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Quasi-Bound States for Circular Bilayer-Graphene Quantum Dots: Subtle Detail of Real and Complex-Valued Analysis

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Graphene quantum dots (GQDs) are assumed to be a perspective systems for quantum computing. The simplest one can be considered as a circular dot described by two-dimensional Dirac-like equation within the known graphene model of massless pseudo-Dirac fermions. The system admits an analytical treatment with a stair-case confining potential. The existence of quasi-bound states for such systems has been declared in a series of papers, an opposite point of view has been proposed by us in [H. Grushevskaya & G. Krylov J NPCS,**25** 21(2022)]. Detailed analysis of eigenfunctions and possibility of quasi-bound states for monolayer and bilayer graphene circular quantum dots with a step like potential is the goal of the current research. It has been demonstrate that anomalous density of states emerge in bilayer graphene cases for the real energies in the vicinity of the point of vanishing determinant of the linear algebraic system for matching eigenfunctions and their derivative at the boundary of the quantum dot. The effect is stipulated by the significant contribution of the Bessel K_m function at the distance up to several dot's radii.

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1. Introduction

Unique electronic properties of graphene already observed experimentally put it forward as a prominent candidate material for future nanoelectronics. Among numerous more or less sophisticated approaches to the theoretical description of this material (see e.g., [1] and references therein) the simplest one is based on known massless pseudo-Dirac fermion model [2]. In this approach in the vicinity of the so called Dirac points the matrix Hamiltonian in tight bind approximation has the form of two-dimensional Dirac one for massless fermion excitations [1] that is $\hat{H} = v_F(\vec{p}\cdot\vec{\sigma})$ where $\vec{p}$ is two-dimensional (2D) momentum, $\vec{\sigma}$ is a 2D vector of Pauli matrixes (σ_x, σ_y), v_F is the Fermi velocity. To model a monolayer graphene quantum dot (MGQD) one can add a confining scalar potential $V(\vec{r})$ to above mentioned Hamiltonian. If this potential is invariant on respect to arbitrary rotation that is $V(r)$ $(r = |\vec{r}|)$ the problem admits variables separation in polar coordinates [5]. The simplest exactly solvable case with such a symmetry corresponds to step-like potential of the form $V(r) = V_0\theta(r - R)$ where θ is the Heaviside function, R is the radius of the dot. Investigation of this model will be primary goal of the first part of the paper whereas in the second part we consider a model of the bilayer graphene quantum dot (BGQD).

The structure of the paper is the following. In Section 2 we start with the MGQD and construct eigenstates and eigenvalues. Continuity conditions for the spinor wave function on the boundary of the quantum dot leads to a linear system (we call it as matching system in what follows) relating expansion coefficients of the wave function on eigensolutions in inner and

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outer regions in respect to the dot. Situation, when the determinant of this system vanishes at definite values of the energy ϵ^* (we call it as a exceptional point), is the so-called quasi-bound state condition proposed in [5, 6]. We consider choice of real or complex energies and see what results it leads for the energy values strictly in exceptional points and in their vicinity.

Section 3 starts with a short description of the BGQD Hamiltonian. The analysis similar to Section 2 will be performed for the BGQD with the same geometry and the confining potential as for MGQD. Discussion and conclusion section finalizes our treatments.

2. Monolayer GQD

Accounting circular symmetry of the problem and with the use of the following representation of the spinor wave function

$$\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix} = \begin{pmatrix} e^{\imath m\phi}\,\psi_1(\rho)\\ \imath\, e^{\imath(m+1)\phi}\,\psi_2(\rho)\end{pmatrix}, \qquad (1)$$

the eigenproblem for the MGQD leads to the following system for a pair of radial functions a, b

$$\xi a(\rho) = -b'(\rho) - \frac{(m+1)b(\rho)}{\rho}, \qquad (2)$$

$$\xi b(\rho) = a'(\rho) - \frac{ma(\rho)}{\rho} \qquad (3)$$

where more convenient variables for the radial distance $\rho = r/R$ and the energy $\epsilon = RE/v_F$ have been introduced, and the parameter $\xi = \epsilon - V(\rho)$ is a local constant in two regions $\rho < 1$ (inner region of the quantum dot) and $\rho > 1$ (outer region) [5].

