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On resonant scattering states in graphene circular quantum dots

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Abstract. Due to the effect of Klein tunneling, two-dimensional graphene quantum dots do not possess genuine bound states but quasi-bound (resonant tunneling) states only. We discuss in detail the attempt to describe these states within the framework of the Dirac pseudo-fermion model for circular dots. We demonstrate explicitly that introduced earlier the so-called "resonance condition" corresponds to the inconsistent system of linear equations obtained from matching conditions on the boundary of the quantum dot when one tries to use it for complex energy values and in the case of total reflection for the energies coincided with the potential well top.
Keywords: graphene, Klein tunneling, massless pseudo-Dirac fermion, quantum dot, quasi-bound states

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1. Introduction

After more than twenty years of experimental observation, graphene still attracts a lot of attention and attempts to use as a base for super-high-speed electronic devices. The masslessness of graphene carriers in the most popular graphene model, the so-called pseudo-Dirac fermion model, from one side seems to be very attractive due to the high value of the Fermi velocity (of about 10^6 m/s) for the material but failed to artificially form a predefined gap in a band structure needed for transistor-like behavior.

Graphene quantum dots are considered as a variant to find a way of the electric current operation. Experimentally, they can be formed with a few different techniques (see, e.g. [1-3] and references therein). The theoretical description is based usually on the simplest analytically treatable case of circular symmetric quantum dot with radial step potential [4,5] (see also other approaches in [3,6] and references therein).

The specific feature of quantum problems for the 2D massless Dirac equation with the circular symmetric finite height potential barrier is the absence of bound eigenstates. This is stipulated by the fact that solutions of the Dirac radial equation, in a region with a flat potential, are a linear combination of the Bessel functions which asymptotically look like sin and cos; therefore the eigenstates are non-normalizable and correspond to unbound particles.

In the cited references [4] it has been stated the existence of the quasi-bound eigenstates of complex energies, the imaginary part of which corresponds to a level's decay time. The

eigenstates were chosen from some sort of a "spectral condition" arisen in consideration. In [4] and [7,8] the deduction of this condition was slightly different, in the first one it has been derived for admissible system eigenstates, in the second paper, the condition was deduced for the scattering problem. In subsequent publications, there were made a lot of experimental work with the result interpretation based on these theoretical predictions [7,9]. Besides a further theoretical analysis of more complicated systems such as bilayer graphene [6], as well as of systems in an electromagnetic field was produced [10-12].

Nevertheless, as we prove with all detail and this is the main goal of the paper, in both cases the statement on the existence of such types of quasi-bound states is erroneous. It appears due to neglecting one of two independent solutions of the corresponding radial Dirac equation when using improper physically ground assumptions.

2. Model

We use 2D massless Dirac fermion model of graphene [13], in tight binding approximation and near the Dirac point excitations, its Hamiltonian operator reads $\hat{H}_0 = \gamma\vec{\sigma}\cdot\vec{k}$ where γ is the band parameter linearly related with the Fermi velocity, $\vec{\sigma} = \{\sigma_x, \sigma_y\}$ is the 2D vector of two Pauli matrixes, $\vec{k}$ is the quasi-momentum. Then, a graphene quantum dot (GQD) can be considered as graphene in some confining potential $V(\vec{r})$. The Hamiltonian reads $\hat{H} = \hat{H}_0 + V(r)$ with a scalar potential incorporated as a diagonal matrix. In the matrix form we have [5]

$$\hat{H} = \begin{pmatrix} V(\vec{r}) & \hat{p}_- \\ \hat{p}_+ & V(\vec{r}) \end{pmatrix} \tag{1}$$

with the operators $\hat{p}_\pm$ given by $\hat{p}_- = -i\frac{\gamma}{\hbar}\frac{\partial}{\partial x} - \frac{\partial}{\partial y}$, $\hat{p}_+ = -i\frac{\gamma}{\hbar}\frac{\partial}{\partial x} + \frac{\partial}{\partial y}$.

As a model GQD we consider a circular quantum dot with a radial step potential, region D is the circle of a radius R,

$$V(\vec{r}) = \begin{cases} 0, \vec{r} \notin D \\ V_0, \vec{r} \in D \end{cases} \tag{2}$$

