Klein Bound States in Single-Layer Graphene

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(Dated: April 6, 2020)

The Klein paradox, first introduced in relation to chiral tunneling, is also manifested in the study of bound-states in single-layer graphene with a 1D square-well potential. We derive analytic (and numerical) solutions for bound-state wavefunctions and in the presence of an external transverse magnetic field, analytic expressions for the bound state wavefunctions for a discrete sequence of potential strengths are derived, and are used to determine the measurable areal densities and currents. Based on ideas presented in Refs. [7, 8], our formalism also applies to the occurrence of bound states of light in periodic optical waveguide structures.

Introduction.— Chiral tunneling of electrons through a 1D potential barrier in single layer graphene was first considered in a seminal paper by Katsnelson, Novoselov, and Geim [1]. A closely related and physically motivated problem concerns the formation of electron bound states in a 1D (symmetric) potential well [2-6] (bound-states here refers to bound in one direction and free in the other direction). In this Letter we elucidate several novel aspects of such bound-states amenable to experimental verification. Our main results are: (1) In the absence of a magnetic field, bound-state eigenfunctions and eigenvalues are derived analytically, and electric dipole transition strengths are calculated to determine the absorption spectrum between bound-states. Parity and time reversal symmetry are employed to find the relation between the two (pseudo-)spinor components. (2) In the presence of an external magnetic field, analytic expressions for the bound state wavefunctions for a discrete sequence of potential strengths are derived, and are used to determine the measurable areal densities and currents. Based on ideas presented in Refs. [7, 8], our formalism also applies to the occurrence of bound states of light in periodic optical waveguide structures.

Bound states in a symmetric 1D square-well.— We search for bound states of a massless particle in single-layer graphene using the 2D Dirac equation with 1D square-well symmetric potential $U(x) = U_0 \Theta(|x| - L)$. Employing $L$ as a length unit, we define dimensionless coordinates $x \rightarrow x/L$, $y \rightarrow y/L$, potential $u(x) = LU(x)/(h\nu F)$, where $U_0 \Theta(|x| - 1)$, energy $\varepsilon = LE/(h\nu F)$, (where $E$ is the energy in physical units), and wavenumber $k = \varepsilon$, (where $E/(h\nu F)$ is the Fermi wavenumber in physical units). Klein physics [9] occurs for $U_0 > \varepsilon > 0$ where inside the well $|x| < 1$ the Fermi energy lies in the conduction band while outside the well $|x| > 1$ the Fermi energy lies in the valence band [9, 10]. Near the K’ Dirac point, the time-independent 2D Dirac equation (in dimensionless variables) is,

$$\mathcal{H}\Psi \equiv \left[ -i(\sigma_x \partial_t + \sigma_y \partial_y) + u(x) \right] \Psi(x,y) = \varepsilon \Psi(x,y).$$

(1)

Under parity transformation $(x,y) \rightarrow (-x,y)$, the potential is symmetric, $u(x) = u(-x)$, but the total Hamiltonian is not, $\mathcal{H}(-x,y) \neq \mathcal{H}(x,y)$. The general solution of the wavefunction in the three different regions is,

$$\psi(x,y) = e^{i\theta(y)} \psi(x),$$

$$\psi(x) = \begin{dcases} a_1 e^{ik_1 x} + b_1 e^{-ik_1 x} (x < 1), \\ a_2 e^{ik_2 x} + b_2 e^{-ik_2 x} (x > 1), \\ a_3 e^{ik_3 x} + d_3 e^{-ik_3 x} (x < -1), \\ \end{dcases}$$

(2)

where $\theta$ is the inclination angle and $\theta$ is the refractive angle. The dimensionless momentum vector inside the well (where $u(x) = 0$) is

$$k = (\cos \phi x + \sin \phi y) \equiv k_x x + k_y y,$$

(3)

and $|k| = \varepsilon = \sqrt{k_x^2 + k_y^2}$. The $x$ component of the momentum outside the well (where $u(x) = U_0 > 0$) and the refractive angle are given by

$$q_x = \sqrt{(\varepsilon - U_0)^2 - k_y^2},$$

$$\tan \theta = k_y/q_x = \varepsilon \sin \phi/k_x = \sqrt{(\varepsilon - U_0)^2 - (\varepsilon \sin \phi)^2},$$

(4)