It is evident from the local constancy of the ξ that the solutions in both the regions correspond to a free particle wave function with only different energies. It is easily to obtain the second order equation for the only one function, e.g. $b(\rho)$

$$b'' + \frac{1}{r}b' + \left(\xi^2 - \frac{m+1/2}{r^2}\right) b(\rho) = 0 \qquad (4)$$

which is the equation for the Bessel functions, so that the general solution of the system (2),(3) reads

$$a(\rho) = c_1 J_{m-1/2}(\xi\rho) + c_2 Y_{m-1/2}(\xi\rho), \qquad (5)$$

$$b(\rho) = \imath(c_1(-J_{m+1/2}(\xi\rho)) - c_2 Y_{m+1/2}(\xi\rho)). \quad (6)$$

Here c_1, c_2 are arbitrary constants, J, Y Bessel functions of the first and second kind respectively.

In [3, 4] and in several later publications [8, 9] authors used absolute value $|\xi|$ instead of the original variable and this is a subtle error, but only for the consideration of the problem in complex domain of ϵ. Let us demonstrate this explicitly by an example. We choose $\xi = (1 + \imath)/\sqrt{2}$, then $|\xi|^2 = 1$, $\xi^2 = \imath$ and substituting the last into eq. (4) we just do not obtain the ordinary Bessel functions on ρ as solutions. The reason why some authors did this mistake is that for complex energies and with $|\xi|$ the spatial behavior of the solutions will be finite at infinity.

Further, we construct a solution of radial scattering problem as in [5, 6], then we find radial eigenfunctions on the semi-axis and discuss their behavior. In all cases we need to match solutions on the dot boundary $\rho = 1$ to provide continuity property.

Let us to do this for the scattering case. Then, we have to find a solution which behaves as a scattering wave (oscillating and decaying as $\rho^{-\frac{1}{2}}$ at infinity) in two dimensional space. For such one, the only possible choice is the Bessel function $H_m^2(\xi\rho)$ (with real ξ) [5], but as we have already mentioned this is not true if ξ is complex. In the last case all Bessel functions of complex argument gain exponential component due to imaginary part of the ξ, either growing or decaying one. In fact, with this remark been done, the so-called resonance condition [5] and concept of quasi-bound state [5, 6] with complex values of the energy should not be used.

Let us construct eigenfunctions of the problem for real values of ξ. The condition of finiteness of the solution in the origin requires vanishing coefficient at function $Y_m(\xi\rho)$, that

is $c_2^{(i)} = 0$. Continuity of the radial spinor eigenfunction at $\rho = 1$ leads to the following relations for remaining inner domain coefficient $c_1^{(i)}$ and outer domain ones $c_1^{(o)}$, $c_2^{(0)}$

$$c_1^{(i)} J_{m-1/2}(\epsilon) = c_1^{(o)} J_{m-1/2}(V_0 - \epsilon) + c_2^{(o)} Y_{m+1/2}(V_0 - \epsilon), \tag{7}$$

$$c_1^{(i)} J_{m+1/2}(\epsilon) = c_1^{(o)} (-J_{m+1/2}(V_0 - \epsilon)) + c_2^{(o)} Y_{m+1/2}(V_0 - \epsilon), \tag{8}$$

where we took into account the different constant values for ξ inside and outside the quantum dot.

