Confinement of graphene electrons in the hyperbolic secant potential

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We present exact analytical solutions for the bound modes of two-dimensional massless Dirac fermions confined within a hyperbolic secant potential, which provides a good fit for potential profiles of existing top-gated graphene structures. We show that bound states of both positive and negative energies exist in the energy spectrum and that there is a threshold value of the characteristic potential strength for which the first mode appears.

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I. INTRODUCTION

The carriers within graphene, a single layer of carbon atoms in a honeycomb lattice, behave as two-dimensional massless Dirac fermions. In the presence of an electric field, their massless, relativistic nature results in drastically different behavior to their normal non-relativistic electron counterparts, for example, back scattering is forbidden for carriers which are incident normal to the barrier. However, they can be reflected at non-normal incidence and therefore full confinement is possible. Klein tunneling through p-n junction structures in graphene has been studied both theoretically and experimentally. Quasi-bound states were considered in order to study resonant tunneling through various sharply terminated barriers. In this paper we obtain a hitherto unknown analytical solution for bound modes within the hyperbolic secant potential in pristine graphene and count the number of modes contained within. We show that bound states of both positive and negative energies exist in the spectrum and that there is a threshold value of the characteristic potential strength for which the first mode appears, in striking contrast to the non-relativistic case.

II. BOUND MODES IN A MODEL POTENTIAL

The Hamiltonian operator in the massless Dirac-Weyl model for graphene, which describes the motion of a single electron in the presence of a one-dimensional potential \( U(x) \) is

\[
\hat{H} = v_F (\sigma_x \hat{p}_x + \sigma_y \hat{p}_y) + U(x),
\]

where \( \sigma_{x,y} \) are the Pauli spin matrices, \( \hat{p}_x = -i\hbar \partial_x \) and \( \hat{p}_y = -i\hbar \partial_y \) are the momentum operators in the \( x \) and \( y \) directions respectively and \( v_F \approx 10^6 \text{ m/s} \) is the Fermi velocity in graphene. In what follows we will consider a smooth confining potential, the hyperbolic secant potential, which does not mix the two non-equivalent valleys. All our results herein can be easily reproduced for the other valley. When Eq. \( \text{(1)} \) is applied to a two-component Dirac wavefunction of the form:

\[
e^{ik_y y} \begin{pmatrix} \Psi_A(x) \\ \Psi_B(x) \end{pmatrix}
\]

where \( \Psi_A(x) \) and \( \Psi_B(x) \) are the wavefunctions associated with the \( A \) and \( B \) sublattices of graphene respectively and the free motion in the \( y \)-direction is characterized by the wave vector \( k_y \) measured with respect to the Dirac point, the following coupled first-order differential equations are obtained:

\[
(V(x) - \varepsilon) \Psi_A - i \left( \frac{d}{dx} + k_y \right) \Psi_B = 0 \quad (2)
\]

\[
(V(x) - \varepsilon) \Psi_B - i \left( \frac{d}{dx} - k_y \right) \Psi_A = 0 \quad (3)
\]
Here \( V(x) = U(x)/\hbar v_F \) and energy, \( \varepsilon \), is measured in units of \( \hbar v_F \). For convenience let \( \Psi_A = (\Psi_1 + \Psi_2)/2 \) and \( \Psi_B = (\Psi_1 - \Psi_2)/2 \) therefore Eqs. (2,3) become

\[
\left( V(x) - \varepsilon - i \frac{d}{dx} \right) \Psi_1 + i k_y \Psi_2 = 0
\]

(4)

\[
\left( V(x) - \varepsilon + i \frac{d}{dx} \right) \Psi_2 - i k_y \Psi_1 = 0
\]

(5)

Eqs. (4,5) can then be reduced to a single second order differential equation in \( \Psi_1, \Psi_2 \)

\[
\left[ (V(x) - \varepsilon)^2 - k_y^2 \pm i \frac{dV(x)}{dx} \right] \Psi_{1,2} + \frac{d^2 \Psi_{1,2}}{dx^2} = 0
\]

(6)

The plus and minus signs corresponds to wavefunction \( \Psi_1 \) and \( \Psi_2 \) respectively. The potential under consideration is defined as

\[
V(x) = -V_0 \cosh \left( \frac{x}{l} \right)
\]

(7)

where \( V_0 \) and \( l \) characterize the potential strength and width respectively. This potential is known to admit analytic solutions for the case of \( \varepsilon = 0 \) and is a good representation of experimentally generated potential profiles. For top gated structures, the width of the potential is defined by the geometry of the top gate structure, and the strength of the potential is defined by the voltage applied to the top gate.