In the p-n-junction analyzed here, Klein tunneling occurs for $U_0 > 1$ and $\varepsilon > 0$ (where $q_x$ is real), whereas Klein bound states occur for $U_0 > \varepsilon > 0$ (1 + $\sin \phi$) $>$ 0, for which

$$q_x = i\kappa_x (\varepsilon, \phi) \equiv i \sqrt{(\varepsilon \sin \phi)^2 - (U_0 - \varepsilon)^2},$$

(5)

and $\kappa_x(\varepsilon, \phi) > 0$. The bound state wavefunctions must decay exponentially as $e^{-\kappa_x |x|}$ as $|x| \rightarrow \infty$. In this region $\tan \theta = -i\kappa_x/\kappa_y$ is pure imaginary, and $\tan \theta < 1$. Consequently, $\sin \theta$ is real and $\cos \theta$ is imaginary. To insure asymptotic decay at large $|x|$ we must set $\beta = \gamma = 0$ in Eq. (2). Continuity of $\psi(x)$ at $x = \pm 1$ yields a homogeneous system of four linear equations for the complex coefficient vector $\epsilon \equiv (a, b, \alpha, \delta)^T$ that is an eigenvector with zero eigenvalue of the matrix $A(\varepsilon)$. $A(\varepsilon)c = 0 (A(\varepsilon)$ is explicitly given in the Supplemental Material [11]). The determinant of $A(\varepsilon)$ is given by

$$C \det[A(\varepsilon)] = \kappa_x(\varepsilon, \phi) \cos \phi \cos (2\varepsilon \cos \phi) + [\varepsilon(1 + \sin^2 \phi) - U_0] \sin 2\varepsilon \cos \phi,$$

(6)

where $C$ is a non-vanishing multiplicative constant and the expression on the RHS is real. Bound-states occur at energies $\varepsilon_n$ for which $\det[A(\varepsilon_n)] = 0$. For reasons that will be explained later, we focus on bound states at different energies $\varepsilon_n$ but for the same $k_y = \varepsilon_n \sin \phi_n$. We use the following realistic values for the parameters of graphene: $L = 172$ nm, $U_0 = 50$ meV, which yields $U_0 = 4/\kappa = \approx 16.0$. The pattern of bound state energies in the $(\phi, \varepsilon)$ plane is shown in Fig. 1(a), together with the curve $k_y = \varepsilon \sin \phi = 10 = 0.0581$ nm$^{-1}$. The intersection points indicate bound-state energies $\{\varepsilon_n\}$ with the same value of $k_y = \varepsilon_n \sin \phi_n$. Bound state wavefunctions.— Now we compute the wavefunctions for $\{\varepsilon_n, \phi_n\}$, $n = 0, 1, \ldots, 7$, see Fig. 1(a). The pairs $(\varepsilon_n, \phi_n)$ are inserted into the matrix $A$ and the spinor bound-state wavefunctions
$\psi_n(x) = \psi_n^{(1)}(x)$ are determined in terms of the four coefficients $c_0 \equiv (\alpha_n, \beta_n, \gamma_n, \delta_n)$, i.e., the solution of the eigenvalue equation $\mathcal{A}_n \psi_n(x) = 0$. Due to parity symmetry (see below), the components of the spinors are subject to the constraints,

$$\text{Im}[\psi_n^{(1)}(x)] = \text{Re}[\psi_n^{(2)}(x)] = 0,$$

$$\text{Im}[\psi_n^{(2)}(x)] = (-1)^n \text{Re}[\psi_n^{(1)}(-x)].$$

Analytic expressions for the ground and excited state wavefunctions are derived by choosing

$$a = b^* = A_n e^{i\eta_n}, \quad \eta_n = (2n + 1) \frac{x}{2} - \frac{1}{2} \phi.$$  

where $A_n$ are real normalization constants and the phase $\eta_n$ is chosen to satisfy the symmetries in Eq. (7). Combining Eqs. (2) and (8), the bound-state wavefunctions, $\Psi_n(x,y) = e^{i\phi} \psi_n(x)$ for $|x| < 1$ are,

$$\psi_n(x,y) = A_n \begin{pmatrix} \psi_n^{(1)}(x) \\ -i \psi_n^{(1)}(x) \end{pmatrix},$$

$$= A_n \begin{pmatrix} \cos[\gamma_n(x)] + i \sin[\gamma_n(x)] \\ -i \cos[\gamma_n(x)] + \sin[\gamma_n(x)] \end{pmatrix}, \quad (9)$$

where $k_n = \epsilon_n \cos \phi$. The decaying parts of the wavefunctions for $|x| > 1$ are determined by the coefficients $\beta, \delta$, and the symmetry specified in Eq. (7) is fulfilled for all $x$. The two upper components of the spinor wavefunctions $\psi_{n=0,1}(x)$ are shown in Fig. 1(b).