Due to linearity of the system (2),(3) the normalization of the solutions should be added in some way, e.g., by putting one of the coefficient $c_1^{(i)} = 1$. The latter does not lead to a finite norm of the spinor wavefunction, but is one of possible choice. Then the determinant of the matching system reads

$$\det(\epsilon) = J_{m+\frac{1}{2}}(V_0 - \epsilon) Y_{m-\frac{1}{2}}(V_0 - \epsilon) - J_{m-\frac{1}{2}}(V_0 - \epsilon) Y_{m+\frac{1}{2}}(V_0 - \epsilon) \tag{9}$$

and it is strictly non-zero in the interval $\epsilon \in [0, V_0]$. It also diverges at the right end of the interval because Y function is divergent in the origin.

Another variant emerges if one chooses the following normalization condition: $c_i^{(o)} = 1$ either for $i = 1$ or for $i = 2$ for outer region coefficients. As for an incident wave of the original problem one should use the plane wave $\exp\{\imath kx\}$, then the known expansion with the Bessel functions [11]

$$\exp\{\imath kr\} = \sum_{n=-\infty}^{\infty} \imath^n J_n(kr) \tag{10}$$

leads to a constant value of the expansion coefficient for partial radial scattering problem for a given m. This precisely corresponds to the choice been done above.

Then, one finds that the system determinant

$$\det(\epsilon) = J_{m+\frac{1}{2}}(\epsilon) Y_{m-\frac{1}{2}}(V_0 - \epsilon) - J_{m-\frac{1}{2}}(\epsilon) Y_{m+\frac{1}{2}}(V_0 - \epsilon) \tag{11}$$

may possesses non-trivial real roots ϵ^* so that $\det(\epsilon^*) = 0$. As for example we demonstrate this for the following parameters $V_0 = 5, m = 1/2$ in Fig. 1. It can be checked that the linear system (7),(8) is inconsistent for this root.

The absence of the solution of the system (7),(8) does not lead to paradox at ϵ^*, it simply

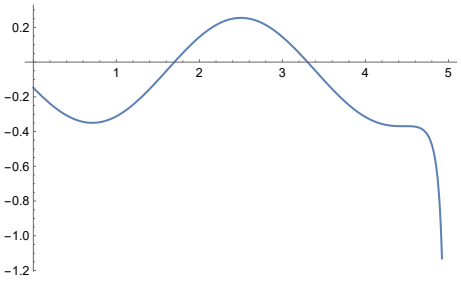

FIG. 1: Energy dependence of the matching system determinant for $m = 1/2,\ V_0 = 5$.

means that the term with the coefficient $c_1^{(i)}$ which we put to unity, is negligible in respect to the rest ones. This can be understood from the consideration when ϵ is in the vicinity of the point ϵ^*. Indeed, one component of the outer region solution with the Bessel function J turned out to be very small on the respect to all other components, whereas the large components diverge at $\epsilon \to \epsilon^*$. It means that the original choice of the normalization condition was poor.

In [12] it has been shown that the same situation of system's inconsistency takes place for the scattering case for $\epsilon = \epsilon^*$ and for complex values for the energy. In the vicinity of such a point the coefficients are high but finite. As it was already mentioned, for complex energy values

at least one term in the outer region solution diverges at $\rho \to \infty$ due to properties of the Bessel functions that breaks the construction of the quasi-bound state in the considered case.

Now, we switch to BGQD and demonstrate that in the vicinity of real valued ϵ^* a whole band of states looking like a quasi-bound ones appears.

3. Bilayer GQD

The Hamilton operator in two component wave function approximation reads [5, 10]

$$\hat{H} = \frac{1}{2}\begin{pmatrix} V(\vec{r}) & \hat{p}_-^2 \\ \hat{p}_+^2 & V(\vec{r}) \end{pmatrix} \tag{12}$$

where the operators $\hat{p}_\pm$ are given by the relation $\hat{p}_- = -i\frac{\partial}{\partial x} - \frac{\partial}{\partial y}$, $\hat{p}_+ = -i\frac{\partial}{\partial x} + \frac{\partial}{\partial y}$, the scalar potential $V(\vec{r})$ is of the same form as for MGQD.

