding state of the circle, but is quite different at the edges. The two components have the same absolute value at the edges, as required by the BC, and both vanish at the corners, as that is the only way the BC of the edges that meet at the corner can be satisfied.

To finalize the analysis of the method, we tested it in a problem with BCs analogous to those found in zigzag-terminated hexagonal graphene flakes.

3.5. Dirichlet hexagonal enclosure

We applied this method to the study of an hexagonal enclosure with the BCs equivalent to those of an hexagonal graphene flake whose edges are all zigzag-terminated\(^1\). This specific set of BCs can be expressed by alternating $t$ between $t = 0$ and $t \to \infty$, depending on the termination sublattice.

As we are working with Dirichlet boundaries in alternating sides for each spinor component, we can construct the initial polynomial as in equation (5). Considering a regular hexagon centered at the origin of side-length $L$, the two spinor components for the starting state will be defined as

$$
\psi_{0,A}(x, y) = \left[ \sqrt{3}L/2 + y \right] \left[ L + \left( x - \frac{y}{\sqrt{3}} \right) \right] \left[ L - \left( x + \frac{y}{\sqrt{3}} \right) \right]$

$$
\psi_{0,B}(x, y) = \psi_{0,A}(x, -y).$$

(39)

With this, we diagonalize the Hamiltonian

$$
\langle \Psi_i | H^\dagger H | \Psi_j \rangle = \langle \psi_{iA} | \left( -\hbar^2 c^2 \nabla^2 \right) | \psi_{jA} \rangle + \langle \psi_{iB} | \left( -\hbar^2 c^2 \nabla^2 \right) | \psi_{jB} \rangle.$$

(40)

The resulting spectrum is visible in figure 8 for different basis sizes. The numerical solution was obtained via Wolfram Mathematica\(^6\) by imposing Dirichlet BCs on three alternating sides of the enclosure in question, leaving the remaining free.

\(^1\) Armchair edges in graphene couple two Dirac cones of graphene [25], and boundary conditions can only be expressed in terms of a 4-component spinor. Our method can, in principle, be extended to that situation.
Finally, we will compare these results with the ones obtained by Gaddah [14] for the problem of the triangular billiards with boundary condition $\psi_A = 0$ (in our notation, $t \to \infty$). The exact spectrum described by the author follows the relation ($L$ is the side-length of the equilateral triangle in question)

$$E_{n_1,n_2} = \pm \frac{4 \pi}{3} h \nu \sqrt{n_1^2 + n_1 n_2 + n_2^2},$$

(41) where $n_2 \geq n_1 > 0$. As described in the article, the states with $n_2 > n_1$ are (at least) $2n$ degenerate. The BCs we imposed on a hexagon, $\psi_A = 0$ on three alternating sides (equation (39)), also enforce $\psi_A = 0$ on the edges of an equilateral triangle, that contains the hexagon region in question. The condition for $\psi_B$ is the same, as it is a simple inversion of this same triangle. As a consequence, after re-scaling the exact spectrum for the triangle by $\sqrt{A_{hex}/A_{triang}}$, we obtain a match between the two as shown in figure 9. We also compare the density plots for the first three approximate eigenfunctions to those present in Gaddah’s work. This comparison (using 10 polynomials) is presented in figure 10 for $|\psi_A|^2$, with the corresponding regions highlighted.

4. Summary and conclusions

With the polynomial method we have been able to construct approximate solutions to Schrödinger and Dirac-Weyl equations for planar convex polygonal enclosures. The method has been applied before to the determination of frequencies of plate vibrations in the Mechanical Engineering community, but as far as we know its generalization to the Dirac billiards has not been reported before. In this case we considered different types of BC, including situations where only the ratio of spinors components is specified.

The method is based on constructing a truncated basis of states, all of which satisfy the prescribed BC from the start. By comparing with cases where the exact solution is known (most often by separation of variables) we were able to ascertain the convergence of the method. Typically, a basis size of order $3n$ is required to obtain $n$ eigenvalues with close to 1% accuracy. The method provides not only the lowest energies (or lowest absolute energies for the Dirac–Weyl case) but also eigenstates as finite order polynomials in the coordinates.
Acknowledgments

M. F. C. M. Quintela thanks Dr. J. Viana Lopes, J. P. Pires, and S. M. João for the enlightening and extensive discussions about this work. The authors acknowledge financing of Fundação da Ciência e Tecnologia, of COMPETE 2020 programme in FEDER component (European Union), through projects POCI-01-0145-FEDER-028887 and UID/FIS/04650/2019. The authors also acknowledge financial support from Fundação para a Ciência e Tecnologia, Portugal, through national funds, co-financed by COMPETE-FEDER (Grant M-ERA-NET/20002/2016—UltraGraf) under the Partnership Agreement PT2020.

Appendix A. General BC for a non-symmetrical gap

We consider a generalization of the Hamiltonian of equation (16)

\[ -i\hbar\sigma \cdot \nabla \Psi + m(\mathbf{r})(\sigma^z - \cos \theta) \Psi = E \Psi. \]

Choosing the y coordinate normal to the interface with the forbidden region, and trying \( \Psi(x, y) = \exp(ik_x x) \Phi(y) \)

\[ \hbar \sigma^y \left( -i\sigma^y \partial_y + k_x \sigma^x \right) \Phi = \left[ E - m(\sigma^z - \cos \theta) \right] \Phi. \]  \hspace{1cm} (42)

In spinor components,

\[ \partial_y \phi_B - k_x \phi_B = -\frac{[E - m(1 - \cos \theta)]}{\hbar \sigma^y} \phi_A \]

\[ \partial_y \phi_A + k_x \phi_A = \frac{[E + m(1 + \cos \theta)]}{\hbar \sigma^y} \phi_B \]  \hspace{1cm} (43a) \hspace{1cm} (43b)

A confined state requires

\[ \phi_B(y) = B \ e^{\eta y} \]

\[ \phi_A(y) = A \ e^{\eta y} \]  \hspace{1cm} (44a) \hspace{1cm} (44b)

with \( \kappa > 0 \). Therefore,

\[ (\kappa - k_x)B = -\frac{[E - m(1 - \cos \theta)]}{A} \]

\[ (\kappa + k_x)A = \frac{[E + m(1 + \cos \theta)]}{B}. \]  \hspace{1cm} (45a) \hspace{1cm} (45b)

As \( m \to \infty \) we can drop \( E \) compared to \( m \) and \( k_x \) compared to \( \kappa \),

\[ \left( \frac{B}{A} \right)^2 = \frac{m(1 - \cos \theta)}{m(1 + \cos \theta)} = \sin^2 \left( \frac{\theta}{2} \right) \]

\[ \cos^2 \left( \frac{\theta}{2} \right). \]  \hspace{1cm} (46)

The BC becomes

\[ \frac{B}{A} = \pm \tan \left( \frac{\theta}{2} \right) = \eta \hspace{1cm} \eta = \pm 1. \]  \hspace{1cm} (47)

But

\[ \kappa B = \frac{m(1 - \cos \theta)}{\hbar \sigma^y} A. \]  \hspace{1cm} (48)

In summary, the boundary condition has the form

\[ \phi_B = \eta \phi_A. \]  \hspace{1cm} (49)

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