The symmetry specified in Eq. (7) also implies that $\psi_n^{(1)}(x)$ is an odd function of $x$. Hence, $\langle 0 | \psi_0 | 1 \rangle = 0$, i.e., the two states are orthogonal, as have any two different eigenfunctions.

**Currents.**— Bound states, with wavefunctions $\psi_n(x) = (\psi_n^{(1)}(x), \pm \psi_n^{(2)}(x))$, do not carry current along $x$: $J_{n\mu}(x) \equiv \psi_n^{(1)}(x) \sigma_\mu \psi_n(x) = 0$, however, they do carry current along $y$, $J_{ny}(x) \equiv \psi_n^{(1)}(x) \sigma_y \psi_n(x) \neq 0$, $(n = 0, 1)$, that is symmetric under $x \rightarrow -x$ and it quickly decays for $|x| > 1$. As we discuss below in connection with time reversal invariance, all states are Kramers degenerate, and the two degenerate states forming a Kramers pair carry currents in opposite directions.

**Parity.**— The importance of parity in the physics of graphene is discussed in Ref. [12], where it is shown that parity operator in $(1+2)$ dimensions plays an interesting role and can be used for defining conserved chiral currents (see also Ref. [15]). Here we concentrate on bound states, wherein the current along $x$ should vanish, and consider the role of the parity transformation under which the Hamiltonian is not invariant. For a symmetric potential, $u(x) = u(-x)$, we consider the static (time-independent) case with Hamiltonian $\mathcal{H}(x,y)$ introduced in Eq. (1). The parity transformation in 2+1 dimensions is taken to mean the transformation $(x,y) \rightarrow (-x,y)$. For massless Dirac fermions this transformation is realized by the operator $\sigma_y$. Explicitly,

$$\mathcal{H}'(x,y) \equiv \sigma_y \mathcal{H}(x,y) \sigma_y = i \sigma_y \partial_x - i \sigma_y \partial_y + u(x) = \mathcal{H}(-x,y) \neq \mathcal{H}(x,y).$$

Thus, near a given Dirac point, say $K^\prime$, $\mathcal{H}$ is not parity invariant [despite the fact that $u(x) = u(-x)$] [18]. However, for a symmetric potential the wavefunctions $\psi_n(x)$ in Eq. (9) obey the symmetry relations,

$$\sigma_y \psi_0(x) = -\psi_0(-x),$$

$$\sigma_y \psi_1(x) = -\psi_1(-x). \quad (11)$$

Equation (11) is a concrete realization of Eq. (14) in Ref. [12]. Hence, we define $\psi_n(x)$ as being $\text{Re}^{(ny)}$ under parity if and only if $\sigma_y \psi_n(x) = \pm \psi_n(-x)$. With this assignment, Eq. (11) is consistent with (albeit different than) the non-relativistic one-dimensional problem, where, in a symmetric potential, the parity of eigenstates is such that $\psi_n(-x) = (-1)^n \psi_n(x)$, $n = 0, 1, 2, ...$, and the ground-state is symmetric. By definition,

$$\mathcal{H} \psi_n(x) = \epsilon_n \psi_n(x) \Rightarrow \mathcal{H}' \psi_n(-x) = \epsilon_n \psi_n(-x). \quad (12)$$

Thus, $\psi_n(x)$ and $\psi_n(-x) \neq \pm \psi_n(x)$ are respectively eigenfunctions of $\mathcal{H}$ and $\mathcal{H}' \neq \mathcal{H}$ with the same eigenvalue $\epsilon_n$.

**Time Reversal Invariance.**— The time reversal operator is $T = i\sigma_y K$, where $K$ is the complex conjugation operator. It is easy to check that $[\mathcal{H}, T] = 0$, so that each state is doubly (Kramers) degenerate. Applying the operator $T$ on a wavefunctions $\Psi_n(x,y)$, Eq. (9) we obtain [recall that $\psi_n^{(1)}(x)$ is real and $\psi_n^{(2)}(x) = (-1)^n i \psi_n^{(1)}(-x)$ is purely imaginary],

$$\Psi_n^T(x,y) = A_n e^{-i\omega y} \begin{pmatrix} (-1)^n i \psi_n^{(1)}(-x) \\ i \psi_n^{(1)}(x) \end{pmatrix}, \quad (13)$$

which is the Kramers partner of $\Psi_n(x,y)$, i.e., $\mathcal{H} \Psi_n^T(x,y) = \epsilon_n \Psi_n^T(x,y)$.

