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BOUND STATES IN 2D FERMION SYSTEMS OF GRAPHEN

Analytical solutions for the zero-energy modes of two-dimensional massless Dirac fermions confined within the one-dimensional Lorentz-like potential, which provides a reasonable fit for potential profiles of existing top-gated graphene structures is performed. On the basis of obtained hypergeometrical equations we have studied the conditions for formation of quantum bound states providing an one-dimensional fermion localization. A simple relations between the potential parameters and number of modes within the potential are established. Possibility of realization of the external controlled charge transport in the studied 2D system is considered.

1. Introduction

Carriers within graphene behave as two-dimensional (2D) massless Di1rac fermions, exhibiting relativistic behavior at sub-light speed owing to their linear dispersion, which leads to many optical analogies (see [1]). For them as for relativistic particles there is the known problem of the spatial localization (see [1-5]). The relativistic particles do not experience exponential damping within a barrier like their non relativistic counterparts and that as the barrier height tends towards infinity, the transmission coefficient approaches unity. This inherent property of relativistic particles makes confinement non-trivial. Carriers within graphene behave as two-dimensional (2D) massless Dirac fermions, exhibiting relativistic behavior at sub-light speed owing to their linear dispersion, which leads to many optical analogies. Features of particle tunneling through p-n junction structures in graphene has been studied both theoretically and experimentally (see [1,5,6]). Quasi-bound states were considered in order to study resonant tunneling through various sharply terminated barriers (see [1,5,7]).

In the presented paper the changed geometry of the problem is considered in order to study the propagation of fully confined modes along a smooth electrostatic potential, much like photons moving along an optical fiber (see [1,8,9]). The Lorentz-like potential is used for confinement of carriers within graphene. The bound modes within such a channel are analyzed on the basis of the hypergeometrical equations describing wave states of fermions.

Recently quasi-one-dimensional channels have been achieved within graphene nanoribbon (see [4]), however the control of their transport properties requires precise tailoring of edge terminations, currently unachievable. The solution of this problem can be with the help of truly bound modes creating within bulk grapheme by top gated structures (see [1]).

The key to the realization of truly bound modes within a graphene waveguide as zero-energy modes is related to possibility to control of the Fermi level using the back gate. Then as in an ideal graphene sheet at half-filling, the Fermi level is at

the Dirac point and the density of states for a linear 2D dispersion vanishes. Cannot escape into the bulk as there are no states to tunnel into.

The model Lorentz potential allows leads an exact analytical solution of bound modes within a smooth electrostatic potential at half-filling, count the number of modes and calculate the conductivity of the channel. The conductivity carried by each of these modes is comparable to the minimal conductivity of a realistic disordered grapheme system (see [2]). For the considered model potential there are threshold potential parameters for which bound modes appear.

Thus we present an exact analytic solution for the fully confined zero-energy modes of massless 2D Dirac fermions in a model smooth potential vanishing at infinity and then describe the experimental geometry required for the observation of confined modes within such grapheme waveguides.

2. The Hamiltonian and dispersion

The two-dimensional system of the graphene is consisted of carbon atoms arranged in hexagonal structure via atomic sp^2 bonds (see [1,10]). The structure can be seen as a lattice with a basis of two atoms per unit cell, and two lattice vectors $a_1 = \left(\sqrt{3}/2, -a/2\right)$, $a_2 = \left(0, a\right)$, as shown in Fig.1.

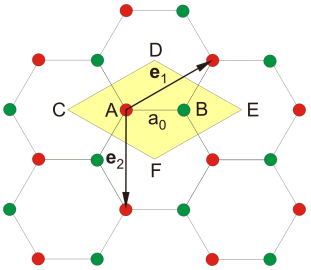

Fig.1. A plane structure of the graphene. The circles represent carbon atoms, e_1 and e_2 represent lattice vectors.