Eigenproblem for a spinor function (A, B) leads to the system

$$(V(r) - E)\, A(x,y) = \frac{1}{2}\hat{p}_-^2 B(x,y), \tag{13}$$

$$(V(r) - E)\, B(x,y) = \frac{1}{2}\hat{p}_+^2 A(x,y), \tag{14}$$

that can be transform into an equation for a single function e.g., A as

$$\frac{1}{4}\hat{p}_+^2\hat{p}_-^2 A = (V(r) - E)^2 A \tag{15}$$

In a similar manner as for the MGQD, the eigenproblem is separable in polar coordinates. After variable separation of the following form: $A = a(r)\exp(\imath m\phi)$ and $B = b(r)\exp(\imath(m+2)\phi)$, the 4th-order differential equation for a single function $a(r)$ reads [5]

$$\left[\frac{1}{2}\frac{d^2}{d\rho^2} + \frac{1}{2\rho}\frac{d}{d\rho} + \left(\xi - \frac{m^2}{\rho^2}\right)\right]\left[\frac{1}{2}\frac{d^2}{d\rho^2} + \frac{1}{2\rho}\frac{d}{d\rho} + \left(-\xi - \frac{m^2}{\rho^2}\right)\right] a(\rho) = 0 \tag{16}$$

with the same designation of locally constant ξ as for MGQD in the internal and outer regions.

The most interesting feature of eq. (16) is that the two operators representing content of every square bracket commute and every of them separately admits the Bessel functions as its eigenfunctions. For the left operator these are ordinary Bessel functions $J_m(\kappa\rho), Y_m(\kappa\rho)$, for the right one the appropriate eigenfunctions are the Bessel functions of imaginary argument $I_m(\kappa\rho), K_m(\kappa\rho)$ with $\kappa = \sqrt{2\xi}$. We also will use and additional prime for the κ constant in the outer region. A linear combination of all these four functions is the general solution of the problem, so that the eigenfunctions both for $a(r)$ and $b(r)$ are expressed through them. To construct an eigenstate we have to match the eigenfunctions and their derivatives at the dot boundary $\rho = 1$. One more aspect should be taken into account is that in both regions we have to discard some functions which have singular behavior therein provided working with real energies. Then for the interior region ($\rho < 1$) of the dot we discard the Bessel functions Y_m, I_m as singular ones in the origin and arrive to the following form of the eigenstate inside the dot

$$a(\rho) = c_1 J_m(\kappa\rho) + c_2 I_m(\kappa\rho), \tag{17}$$

$$b(\rho) = c_1 J_{m+2}(\kappa\rho) + c_2 I_{m+2}(\kappa\rho). \tag{18}$$

The formula for b has been obtained from the system (13),(14) after the substitution of eq. (17) into eq. (14).

With above mention arguments, for the outer region with $r \geq 1$ we omit the only one Bessel function I_{m+2} as singular at infinity and

arrive at the following form for the eigenstate

$$a(\rho) = C_1 J_m(\kappa'\rho) + C_2 Y_m(\kappa'\rho), \tag{19}$$

$$b(\rho) = \text{sign}(\epsilon - V_0)(C_1 J_{m+2}(\kappa'\rho), \\ C_2 + Y_{m+2}(\kappa'\rho) + C_3 K_{m+2}(\kappa'\rho) \tag{20}$$

where the sign function is introduced in the second equation of the system.

Both eigenfunctions and their derivatives should be continuous on the dot's boundary. Therefore, there exist the following four matching conditions for the coefficients c_1, c_2, C_2, C_3 (we again put the coefficient at Y_m to unity as normalization for outer region):

$$c_1 J_m(\kappa) + c_2 I_m(\kappa) - C_2 Y_m(\kappa') - C_3 K_m(\kappa') - J_m(\kappa') = 0, \tag{21}$$