**Electromagnetic Transitions.**— Consider $E1$ transitions induced by $x$ polarized light such that the dipole operator is $\mathcal{O}(x) = e E_x x$, where $E_x$ is the

**FIG. 1:** (a) Nodes of det $\mathcal{A}(\phi, x)$, Eq. (6), in the $(\phi, x)$ plane (blue curves), and the curve $k_0 = \epsilon \sin \phi = 10$ (orange curve). The pairs $(\epsilon_n, \phi_n)$ specified by blue and red dots are the bound state energies for $k_0 = \epsilon_0 \sin \phi_0 = 10$. (b) Upper components of $\psi_0(x)$ (red solid curve) and $\psi_1(x)$ (blue dot-dashed curve) versus $x$. The lower components are related to the upper ones via Eq. (9). Note that the wavefunctions do not have a definite symmetry around $x = 0$ (see discussion on the role of parity below).
electric field amplitude. The parity of the product \(\psi^*_y(x)\psi_y(x)\) is \((-1)^{l+m+1}\). Because \(k_y\) is conserved and is the same for \(\Psi_m(x, y)\) and \(\Psi_y(x, y)\), we have,

\[
\langle \Psi_m | \hat{O} | \Psi_n \rangle = \frac{1}{2}(1 - (-1)^{n+m})\epsilon E_v(x, y)_{n,m}. \quad (14)
\]

Figure 2 shows the absorption spectrum of the transitions \(0 \rightarrow 1, 1 \rightarrow 2, 0 \rightarrow 3, 1 \rightarrow 4, 0 \rightarrow 5, 1 \rightarrow 6, 0 \rightarrow 7, \), where the absorption rates in arbitrary units are proportional to \(\omega_{nm}^2 \left[|\langle \psi_n | \psi_m \rangle|\right]^2\) where \(\omega_{nm} = \epsilon_m - \epsilon_n\). [13]

Strictly speaking, electrons can occupy orbits with arbitrary \(k_y < \epsilon\) and transitions can occur between the pertinent energy states. However, practically, an experiment can be carried out in a graphene nano-ribbon of width \(L_y\), such that \(k_y = \pm \frac{2\pi n}{L_y}\) for \(n = 1, 2, \ldots\) is quantized. If \(L_y\) is small enough, only the lowest mode is occupied. In our example, \(k_y = 10\) and \(\epsilon < \omega = 16\) (in dimensionless units). If this value of \(k_y\) corresponds to the lowest mode \(\rho = 1\), then the second mode \((\rho = 2)\) has \(k_y = 20 > \epsilon\). In physical units, this implies \(k_y = 0.0581\) nm\(^{-1}\) and \(L_y = 108\) nm. Experimental fabrications of much lower nano-ribbon widths have already been reported [14].

Bound States in a perpendicular magnetic field and square well.—Analysis of bound states in the presence of uniform perpendicular magnetic field and a square well potential enables an access to “unquantized” Landau functions in graphene. First recall the extensively studied case \(U(x) = 0\) (see e.g., Ref. [16]). In the Landau gauge, \(A_y = Bx\), the spinor wavefunction is \(\Psi(x, y) = e^{i\phi}y\psi(x)\).

Introducing the magnetic length \(\ell = \sqrt{\hbar/eB}\) enables formulation in terms of the dimensionless position, wave number and binding energy: \(x \rightarrow x/\ell, k_y \rightarrow k_y/\ell\), and \(\epsilon \rightarrow \ell \epsilon\). The bare equation with dimensionless variables and parameters then reads,

\[
[\epsilon_{2D} \partial_x^2 + \partial_y^2 + k_x] \psi(x) = \epsilon \psi(x).
\]

It is simplified after a shift and scaling of the position coordinate, \(x \rightarrow \sqrt{\hbar} + k_y\).

\[
\mathcal{H} \psi(z) \equiv -\epsilon_{2D} \partial_x^2 - \frac{1}{2} \partial_y^2 \phi \psi(z) = \epsilon \psi(z),
\]

whose general solution is (with \(\delta \equiv 1 - \delta\))

\[
\psi^{(1)}(z) = c_1 \left( \frac{D_{c_1}(iz)}{D_{-1}(iz)} \right) + c_2 \partial_x \left( \frac{D_{c_2}(iz)}{D_{-1}(iz)} \right),
\]

where \(D_{c}(z)\) is the parabolic cylinder function, \(\delta \equiv 2\) (because \(\psi^{(1)}(z)\) is square integrable on the whole interval \(-\infty < z < \infty\)), we must set \(\epsilon^2 = n\) (where \(n\) is a non-negative integer), and \(c_2 = 0\) (because wavefunctions with imaginary arguments blow up). These constraints determine the Landau quantized energies \(\epsilon = \pm \sqrt{n}\) and wavefunctions for electrons in graphene.