The reciprocal lattice vectors are given by $b_1 = \left(2/(a\sqrt{3}), 0\right)$ and $b_2 = \left(1/(a\sqrt{3}), 1/a\right)$. The tight-binding Hamiltonian for electrons in graphene considering that electrons can hop to both nearest- and next-neighbor atoms can be represented in the form

$$H = -t \sum_{(i,j),\sigma} \sum_{j=1}^{3} \left(a_{\sigma i}^{+} b_{\sigma j} + \text{H.c.} \right) - t' \sum_{(i,j),\sigma} \sum_{j=1}^{3} \left(a_{\sigma i}^{+} a_{\sigma j} + b_{\sigma i}^{+} b_{\sigma j} + \text{H.c.} \right), \qquad (1)$$

where $a_{\sigma i}$ ($a_{\sigma i}^{+}$) annihilates (creates) an electron with spin $\sigma = (\uparrow, \downarrow)$ on site R_i on sublattice A (an equivalent definition is used for sublattice B); $t (\approx 2.8 eV)$ is the

nearest-neighbor hopping energy (hopping between different sublattices), t' is the next nearest -neighbor hopping energy (hopping in the same lattice). The Fourier expansion of the mentioned second quantization operators:

$$a_i = \int_{Bz} \frac{d^2k}{2\pi} e^{ikR_i} \bar{a}(k),\ b_i = \int_{Bz} \frac{d^2k}{2\pi} e^{ikR_i} \bar{b}(k),$$

where wave vector integration operators is executed within the first Brillouin zone (Bz) and introduction of the two-component operators

$$\psi(k) = (\bar{a}(k), \bar{b}(k))^T,\ \psi^+(k) = (\bar{a}^+(k), \bar{b}^+(k))$$

allow rewrite the Hamiltonian (1) in the form

$$H = \int_{Bz} \frac{d^2k}{(2\pi)^2} \psi^+(k) H' \psi(k), \tag{2}$$

where H' is a two-dimensional matrix dependent on a wave vector k.

The eigenvalue of the Hamiltonian (2) determines the dispersion of the studied system

$$E_{\pm}(k) = \pm\sqrt{\left(3 + 2\cos(k_y a) + 4\cos\left(\frac{\sqrt{3}}{2}k_y a\right)\cos\left(\frac{3}{2}k_y a\right)\right)} - \\ -t'\left(3 + 2\cos(k_y a) + 4\cos\left(\frac{\sqrt{3}}{2}k_y a\right)\cos\left(\frac{3}{2}k_y a\right)\right), \tag{3}$$

where the plus sign applies to the upper (π^*) and the minus sign the lower (π) band corresponding to electrons and holes.

The dispersion (3) is characterized by the linear dependence close of six vertex points of the type $K_{\pm} = (0, \pm\frac{4\pi}{3\sqrt{3}a})$ (so-called by Dirac points) in the first Brillouin zone of the hexagonal reciprocal lattice. Such the linear dispersion is described by the expression [w]

$$E_{\pm}(q) = \pm v_F |q| + O[(q/K)^2],\ q = k - K, \tag{4}$$

where $|q| \ll |K|$, $v_F = 3ta/2$ is the Fermi velocity [w].

The most striking difference between this result and the usual dispersion, $\varepsilon(q) = q^2/(2m)$, is that Fermi velocity in (4) does not depend on the energy or momentum. The expansion of the spectrum around the Dirac point including t' up to second order in q/K is given by

$$E_{\pm}(q) = \pm v_F + \left(3t' - 9t'a^2/4 \pm (3ta^2/8)\sin(3\arctan(q_x/q_y))\right)$$

Whence it follows that presence of t' shifts in energy the position of the Dirac point and breaks electron-hole symmetry.

Dirac fermions can be obtained from the Hamiltonian (1) with $t' = 0$ using expanding the Fourier sum around K and K'. Then

$$a_n \to e^{-KR_n} a_{1n} + e^{-K'R_n} a_{2n},\ b_n \to e^{-KR_n} b_{1n} + e^{-K'R_n} b_{2n}$$

Where the index $i = 1$ ($i = 2$) refers to the K (K'') point. The new operators, a_{in} and b_{in} are assumed to vary slowly over the unite cell. Transition in (2) to coordinate representation in the considered case result in effective Hamiltonian of the form

$$H = -iv_F \int dxdy \left[\psi_1^+(r)\sigma\nabla\psi_1 + \psi_2^+(r)\sigma\nabla\psi_2(r) \right],$$

with Pauli matrices $\sigma = (\sigma_x, \sigma_y)$, and $\psi_i = (a_i, b_i)$. In first quantized language the two-component electron function $\psi(r)$ close to the Dirac point K obeys 2D Dirac equation

$$-iv_F\sigma\nabla\psi(r) = E\psi(r),$$

which corresponds to the Dirac-like Hamiltonian

$$H = v_F\sigma\nabla .$$

Note that wave function, in momentum space, for the momentum around K has the form

$$\psi_{\pm K}(k) = \begin{pmatrix} \exp(-i\vartheta_k / 2) \\ \pm\exp(-i\vartheta_k / 2) \end{pmatrix},$$

where $\vartheta_k = q_x / q_y$ and the $\pm$ signs correspond to the eigenenergies $E = \pm v_F k$, that is for the π^* and π bands, respectively.