Due to the system's symmetry, for the eigenproblem $\hat{H}\psi = E\psi$, and the spinor function ψ with components $\psi = (A, B)$, the separation of variables can be achieved in the polar coordinates (ρ, ϕ) introduced via the ordinary relations $x = \rho\cos\phi,\ y = \rho\sin\phi$. Then, with dimensionless variables $\rho \to \rho / R, \epsilon = RE/\gamma$ we have

$$(V(\rho) - \epsilon)A(\rho,\phi) = -ie^{-i\phi}\left(\frac{\partial B(\rho,\phi)}{\partial\rho} - \frac{i}{\rho}\frac{\partial B(\rho,\phi)}{\partial\phi}\right), \tag{3}$$

$$(V(\rho) - \epsilon)B(\rho,\phi) = -ie^{i\phi}\left(\frac{\partial A(\rho,\phi)}{\partial\rho} + \frac{i}{\rho}\frac{\partial A(\rho,\phi)}{\partial\phi}\right). \tag{4}$$

Substitution

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} e^{im\phi}a(\rho) \\ \imath e^{\imath(m+1)\phi}b(\rho) \end{pmatrix}, \tag{5}$$

designation $\xi = \epsilon - V(\rho)$ and account of the fact that ξ is different but constant in both two regions $\rho < 1$ (inner region of the quantum dot) and $\rho > 1$ (outer region), leads to the following system of the radial equations

$$\xi a(\rho) = -b'(\rho) - \frac{(m+1)b(\rho)}{\rho}, \tag{6}$$

$$\xi b(\rho) = a'(\rho) - \frac{ma(\rho)}{\rho}. \tag{7}$$

Since the potential V is step-like flat, expressing $b(\rho)$ from the second equation (7) of the radial system and substituting it into the first one, we get the equation for $a(\rho)$ in the form

$$a(\rho)\left(m^2 - \xi^2\rho^2\right) - \rho\left(\rho a''(\rho) + a'(\rho)\right) = 0, \tag{8}$$

with the general solution given by the superposition of two Bessel functions [15]

$$a(\rho) = c_1 J_m(\rho\,|\,\xi\,|) + c_2 Y_m(\rho\,|\,\xi\,|). \tag{9}$$

The latter can be substituted into equation (7) and one gets

$$b(\rho) = c_1(-J_{m+1}(\rho\,|\,\xi\,|)) - c_2 Y_{m+1}(\rho\,|\,\xi\,|). \tag{10}$$

The boundary condition at $\rho = 0$ for the radial system demands the finiteness of the solution so that one has to omit the second term in (10) as the function Y_m is singular at zero. Outside the quantum dot ($\rho > 1$) one has to use both functions in the solution. The only requirement left is the continuity of the eigenfunctions at the boundary $\rho = 1$ of the quantum dot. The important point of the problem is that the eigenfunctions can not belong to the bound state because, independent of the potential values in both regions, all the Bessel functions asymptotically at infinity ($\rho \to \infty$) trend to plane waves and therefore they are non-normalizable.

Let us designate the coefficients c in the solution by additional upper indexes i and o for the inside region and outside one of the quantum dots respectively. Matching solutions for both spinor components at $\rho = 1$ and choosing the normalization constant in the interior region with $c_1^i = 1$ (due to the equation linearity one can choose an arbitrary normalization) we get the following linear system for the determination of the coefficients

$$J_m(|V_0 - \epsilon|) = c_1^o J_m(|\epsilon|) + c_2^o Y_m(|\epsilon|), \tag{11}$$

$$-J_{m+1}(|V_0 - \epsilon|) = c_1^o(-J_{m+1}(|\epsilon|)) - c_2^o Y_{m+1}(|\epsilon|). \tag{12}$$

It can be shown that the determinant of the matrix of this linear system is given by the formula

$$J_{m+1}(|\epsilon|)Y_m(|\epsilon|) - J_m(|\epsilon|)Y_{m+1}(|\epsilon|), \tag{13}$$

it does not depend on V_0 and is non-zero for all real values of m, and ϵ (see e.g., the energy dependence for $m = 0$ in Fig. 1).

It means that we get the real-value solution of the eigenproblem which is continuous in the space. As an example, both spinor components of the solution are shown in Fig. 2 for $V_0 = 3,\ m = 0,\ \epsilon = 0.09$.