In the scaled variable \(z\) the square-well potential \(U(z) = U_0 \Theta(|z| - L)\) reads,

\[
u (z) = \begin{cases} 0, & z(-L) < z < z(L), \\ u_0, & \text{otherwise}. \end{cases}
\]

where \(u_0 = \frac{\omega}{2} L^2\) and \(z(L) = -\sqrt{2}L - k_y \equiv L_1,\)

\[
\frac{d}{dz} \epsilon \psi(z) = \epsilon \psi(z), \quad z \in [L_2, L_1]
\]

where \(\epsilon(z) = \epsilon(z(0))\), and \(\epsilon\) is the energy eigenvalue that needs to be determined. As in Eq. (16), the solutions can be expressed in terms of parabolic cylinder functions \(D_{\nu}(\cdot)\), and the spinor wavefunction is required to be continuous everywhere and square-integrable. For \(z \in [L_2, L_1]\) the solution reads,

\[
\psi(z) = c_1 \left( \frac{D_{\nu}(iz)}{D_{-1}(iz)} \right) + c_2 \partial_x \left( \frac{D_{\nu}(iz)}{D_{-1}(iz)} \right),
\]

Generically, the orders \(\nu_1 = \epsilon^2, \nu_2 = (-\epsilon^2 + 1)\) in Eq. (19) are not (non-negative) integers. In the external regions \(z \notin [L_1, L_2]\), the only solutions of the second of Eq. (18) that decay as \(|z| \rightarrow \infty\) are such that: (1) the order \(\nu\) of \(D_{\nu}(\cdot)\) should be a non-negative integer, and (2) the argument of \(D_{\nu}(\cdot)\) must be real. The most general solution is then an infinite linear combination of Landau functions \(L_{\nu}(z) = \left( \omega / \sqrt{2 \pi} \right) \Theta\), \(n = 0, 1, \ldots, s = \pm \infty\). A general numerical solution is worked out in the supplementary material [11]. Here we show that analytic solutions exist for specific discrete values of the potential strength \(u_0\). We employ the following solutions of Eq. (18) for \(z \notin [L_1, L_2]\), with \(\epsilon = u_0 = \pm \sqrt{\hbar}\), that is, \(\nu = (\epsilon - u_0)\) to:

\[
\psi_{\text{left}}(z) = c_3 \Theta(z - L_1) \left( \frac{D_{\nu}(iz),}{\partial_x D_{\nu}(iz)} \right),
\]

\[
\psi_{\text{right}}(z) = c_5 \Theta(L_2 - z) \left( \frac{D_{\nu}(iz),}{\partial_x D_{\nu}(iz)} \right).\]

Matching Equations.—Following Eqs. (19) and (20), for fixed \(\pm \sqrt{\hbar}\), the wavefunction is determined by the coefficients vector \(c = (c_1, c_2, c_3, c_4)^T\). Continuity requires \(\psi_{\text{left}}(L_1) = \psi_{\text{right}}(L_1)\) and \(\psi_{\text{left}}(L_2) = \psi_{\text{right}}(L_2)\), where each relation yields two equations. This set of four linear homogeneous equations can be formally written as \(A_{\text{left}}(u_0)c = 0\). The potential strength \(u_0\) must satisfy \(\det(A_{\text{left}}(u_0)) = 0\), and the roots \(u_{nm}\) determine the bound-state energies \(\epsilon_{nm} = u_{nm} \pm \sqrt{\hbar}\). The eigenvector \(c_{nm}\) of \(A_{\text{left}}(u_{nm})\) corresponding to eigenvalue zero determines the wavefunction in all space. Figure 3(a) plots \(\det(A_{\text{left}}(u_0))\) versus \(u_0\). For each \(0 < n \in \mathbb{Z}\) there, in principle, an infinite number of zeros \(u_{nm}\) and infinite number of bound-state energies \(\epsilon_{nm} = u_{nm} \pm \sqrt{\hbar}\), where \(s = \pm\). A few bound state energies are shown in Fig. 3(b).