3. Equation and bond quantum states

The Hamiltonian of graphene for the two-component Dirac wavefunctions in the presence of a one dimensional potential $U(x)$ can be write in the form

$$H = v_F \left(-i\sigma_x \hbar\partial_x \mp i\sigma_y \hbar\partial_y \right) + U(x)$$

where the $\mp$ sign denotes the two nonequivalent Dirac points, $v_F \approx 1\times 10^6$ m/s is the Fermi velocity in graphene. An usage of representation of the Dirac function in the form $\exp(iq_y)(\psi_A(x), \psi_B(x))^T$, where A and B correspond two sublattice, leads to coupled first-order differential equations for the wave functions, which can be represented in the form

$$\left(V(x) - \varepsilon\right)\psi_A(x) - i\left(\frac{d}{dx} + q_y\right)\psi_B(x) = 0,$$

$$-i\left(\frac{d}{dx} + q_y\right)\psi_A(x) + \left(V(x) - \varepsilon\right)\psi_A(x).$$

Here $V(x) = U(x) / \hbar v_F$ and $\varepsilon = E / \hbar v_F$.

Carrying out symmetrization of the wave functions with the help the substitutions: $\psi_1 = \psi_A(x) - i\psi_B(x)$ and $\psi_2 = \psi_A(x) + i\psi_B(x)$ we can represent the last system to the system of equations

$$\begin{aligned} \Big(V(x) - (\varepsilon - q_y)\Big)\psi_1(x) - \frac{d}{dx}\psi_2(x) = 0, \\ \frac{d}{dx}\psi_1(x) + \Big(V(x) - (\varepsilon + q_y)\Big)\psi_2(x) = 0. \end{aligned} \tag{5}$$

This system describes the potential dependent and free wave propagation along the x and free directions, respectively, i.e. the propagation in a waveguide.

Differentiation of the second equation of the system (5) and substitution of the expressions

$$\begin{aligned} \frac{d}{dx}\psi_2(x) = \Big(V(x) - (\varepsilon - q_y)\Big)\psi_1(x), \\ \psi_2(x) = -\frac{1}{\Big(V(x) - (\varepsilon + q_y)\Big)}\frac{d}{dx}\psi_1(x), \end{aligned}$$

allow to reduce (5) to the second order differential equation

$$\psi_1''(x) - \frac{V'(x)}{(V-\varepsilon) - q_y}\psi_1' + \Big((V-\varepsilon)^2 - q_y^2\Big)\psi_1 = 0\,. \tag{6}$$

If the Fermi energy is at the Dirac Point there no charge carriers within the system so graphene is insulator. Nonzero conductivity of the graphene waveguide can be caused by coupled states within the potential well that is controlled via change of the potential parameters (see [8]). It is shown [pro] possibility of an experimental fixation of the zero Fermi level. So in the equation (6) we take the value $\varepsilon = 0$.

As known (see [8]) smooth potentials with controlled parameters which admit the exact solution of considered problem represent the special physical interest. To such a type of potential can belong of the Loretz-like potential of the form

$$V(x) = -\frac{\gamma}{x^2 + \mu^2} + \beta \tag{7}$$

where $\gamma > 0, \beta > 0$; the negative value reflects a potential well for electron (see [Pos].)

Substituting the expression (7) into the equation (6) result in the equation which at the condition $\beta = q_y$ takes the form of the differential equation of the hypergeometrical type (see [11-13])

$$\psi_1'' + \frac{\tilde{\tau}(x)}{\sigma(x)}\psi_1' + \frac{\tilde{\sigma}(x)}{\sigma^2(x)}\psi_1 = 0\,, \tag{8}$$

Where $\sigma(x) = (x^2 + \mu^2)$, $\tilde{\tau}(x) = 2x$ and $\tilde{\sigma}(x) = \beta\gamma x^2 + \beta\mu^2 + \gamma^2$.