Let us search for solutions of Eq. (6) with the potential given by Eq. (7) in the form

\[
\Psi_{1,2} = A_{1,2} V^\kappa \psi_{1,2} (x),
\]

(8)

where

\[
\kappa = l \sqrt{k_y^2 - \varepsilon^2}
\]

(9)

and \( A_{1,2} \) is a constant. Substitution of Eq. (8) into Eq. (6) yields

\[
\frac{d^2 \psi_{1,2}}{dz^2} - 8 \kappa \frac{\tanh (z)}{1 + \tanh^2 (z)} \frac{d \psi_{1,2}}{dz} + 4 \left[ 2w \left( S_E \sqrt{\Delta^2 - \kappa^2} + S_\Psi \frac{\tanh (z)}{1 + \tanh^2 (z)} \right) \frac{1 - \tanh^2 (z)}{1 + \tanh^2 (z)} + \left[ w^2 - \kappa (\kappa + 1) \right] \frac{1 - \tanh^2 (z)}{1 + \tanh^2 (z)} \right] \psi_{1,2} = 0
\]

(10)

where we use the dimensionless variables \( w = V_0 l, \Delta = k_y l, E = \varepsilon l \) and \( z = x/2l \). \( S_E = 1 \) for \( E > 0 \) and \( S_E = -1 \) for \( E < 0 \). \( S_\Psi = 1 \) for \( \Psi_1 \) and \( S_\Psi = -1 \) for \( \Psi_2 \). Using the transformation \( \psi_{1,2} = (\xi - \frac{1}{2})^\mu H_{1,2} (\xi) \) with the change of variable

\[
\xi = e^{-i\frac{\theta}{2}} \frac{\tanh (z) + 1}{\sqrt{2} \tanh (z) - i}
\]

where

\[
\mu = \kappa + S_\mu w + \frac{1}{2} (1 + S_\mu S_\Psi)
\]

(11)

and \( S_\mu = \pm 1 \), allows Eq. (10) to be reduced to

\[
\frac{d^2 H_{1,2}}{d\xi^2} + \left[ \frac{\gamma}{\xi} + \frac{\delta}{\xi - 1} + \frac{\epsilon}{\xi - a} \right] \frac{dH_{1,2}}{d\xi} + \frac{\alpha \beta \xi - q}{\xi (\xi - 1) (\xi - a)} H_{1,2} = 0,
\]

(12)
where

\[ \epsilon = \alpha + \beta - \gamma - \delta + 1 \]
\[ \gamma = \delta = 1 + 2\kappa \]
\[ a = \frac{1}{2} \]
\[ \beta = \frac{2}{\alpha} [S_{\Psi} w + (1 + 2\kappa) \mu] \]
\[ 2\alpha = 2\mu + 2\kappa + 1 \pm \sqrt{(2\mu + 2\kappa + 1)^2 - 8[S_{\Psi} w + (1 + 2\kappa) \mu]} \]
\[ q = S_{\Psi} w + (1 + 2\kappa) \mu + i2S_{E} w \sqrt{\Delta^2 - \kappa^2} \]

and \( H_{1,2} \) is the Heun function given by the expression:

\[ H_{1,2} = H_{1,2} (a, q; \alpha, \beta, \gamma, \delta, \xi) = \sum_{j=0}^{\infty} c_j \xi^j \]

where

\[ c_0 = 1, \quad a\gamma c_1 - qc_0 = 0, \quad R_j c_{j+1} - (Q_j + q) c_j + P_j c_{j-1} = 0 \]

with

\[ P_j = (j - 1 + \alpha)(j - 1 + \beta) \]
\[ Q_j = j [(j - 1 + \gamma) (1 + a) + a\delta + \epsilon] \]
\[ R_j = a (j + 1)(j + \gamma) \]