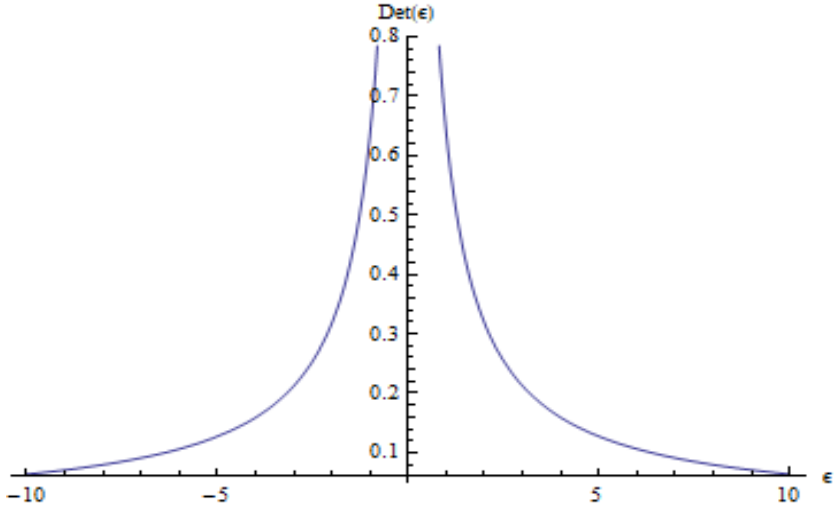

Fig. 1. Dependence of the determinant on energy for $m = 0$

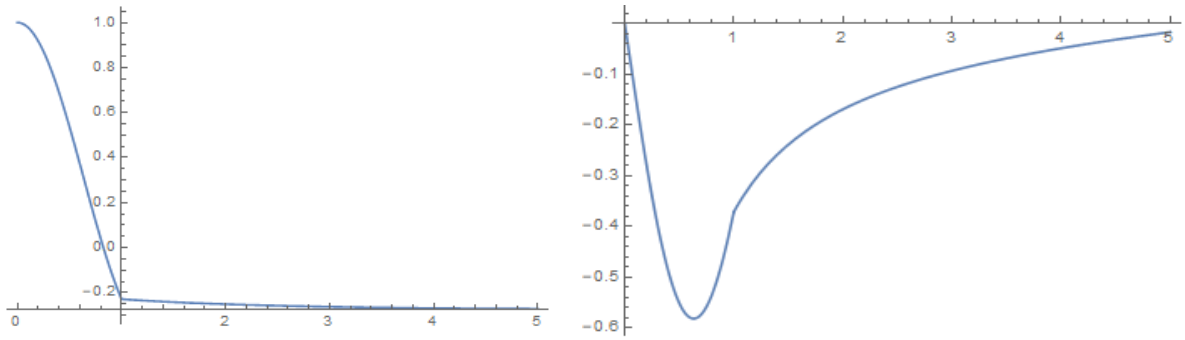

Fig. 2. Upper and lower components of the spinor eigenfunction for $m = 0$, $\epsilon = 0.09$, $V_0 = 3$

Of course, instead of the Bessel functions J_m, Y_m one can use the Hankel functions of the first and second kind $H_m^{(k)}(z) = J_m(z) \pm \imath Y_m(z), k = 1,2$ for the outer region as it has been done in [5] resulting in complex coefficients. However, all eigenfunctions are functions of a real variable and belong to a continuous spectrum. The authors of [5] put the additional requirement that the eigenfunction should asymptotically behave as $\exp\{\imath\,|\,\xi\,|\,r\}$. From the physical point of view, it means that one fixes the phase of the exponential function because a linear combination of the Bessel (or Hankel) functions asymptotically can be represented as $\mathrm{Re}(a\exp\{i(kr+\phi)\})$. This additional restriction leads to the specific condition which was stated in [5] as a "spectral condition"

$$J_{m+1}(|\,\epsilon - V_0\,|)H_m^{(1)}(|\,\epsilon\,|) - J_m(|\,\epsilon - V_0\,|)H_{m+1}^{(1)}(|\,\epsilon\,|) = 0\,. \tag{14}$$

This equation has no real solutions for ϵ, except of those for $m > 1, \epsilon = 0$, but has complex ones which were interpreted in [5] as quasi-bound states with a finite lifetime.

As we intend to demonstrate condition (14) is meaningless because corresponds to an inconsistent system of linear equations followed by the matching conditions at the quantum dot boundary $\rho = 1$. With this in mind, we follow the "scattering scheme" of [7,8] to obtain the matching condition system. For the radial scattering problem inside the GQD, the solution consists of the transient wave and still is described by the Bessel J function with some amplitude $tJ_m(|\,\xi\,|\,r)$ (e.g., for the upper component, letter t is used for transmission coefficient).

The solution outside the GQD is a superposition of two Hankel functions describing the incident and scattered waves, that is $H_m^{(1)}(\epsilon)+rH_m^{(2)}(\epsilon)$ again for the upper component (with "r" letter to designate the reflection coefficient). Then the matching system reads

$$tJ_m(|V0-\epsilon|)-rH_m^{(1)}(|\epsilon|)-H_m^{(2)}(|\epsilon|)=0\,, \tag{15}$$

$$-tJ_{m+1}(|V0-\epsilon|)+rH_{m+1}^{(1)}(|\epsilon|)+H_{m+1}^{(2)}(|\epsilon|)=0\,. \tag{16}$$