The equation (8) with the help of the substitution $\psi_1(x)=\varphi(x)y(x)$ where the function $\varphi(x)$ by the relation of the form $\varphi'/\varphi=\pi(x)/\sigma$ can be reduced to the canonical hypergeometrical equation of the form

$$\sigma(x)y''+\tau(x)y'+\lambda y=0\,, \tag{9}$$

where (see [13])

$$\begin{aligned}
&\pi(x)=\frac{\sigma'-\tilde{\tau}}{2}\pm\sqrt{\left(\frac{\sigma'-\tilde{\tau}}{2}\right)^2-\bar{\sigma}+k\sigma}\,,\ k=\lambda-\pi'(x),\\
&\tau(x)=\tilde{\tau}(x)+2\pi(x),\ \ \bar{\sigma}(x)=\bar{\sigma}+\pi(x)[\tilde{\tau}(x)-\sigma'(x)],\\
&k=\lambda-\pi'(x).
\end{aligned} \tag{10}$$

Taking into account that $\pi(x)$ is a first order polynomial, from the first equation of the system (10) we obtain two solutions: $k=\beta\gamma$ and $k=(\gamma/\mu)^2+\beta\gamma$. In the first case $\pi(x)=\pm i\gamma\sqrt{\beta\gamma}$ and in the second case $\pi(x)=\pm(\gamma/\mu)x$. From these solutions $\pi(x)=-(\gamma/\mu)x$ correspond to the localization condition.

In according with the mentioned solution the system (9) yields

$$\begin{aligned}
&\tau(x)=2\left(1-\frac{\gamma}{\mu}\right)x,\ \ \varphi(x)=(x^2+\mu^2)^{-\gamma/(2\mu)},\\
&\lambda=k+\pi'(x)=\left(\frac{\gamma}{\mu}\right)^2-\left(\frac{\gamma}{\mu}\right)+\beta\gamma.
\end{aligned} \tag{11}$$

Polynomial solution of the equation (9) is built on the basis of the equation of the form

$$\sigma(x)v_n''+\tau_n v_n'+\mu_n v_n=0\,, \tag{12}$$

where $\tau_n(x)=\tau(x)+n\sigma'$, $\mu_n=\lambda+n\tau'+\frac{n(n-1)}{2}\sigma''$ and v_n is the derivative of the n-the order of the solution of the equation (9) ($v_n=y^{(n)}$). Polynomial solutions of the equation (9) are described by the formulae of the form

$$y_n(x)=\frac{B_n}{\rho(x)}\left(\sigma^n\rho(z)\right)^{(n)},$$

where the function $\rho(x)$ is determined by the equation

$$(\sigma\rho)'=\tau\rho \tag{13}$$

In the considered case the solution of the equation (13) has the form

$$\rho(x)=(x^2+\mu^2)^{-\gamma/\mu}\,.$$

The bound modes in the system obey the condition

$$\mu_n = \lambda + n\tau' + \frac{1}{2}n(n+1)\sigma'' = \\ + \left(\left(\frac{\gamma}{\mu} \right)^2 - \frac{\gamma}{\mu} + \beta\gamma \right) + n^2 + \left(3 - 2\frac{\gamma}{\mu} \right) n = 0,\ n = (0,1,2...) \tag{14}$$

which determine the dependence of number of the bound quantum states on the potential parameters. From the equation (14) we can obtain corresponding relation

$$n = \frac{1}{2}\left(3 - 2\frac{\gamma}{\mu} \right) \pm \sqrt{\frac{1}{2}\left(\frac{\gamma}{\mu} \right)^2 - 2\frac{\gamma}{\mu} + \left(\frac{3}{4} - \beta\gamma \right)} \ . \tag{15}$$

Thus change of the ratio γ / μ, characterizing a shape of the one-dimensional potential $V(x)$, leads to the change of the limit number of bounded quantum states of electron in the waveguide. Appear of the bound states occurs by discrete leading to increasing of the density of electron states and the increasing of conductivity of the waveguide/ Appear of the first bound states is accompanied by a transition from the non- to conductive electron state.

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