We shall now solve for \( \Psi_1 \). For \( \Psi_1 \) to be a non-divergent function we require that \( H_{1,2} \) is reduced to a finite polynomial. This occurs when two conditions are met:

\[ \alpha = -n \quad (13) \]

and

\[ q = q_{n,m}, \quad (14) \]

where \( n \) and \( m \) are non-negative integers and \( m \leq n \), and \( q_{n,m} \) are the eigenvalues of the tridiagonal matrix

\[
\begin{bmatrix}
0 & a\gamma & 0 & \cdots & 0 \\
0 & -Q_1 & R_1 & \cdots & 0 \\
0 & P_2 & -Q_2 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & R_{n-1} \\
0 & 0 & 0 & \cdots & P_n - Q_n \\
\end{bmatrix}
\]

In this instance,

\[ H_1 = H (a, q_{n,m}; -n, \beta, \gamma, \delta, \xi) \quad (15) \]

is a polynomial of degree \( n \), these solutions are the Heun polynomials, which have attracted a lot of recent attention in relation to various exactly solvable quantum mechanics problems. Since \( w \) and \( \kappa \) are positive quantities, in order to satisfy the termination condition, Eq. (13), \( S_{\mu} \) must take upon the value of \(-1\) therefore Eq. (11) becomes

\[ \mu = \kappa - w. \]

The first termination condition, Eq. (13), also requires

\[ \kappa = w - \frac{n + 1}{2} \quad (16) \]
therefore the exponent parameters become

\[ \alpha = -n, \quad \beta = 2w - n - 1, \quad \gamma = \delta = 2w - n \]

and the accessory parameter becomes

\[ q_{n,m} = iS_E 2w \sqrt{\Delta^2 - \left( w - \frac{n + 1}{2} \right)^2} - n \left( w - \frac{n + 1}{2} \right). \]  

(17)

Since \( \kappa \geq 0 \) we obtain the condition that \( w \geq \frac{(n+1)}{2} \). It should be noted that this puts an upper limit on \( n \), the order of termination of the Heun polynomial. Notably the first mode occurs at \( n = 0 \), thus there is a lower threshold of \( w \geq \frac{1}{2} \) for which bound modes appear. Hence within graphene, quantum wells are very different to the non-relativistic case; bound states are not present for any symmetric potential, they are only present for significantly strong or wide potentials, such that \( V_0 l > \frac{1}{2} \).

From Eqs. (9,16) the exact Dirac energy spectra is found to be

\[ E_{n,m} = \pm \sqrt{\Delta_{n,m}^2 - \left( w - \frac{n + 1}{2} \right)^2} \]  

(18)

where \( \Delta_{n,m} \) is a function of \( w \) and \( n \) and is found via the satisfaction of the second termination condition, Eq. (14). Let us first consider the case of \( E = 0 \), in this instance the termination condition, Eq. (14), is satisfied when \( q_{n,m} = 0 \), which requires \( w = (n + 1)/2 \), resulting in unbound states since in this instance \( \Delta_{n,m} = 0 \), or when

\[ q_{n,m} = -n \left( w - \frac{n + 1}{2} \right) = \frac{\alpha \beta}{2}, \]  

(19)

which requires \( \Delta = \pm \left( w - \frac{n + 1}{2} \right) \) and in this case Eq. (15) becomes

\[ H \left( \frac{1}{2}, \frac{\alpha \beta}{2}; \alpha, \beta, \gamma, \gamma, \xi \right). \]  

(20)

Using the identity 31

\[ H \left( a, q; \alpha, \beta, \gamma, \delta; z \right) = H \left( \frac{1}{a}, \frac{q}{a}; \alpha, \beta, \gamma, \alpha + \beta + 1 - \gamma - \delta; \frac{z}{a} \right) \]  

allows Eq. (20) to be re-expressed as

\[ H \left( 2, \alpha \beta; \alpha, \beta, \gamma, \alpha + \beta + 1 - 2\gamma; 2\xi \right) \]

which reduces to the Gauss hypergeometric function 32

\[ _2F_1 \left( \frac{1}{2}, \frac{1}{2}; \alpha, \beta; \gamma; 4\xi (1 - \xi) \right). \]

In order to terminate the hypergeometric series and therefore obtain bound solutions it is necessary to satisfy the condition \( \alpha = -2N \), where \( N \) is a positive integer, therefore,

\[ \Delta = \pm \left( w - N + \frac{1}{2} \right), \]

where \( n = 2N \) which restores the results obtained in Ref. 6.