$$\frac{1}{2}c_1\kappa(J_{m-1}(\kappa) - J_{m+1}(\kappa)) + \frac{1}{2}c_2\kappa(I_{m-1}(\kappa) + I_{m+1}(\kappa)) - \frac{1}{2}C_2\kappa'(Y_{m-1}(\kappa') - Y_{m+1}(\kappa')) \\ -\frac{1}{2}C_3\kappa'(-K_{m-1}(k') - K_{m+1}(\kappa')) - \frac{1}{2}\kappa'(J_{m-1}(\kappa') - J_{m+1}(\kappa')) = 0, \tag{22}$$

$$c_1 J_{m+2}(\kappa) + c_2 I_{m+2}(\kappa) + \text{sign}(E - V_0)(C_2 Y_{m+2}(\kappa') + C_3 K_m(\kappa') + J_{m+2}(\kappa')) = 0, \tag{23}$$

$$\frac{1}{2}c_1\kappa(J_{m+1}(\kappa) - J_{m+3}(\kappa)) + \frac{1}{2}c_2\kappa(I_{m+1}(\kappa) + I_{m+3}(\kappa)) + \text{sign}(E - V_0)\left(\frac{1}{2}C_2\kappa'\right. \\ \left.\times(Y_{m+1}(\kappa') - Y_{m+3}(\kappa')) + \frac{1}{2}C_3\kappa'(-K_{m-1}(\kappa') - K_{m+1}(\kappa')) + \frac{1}{2}\kappa'(J_{m+1}(\kappa') - J_{m+3}(\kappa'))\right) = 0. \tag{24}$$

In the monolayer GQD case, we were interested in the condition of vanishing determinant of the matching system. This is assumed as a condition of the existence of quasi-bound states. This can be done for the system under investigation step by step for definite values of m, V_0 numerically. Let us do it for $m = 0$, $V_0 = 1$. In Fig. 2, we demonstrate the dependence of the matching system determinant upon the energy. As one can see, the root is at $\epsilon^* = 0.87$.

It turns out that as for the monolayer GQD case, the matching system is also inconsistent in the point ϵ^*, that there is no solution at all. Now we try to look at the solution behavior near the root, e.g., let us define the deviation $\delta\epsilon$ from the root ϵ^*. Then we expand the system (21-24) into a series on $\delta\epsilon$ near the point ϵ^*, keep only linear terms. In this way, we find for c_1, c_2, C_2, C_3

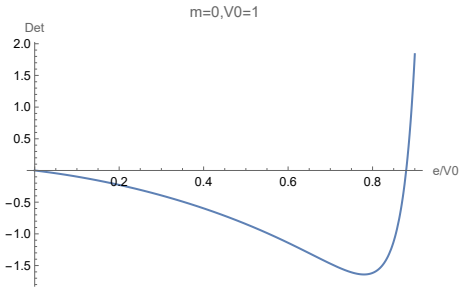

FIG. 2: Energy dependence of the matching system determinant for $m = 0$, $V_0 = 5$.

divergent at $\delta\epsilon \to 0$ formula of the form

$$c_1 = \frac{0.8169\delta\epsilon^2 + 0.2367\delta\epsilon + 0.01245}{\delta\epsilon^2 + 0.02751\delta\epsilon} \tag{25}$$

$$c_2 = \frac{0.3993\left(0.1637\delta\epsilon^2 + 0.0091\delta\epsilon + 0.00017\right)}{(\delta\epsilon + 0.07022)\left(\delta\epsilon^2 + 0.02751\delta\epsilon\right)} \tag{26}$$

$$C_2 = \frac{\left(0.0011\delta\epsilon^2 + 0.000024de + 1.6886\times10^{-7}\right)}{0.000377\delta\epsilon^2 + 3.731\times10^{-6}\delta\epsilon} \tag{27}$$

$$C_3 = \frac{0.25432\delta\epsilon^2 + 0.0264951\delta\epsilon + 0.0007}{0.0977\delta\epsilon^2 + 0.0019\delta\epsilon} \tag{28}$$

Let us demonstrate eigenfunction for some value of $\delta\epsilon$. In Fig. 3 the radial dependence of the