Wavefunctions and Currents. The spinor wavefunctions and the currents along \(y\) corresponding to well height \(u_{nm}\) for \((n, m) = (0, 0)\) are shown in Fig. 4. The main properties of the wavefunctions are: (1) It is possible to choose the phase such that the upper component of the spinor is real while the
The consequences of parity non-invariance and time reversal invariance are elucidated, and photon absorption inducing $E1$ transition between two levels is worked out. In the presence of an external uniform perpendicular magnetic field, an analytic expression for the wavefunctions is derived for a discrete (albeit infinite) sequence of potential strengths $u_0 = \{u_{n,m}\} n, m = 0, 1, 2, \ldots$. The Landau functions (in graphene) with non-integer orders and imaginary argument appearing in Eq. (19) are thereby exposed to experimental probes. Exact numerical calculations valid for every potential strength are carried out in the supplemental material [11], and the importance of the symmetry (21) is stressed.

Our results apply directly to the propagation of light waves in periodic waveguide optical structures. Transport of light in a 2D binary photonic superlattice with two interleaved lattices $A$ and $B$ is realized by a sequence of equally spaced waveguides with alternating deep/shallow peak refractive index changes. Propagation of monochromatic light waves is well-described by the scalar wave equation in the paraxial approximation. The tight-binding limit results in coupled-mode equations for the fundamental-mode field amplitudes which are functions of a discrete set of integer variables, and approximating these with a continuous variable rather than as an integer index yields a 2D Dirac equation with an external electrostatic potential [7, 8]. This yields the same mathematical formalism used to describe graphene.

Acknowledgments: We would like to thank Mikhail I. Katsnelson, Jean Noël Fuchs Ken Shiriozaki and Ady Stern for illuminating discussions. This work was supported in part by a grant from the DFG through the DIP program (FO703/2-1).
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The reason is that there are two inequivalent representations of the 2D Dirac $\gamma$ matrices. Parity operation carries valley $K \rightarrow K'$, and its conservation can be restored if valley degeneracy is incorporated in the Lagrangian, when it is built upon both representations [12].
Supplemental Material for “Klein Bound States in Single-Layer Graphene”

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Here we elaborate on several points discussed in the main text (MT) \cite{1}. Section I contains additional information regarding the matrix $A(\varepsilon)$ introduced in Eq. (6) of the MT. Section II considers the numerical solution of Eq. (18) in the MT, and Sec. III discusses the electric dipole ($E_1$) transitions between bound states.

I. THE MATRIX $A(\varepsilon)$ RELATED TO EQ. (6)

In this section we give an explicit expression for the matrix $A(\varepsilon)$ that determines the bound state energies and wavefunction coefficients specified by the vector $\mathbf{c} \equiv (a, b, a, \delta)$ appearing in Eq. (2). The pertinent quantities are introduced in the discussion near Eqs. (3), (4), and (5) in the MT. The matching conditions at $x = \pm 1$ lead to a homogeneous system of four linear equations for the complex coefficients $a, b, a, \delta$. Bound-state solutions occur at energies $|\varepsilon_n|$ for which the determinant of $A(\varepsilon)$ vanishes, and the corresponding coefficient vector $\mathbf{c}_n$ is determined by the set of homogeneous equations $A(\varepsilon_n)\mathbf{c}_n = 0$. The explicit form of the matrix $A(\varepsilon)$ in the system of equations, $A(\varepsilon)\mathbf{c} = 0$, is given by

$$A(\varepsilon) = \begin{pmatrix}
e^{i\varepsilon n_0 \phi} & e^{-i\varepsilon n_0 \phi} & -e^{-\kappa_z} & 0 \\
e^{i(z\cos \phi + \phi)} & e^{-i(z\cos \phi + \phi)} & 0 & 0 \\
e^{-i(z\cos \phi - \phi)} & e^{i(z\cos \phi - \phi)} & 0 & 0 \\
e^{-i\varepsilon n_0 \phi} & e^{i\varepsilon n_0 \phi} & 0 & -e^{-\kappa_z} \end{pmatrix}. \quad (1)$$

II. NUMERICAL SOLUTION OF EQ. (18)

The set of Landau functions is complete on the interval $(-\infty, \infty)$ so we can expand $\psi(z)$:

$$\psi(z) = \sum_{n=0}^{\infty} \sum_{s=\pm} a_{ns} L_{ns}(z), \quad \text{where} \quad L_{ns}(z) = N_{ns} \begin{pmatrix} D_n(z) \\ i\sqrt{n}D_{n-1}(z) \end{pmatrix}; \quad (2)$$