Precisely, the determinant of this system is just the left hand side of condition (14). So, our goal is to construct the system in the vicinity of the vanishing determinant. First, we do it for the energy values $\epsilon=V_0$ corresponding to the top of the potential well. The determinant of the matrix, in this case, vanishes due to the properties of Bessel J functions at zero argument. But we apply this energy value directly to the system to get

$$t\times 0-rH_m^{(1)}(|V_0|)-H_m^{(2)}(|V_0|)=0\,, \tag{17}$$

$$-t\times 0+rH_{m+1}^{(1)}(|V_0|)+H_{m+1}^{(2)}(|V_0|)=0\,. \tag{18}$$

The latter means that the reflection coefficient has to be expressed as a ratio ($r=H_m^{(1)}(|V_0|)/H_m^{(2)}(|V_0|)$) of Hankel functions but with the orders differ on "one" for the first and the second equations. Taking into account the fact that the Hankel functions of the first and second kind at a given value of the argument are the conjugated complex numbers, the reflection coefficient as their ratio turns out to be unimodal. But the equality of it for both equations can be only approximately satisfied in an asymptotic regime and for small and intermediate values of the confining potential. For example, we represent in Fig. 3 the value $\mathrm{R_{arg}}=\arg\left(\frac{H_{20}^{(1)}(x)}{H_{20}^{(2)}(x)}\right)/\arg\left(\frac{H_{21}^{(1)}(x)}{H_{21}^{(2)}(x)}\right)$ as a function of the potential height V_0 to confirm our statement.

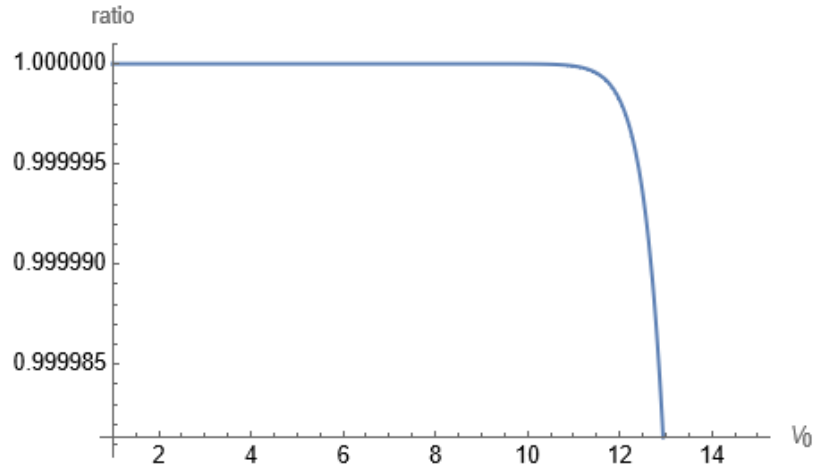

Fig. 3. Dependence of $\mathrm{R_{arg}}$ on the confining potential height V_0. The region with an approximate unity value of the ratio corresponds to the total reflection case

The last regime corresponds to the same amplitudes for the reflected wave as an incident one with only a phase shift and therefore to zero value for the transmitted wave. The latter means the total wave reflection that hardly is considered as "a bound state" as was stated in [5,6].

Now, we try to understand what happens near the non-trivial complex roots of equation (14) when the energy does not coincide with the well height. We choose the following parameters: $V_0 = 20, m = 0$ and find one of the roots of eqs. (17-18) in the vicinity of point $\epsilon = 3$. This gives $\epsilon = 3.95744 - 1.47721I$. Substitution of this value into the matching condition system and normalization of both equations to make coefficients at variable t equal to unity gives

$$1.t - (1.01973 + 0.160047\,\mathrm{I})r = -0.0390394 + 0.0318167\,\mathrm{I}, \quad (19)$$

$$1.t - (1.01973 + 0.160047\,\mathrm{I})r = 0.0409105 - 0.0408179\,\mathrm{I}. \quad (20)$$

As one can see, indeed the determinant of the system vanishes (since left-hand sides of both equations coincide). This means that we really have a root of the "resonance condition" but the right-hand sides are different for both equations. The latter shows that the system is inconsistent and there are no solutions at all in this case. A similar situation holds for other roots too.

3. Conclusion

We explicitly demonstrated that the "resonance condition", introduced in [5] to construct "quasi-bound" states for GQD with a finite lifetime, leads to the inconsistent system of linear equations describing matching conditions for the solution inside and outside GQD. Therefore it can not be considered valid for any application. We also demonstrated that the "exact localization of electron in the quantum dot" considered in [6] and confirmed in [5] in fact can be approximately the case of the total reflection of an electron on a graphene quantum dot at asymptotically high values of magnetic quantum number m and not the very high value of the confining potential (whispering gallery modes).

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