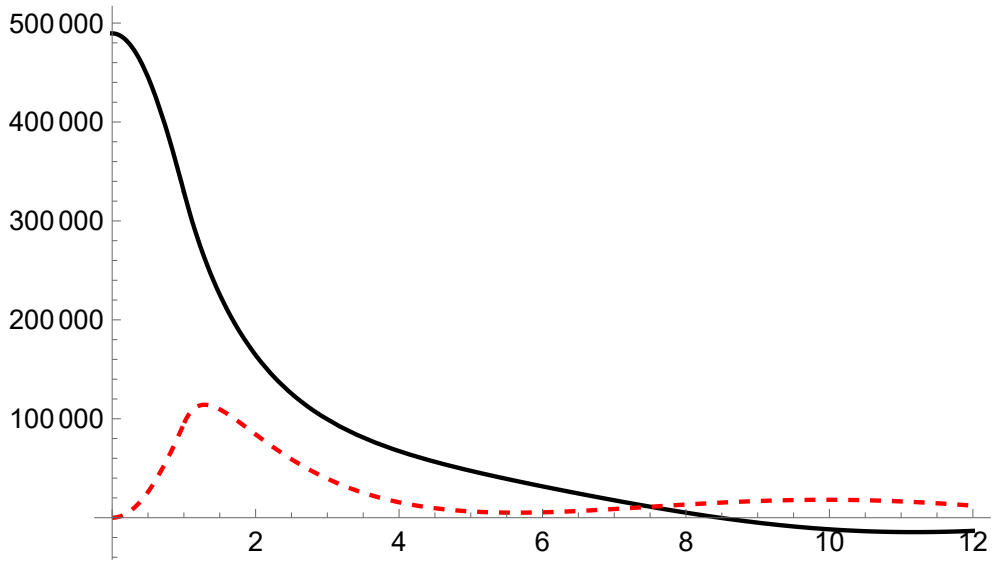

FIG. 3: Spinor eigenfunction $(A(\rho), B(\rho)$ for the energy $e = e^* + de$, $de = 1.0 \times 10^{-6}$, $m = 1,\ V_0 = 1$.

spinor components of eigenfunction is shown for $m = 1, V_0 = 1$. It is clear that the eigenstate does not have a finite norm and belong to continuous spectrum, as Bessel functions J, Y oscillate but do not decrease quickly enough at infinity. But as one can see in the Fig. 3, inside the quantum dot and up to ten of its radius the eigenfunction module is enormous due to c_1 in the inner region and C_3 outside the dot. The component with K Bessel function can be viewed as some sort of the bound state (with a finite norm). In fact, all near region to ϵ^* will demonstrate such a behavior of the eigenstates that can be interpreted as "a resonance band" rather than a single quasi-bound state level.

One could suppose that it is possible to construct a real bound state using the only K component in the outer region of the dot. But this it is not possible because one has to request the continuity properties not only for the spinor function but for its derivative as well. And the last lead to more conditions than can be satisfied even when one try to include system's parameters (e.g. V_0) as variables to be adjusted.

4. Discussion and conclusion

Let us summarize our findings. For the MGQD, complex value of the energy always leads to divergent behavior of at least one of radial eigenfunctions at large distances that spoils the concept of quasi-bound states introduced for this system in some earlier publications. The energy value for which the determinant of the matching system vanishes for real energies that can take place when one fixes the value of an incident radial wave function amplitude, leads to inconsistent matching system in this point. But this does not give serious problems as simply means a poor choice of the normalization condition. In the vicinity of this point one observes regular scattering with no resonant effects revealed.

For the BGQD, the presence of the Bessel function of imaginary argument K with exponentially decaying behavior at infinity among solutions leads to a new quasi-resonant band of states near real energy values corresponding the condition of the vanishing determinant of the matching linear system. Whereas at the strict zero value of the determinant, the matching system is inconsistent, near to this point, the eigensolutions

may gain giant contribution of the K function to the wavefunction. As a result one observes the behavior very similar to a bound states with the density concentrated within a distance of several dot radii.

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