The non-zero energy eigenvalues are obtained by solving Eq. (17). When \( n = 0 \) the eigenvalue is found to be \( E_{0,0} = 0 \) where \( \Delta_{0,0} = \pm (w - \frac{1}{2}) \). For the case of \( n = 1 \), which exists only when \( w \), the characteristic potential strength, exceeds one, the eigenvalues are

\[ E_{1,0} = -\frac{1}{2w} \sqrt{w^2 - w} \]

and

\[ E_{1,1} = \frac{1}{2w} \sqrt{w^2 - w}, \]

where

\[ \Delta_{1,0} = \Delta_{1,1} = \pm \frac{2w - 1}{2w} \sqrt{w^2 - w}. \]
Bound states of both positive and negative energies exist in the energy spectrum, which is markedly different to quantum wells in the non-relativistic case. Each eigenvalue is two-fold degenerate in terms of $\Delta$, the particles momentum along the barrier. It is clear from Eqs. (4,5) that neither $\Psi_1$ nor $\Psi_2$ are symmetrized wavefunctions, so we shall transform to the symmetrized functions:

$$
\Psi_I = (\Psi_1 + \Psi_2) + i(\Psi_1 - \Psi_2), \quad \Psi_{II} = (\Psi_1 + \Psi_2) - i(\Psi_1 - \Psi_2)
$$

In Fig. 1 we present $\Psi_I$, $\Psi_{II}$, and the corresponding electron density profiles for the $E_{10}$ and $E_{11}$ modes. It can be seen from Fig. 1 that upon changing the sign of $\Delta$ the parity of $\Psi_I$ and $\Psi_{II}$ changes. This means backscattering within a channel requires a change in the parity of the wavefunctions and thus should be strongly suppressed. Such suppression should result in an increase in the mean free path of the channel compared to that of graphene. Each component of the spinor wavefunction acts much like the single component wavefunction of a conventional quantum well; when $\Delta > 0$ ($\Delta < 0$), $\Psi_{II}$ ($\Psi_I$) for the lowest energy state, $E_{10}$, is s-like and for the next excited state, $E_{11}$, p-like. Since $\Psi_I$ ($\Psi_{II}$) is the derivative of $\Psi_{II}$ ($\Psi_I$), it must be p-like for $E_{10}$ and d-like for $E_{11}$. The $E_{10}$ mode has a dip in the charge density profile at the middle of the potential well, whereas the $E_{11}$ has a maximum this arises from the complex two-component structure of the wavefunctions.

![Fig. 1](image)

**FIG. 1:** The real part of the wavefunctions $\Psi_I$ (solid line) and $\Psi_{II}$ (dashed line) are shown for $\omega = 2.2$ for: (a) the $E_{1,0}$ mode with $\Delta > 0$, (b) the $E_{1,0}$ mode with $\Delta < 0$, (c) the $E_{1,1}$ mode with $\Delta > 0$ and (d) the $E_{1,1}$ mode with $\Delta < 0$. The insets show the electron density profile for the corresponding modes.

The eigenvalue dependences on the characteristic strength for the case of $n = 0, 1, 2, 3, 4$ are shown in Fig. 2 and their explicit forms are given in the Appendix. It can be seen from Fig. 2 that $m$ new eigenvalues appear when $w$ exceeds $(n + 1)/2$, where $m = n + 1$. The number of eigenvalues, $N_w$, for a fixed value of $w > \frac{1}{2}$ is therefore $(1 + N)(2 + N)/2$ where $N$ is the integer part of $2w - 1$. It should be noted that in the limit that $w \to \infty$, $\Delta = w$ and the eigenvalue spectrum becomes $E = \pm p/2$, where $p$ is an integer. For example, a potential of characteristic strength $w = 2.2$ results in 10 energy states as shown in Fig. 3.

The bound modes which propagate along the potential well each contribute $4e^2/h$ to the channels conductance, where the factor of four accounts for the valley and spin degeneracy. By modulating the parameters of the potential
and or changing the position of the Fermi level one can increase the conductance of the channel by multiples of $4e^2/h$
therefore a change of geometry, from normal transmission to propagation along a potential, allows graphene to be
used as a switching device. The existence of bound modes within smooth potentials in graphene may provide an
additional argument in favor of the mechanism for minimal conductivity, where charge puddles lead to a percolation
network of conducting channels.