Here $N_{ns}$ is a normalization factor. Substitution into Eq. (18) then yields,

$$[-i\sigma_2 \partial_z - \frac{1}{2} z \sigma_3] \psi(z) = M \sum_{n=0}^{\infty} \sum_{s=\pm} a_{ns} \sqrt{n} L_{ns}(z) = [\varepsilon - u(z)] M \sum_{n=0}^{\infty} \sum_{s=\pm} a_{ns} L_{ns}(z). \quad (3)$$

Multiplying by $L_{ml}^\dagger(z)$ (where $t = \mp$) and integrating over $z$, using $(L_{ml}|L_{ns}) = \delta_{mn}\delta_{ls}$ one obtains,

$$t\sqrt{\mathcal{N}} a_{ml} = \varepsilon a_{ml} - M \sum_{n=0}^{\infty} \sum_{s=\pm} A_{mlns} a_{ns}. \quad (4)$$

The infinite sum (as $M \to \infty$) can be cut-off at a sufficiently large $M$. This procedure leads to an eigenvalue problem in a finite Hilbert space of dimension $2M + 1$. The matrix $A$ introduced above can be written as $u_0(I - B)$, where $I$ is the $(2M+1) \times (2M+1)$ unit matrix. The explicit expressions for the matrices $A$ and $B$ are,

$$A_{mlns} = \int_{-\infty}^{\infty} L_{ml}^\dagger(z) u(z) L_{ns}(z) dz = u_0 [\delta_{ml\pm n} - \delta_{ml\mp n}] \int_{-\infty}^{\infty} L_{ml}^\dagger(z) L_{ns}(z) dz; \quad (5)$$

where $u_0$ is the strength of the square well potential defined in Eq. (17) in the MT. Next, we define a diagonal matrix $\Lambda$ by

$$\Lambda_{mlns} = \delta_{ml,ns} \text{Diag}(t\sqrt{\mathcal{N}}) = (0, \sqrt{\mathcal{N}}, \sqrt{\mathcal{N}^2}, \ldots, \sqrt{\mathcal{N}^{2M}}), \quad (6)$$

and a vector $\mathbf{a}$ with $2M + 1$ components, $a_{ns} = (a_0, a_{1+}, a_{2+}, \ldots, a_{M+}, a_{1-}, a_{2-}, \ldots, a_{M-})$. Equation (4) then becomes an eigenvalue problem,

$$[\Lambda + u_0(I - B)] a = \varepsilon a. \quad (7)$$

The matrix $\Lambda + u_0(I - B)$ is real and symmetric. For $u_0 = 0$ the eigenvalues are the Landau energies for graphene $\varepsilon_m = \pm \sqrt{\mathcal{N}}$. In the calculations of density, current and $E_1$ transitions presented below we take
shows the ground-state density symmetrized density \( \rho_0(z) \) of the ground state \( \psi_0(z) \) following incoherent summation over \( \pm k_y \).

(a) \( \frac{1}{2} |\rho_0(z, k_y) + \rho_0(z, -k_y) | \), (b) \( \frac{1}{2} |J_{\rho_0}(z, k_y) + J_{\rho_0}(z, -k_y) | \).

\[ u_0 = \frac{\hbar^2 \omega}{2m} = 10, \ \text{and} \ \frac{-\hbar^2 \omega}{2m} \leq x \leq \frac{\hbar^2 \omega}{2m} \ (\text{in units of } \ell), \ \text{and} \ k_y = \pm 0.5 \ (\text{in units of } 1/\ell). \]

Since \( z = \sqrt{2} x - k_y \), this gives \([L_2, L_1] = [-3, 2]\) for \( k_y = +0.5 \), and \([L_2, L_1] = [-2, 3]\) for \( k_y = -0.5 \). Figure 1 shows the ground-state density symmetrized density \( \rho_0(z) = \frac{1}{2} \sum_{\pm k_y} |\psi_0(\pm k_y)| \) and current density along \( y \), \( J_{\rho_0}(z) = \frac{1}{2} \sum_{\pm k_y} \psi_0^{\dagger}(\pm k_y) \partial \psi_0(z) \). As argued in the discussion of Eq. (21) of the MT, the incoherent sum of contributions from \( \pm k_y \) results in a symmetric density and an antisymmetric current density. In particular, the total current along \( y \), \( I_{\rho_0} = \int_{-\infty}^{\infty} J_{\rho_0}(z) dz \) vanishes (as it should). Similar results for the first excited state \( \psi_1(x) \) are shown in Fig. 2.

III. E1 TRANSITIONS IN THE PRESENCE OF MAGNETIC FIELD

In analogy with the discussion of photon absorption in the absence of an external magnetic field [see Eq. (14) in the MT], we now consider E1 transitions in the presence of the magnetic field. The E1 transition rates \( w_{mn} \) from \( m \) to \( n \) with light polarized along the \( x \) axis are proportional to \( |\varepsilon_n - \varepsilon_m|^4 |\langle \psi_m | x | \psi_n \rangle|^2 \), where \( \{ \varepsilon_n \} \) are the energy eigenvalues obtained from the solution of Eq. (7) and the transition dipole matrix elements are

\[ \langle x | m \rangle = \langle \psi_m | x | \psi_n \rangle = \int_{-\infty}^{\infty} \psi_0^\dagger(z) x \psi_n(z) dx, \]

where \( z(x) = \sqrt{2} (x - k_y) \). The main contribution comes from the interval \(-L \leq x \leq L \) where \( L/\ell = \frac{1}{2}\sqrt{\frac{\hbar^2 \omega}{2m}} \) [see details below Eq. (7)]. Photon absorption spectrum between the lowest eight states \( n = 0, 1, \ldots, 7 \) [determined within the set of parameters specified after Eq. (7)] is shown in Fig. 3. It is interesting to understand the differences between photon absorption spectra in the presence and in the absence of the magnetic field shown in Fig. 2 in the MT. In the latter case, there is the usual parity selection rule, namely, the function \( \psi_0^\dagger(x) x \psi_1(x) \) is even (odd) if \( n + m + 1 \) is odd (even). In particular, transitions \( 0 \to 1, 3, 5, 7 \) are shown but \( 0 \to 2, 4, 6 \) vanish. These parity selection rules do not apply in the presence of magnetic field, hence all transitions \( 0 \to n \ (n = 1, 2, \ldots, 7) \) are allowed.

One can easily convert the E1 transition rates to physical units. Following Ref. [2] (p. 324), the E1 transition rate between states \( |m \rangle \) and \( |n \rangle \) is given, (up to a multiplicative factor \( A \) depending on constants such as \( c \) and \( h \)), by:

\[ w_{mn} = A (E_m - E_n)^4 |\langle \varepsilon_x | x \rangle|^2 |X_{mn}|^2, \]

where \( E_m \) and \( E_n \) are the level energies and \( \varepsilon_x \) is the slowly varying envelope of the electric field. The physical dimension of \( w_{mn} \) is \([w_{mn}] = [A] \times [\text{energy}]^4\). If there is a parameter of length \( d \) in the system, then we can use it as the unit of length and work with dimensionless quantities: \( \varepsilon_x \) for energy \( E_{mn} \), \( u_0 \) for potential height \( U_0 \), \( k_y \to k_y d \) for wave numbers and \( x_{mn} \) for \( X_{mn} \):

\[ E_{mn} = \frac{h \nu F}{d} \varepsilon_m, \quad U_0 = \frac{h \nu F}{d} u_0, \quad X_{mn} = dx_{mn}, \quad \Rightarrow w_{mn} = A \left( \frac{h \nu F}{L} \right)^4 (\varepsilon_n - \varepsilon_m)^4 (\varepsilon_x d)^2 |x_{mn}|^2. \]
FIG. 3: Absorption spectrum of the transitions $0 \rightarrow n, n = 1, 2, \ldots, 7$. The transition rates $w_{0,n}$ (in dimensionless units), which are proportional to $\omega_{0n}^2 \langle \psi_0 | x | \psi_n \rangle^2$, are plotted versus the resonant light photon energy $\hbar \omega_{0n} = \varepsilon_n - \varepsilon_0$ in dimensionless units.

In order to compute $w_{mn}$ we still need to know $E_x$ and compute the energy $eE_x d$ for these values of $d$ and $E_x$. In the absence of an external magnetic field, we can use $d = L$, where $2L$ is the width of the square well. In the presence of a magnetic field, we can use $d = \ell$, the magnetic length. In this case, the dimensionless width of the square well is $2L/\ell$. The relevant energies can be inferred by noting that for a magnetic field of 1 T, $\ell \approx 25 \text{ nm}$ and $\hbar v_F/\ell \approx 21.875 \text{ meV}$.

[1] Y. Avishai and Y. B. Band, “Klein Bound States in Single-Layer Graphene”, Main Text.
[2] Y. B. Band and Y. Avishai, *Quantum Mechanics with Application to Nanotechnology and Information Science*, Elsevier (2013).