![Graph](image1)

**FIG. 2:** (Color online) The eigenvalue spectrum dependance on the potentials characteristic strength, $w$. The dotted (grey),
solid (red), short-dashed (blue), long-dashed (green) and dashed-dotted (maroon) lines correspond to the $n = 0, 1, 2, 3$ and 4
modes respectively.

![Graph](image2)

**FIG. 3:** (Color online) Schematic energy spectrum of $-w / \cosh (x/l)$, for the case of $w = 2.2$, in this instance there are 10
eigenvalues. The solid (red), short-dashed (blue) and long-dashed (green) lines correspond to the $n = 1, n = 2$ and $n = 3$
modes respectively. The dotted (grey) line represents the two $E = 0$ modes (one from $n = 0$ and one from $n = 2$) and the
potential profile is shown in the same scale.

### III. CONCLUSIONS

We have presented the hitherto unknown exact solution to the Dirac equation for the hyperbolic secant potential,
which provides a good fit for potential profiles of existing top-gated graphene structures. It was found that bound
states of both positive and negative energies exist in the energy spectrum and that there is a threshold value of $w$, the characteristic potential strength, for which the first mode appears. A simple relationship between the number of confined modes and the characteristic potential strength $w$ was obtained.

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**Appendix**

List of eigenvalues and their corresponding $\Delta_{n,m}$

\[
E_{0,0} = 0 \\
E_{1,0} = -\frac{1}{2w} \sqrt{w^2 - w} \\
E_{1,1} = -E_{1,0} \\
E_{2,0} = -\frac{1}{2w} \sqrt{4w^2 - 6w + 1} \\
E_{2,1} = 0 \\
E_{2,2} = -E_{2,0} \\
E_{3,0} = -\frac{1}{2w} \sqrt{5w^2 - 10w + 3 + 16w^4 - 64w^3 + 85w^2 - 42w + 9} \\
E_{3,1} = -\frac{1}{2w} \sqrt{5w^2 - 10w + 3 - 16w^4 - 64w^3 + 85w^2 - 42w + 9} \\
E_{3,2} = -E_{3,1} \\
E_{3,3} = -E_{3,0} \\
E_{4,0} = -\frac{1}{4w} \sqrt{40w^2 - 100w + 42 + 6\sqrt{16w^4 - 80w^3 + 140w^2 - 100w + 33}} \\
E_{4,1} = -\frac{1}{4w} \sqrt{40w^2 - 100w + 42 - 6\sqrt{16w^4 - 80w^3 + 140w^2 - 100w + 33}} \\
E_{4,2} = 0 \\
E_{4,3} = -E_{4,1} \\
E_{4,4} = -E_{4,0}
\]

$\Delta_{0,0} = \pm \left( w - \frac{1}{2} \right)$

$\Delta_{1,0} = \Delta_{1,1} = \pm \frac{1}{2w} \sqrt{w^2 - w} \left( w - \frac{1}{2} \right)$

$\Delta_{2,1} = \pm \left( w - \frac{3}{2} \right)$

$\Delta_{2,2} = \pm \frac{1}{2w} \left( 2w^2 - 3w + 1 \right)$

$\Delta_{3,0} = \Delta_{3,3} = \pm \frac{1}{2w} \sqrt{4w^4 - 16w^3 + 21w^2 - 10w + 3 + 16w^4 - 64w^3 + 85w^2 - 42w + 9}$

$\Delta_{3,1} = \Delta_{3,2} = \pm \frac{1}{2w} \sqrt{4w^4 - 16w^3 + 21w^2 - 10w + 3 - 16w^4 - 64w^3 + 85w^2 - 42w + 9}$

$\Delta_{4,2} = \pm \left( w - \frac{5}{2} \right)$

$\Delta_{4,0} = \Delta_{4,4} = \pm \frac{1}{2w} \left( \frac{5}{2} + \frac{1}{2} \sqrt{16w^4 - 80w^3 + 140w^2 - 100w + 33} \right)$

$\Delta_{4,1} = \Delta_{4,3} = \pm \frac{1}{2w} \left( \frac{3}{2} - \frac{1}{2} \sqrt{16w^4 - 80w^3 + 140w^2 - 100w + 33} \right)$

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