ELECTRICALLY CONFINED GRAPHENE QUANTUM DOTS: THEORETICAL TREATMENT

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I. INTRODUCTION

Nanometer sized quasi-circular graphene monolayer patches look very promising as a main component of quantum devices. Such structures can be chemically synthesized [1] but more preferable from the point of operational easiness are those produced by application of an electrical field of the STM tip to a graphene plane which are called tip-induced or electrically confined graphene quantum dots (GQD) [2]. Theoretical treatment of this type of quantum dots attracts a lot of attention last two decades. Theoretical consideration of a quasi-circular GQD with a radius r_0 has been performed in [3,4,5] on the basis of free pseudo-Dirac fermion model with a step-like confining potential $V(r)=V_0\theta(r-r_0)$. The authors of [4,5] assume the existence of quasi-bound states (with a complex energy where the imaginary part of the energy corresponds to the inverse life-time of the state) which represent themselves resonances in a scattering amplitude for the system under consideration. Such an approach attracts much attention both from theoretical point of view [6,7] and from the experimental one [8,9], though its mathematical ground seems not enough clear. Moreover, the pseudo-Dirac fermion models give no consistent description especially for the so called "quasi-zero energy" levels of the system. Natural questions arise what is a precise meaning of the resonance conditions and either exist real reasons to transfer consideration of the problem into the energy complex plane. These are the motives for our reconsideration of the problem. In this report we focus attention on applicability of free pseudo-Dirac fermion models to the problem of GQDs and the existence of quasi-bound states for the GQDs.

II. THEORETICAL APPROACH

For two dimensional systems, solutions of the radial part of the pseudo-Dirac equation in a regions with a constant potential are given as a linear combination of the Bessel functions $J_m(|\xi|r)$, $Y_m(|\xi|r)$ of the first and second kind (m is a magnetic quantum number related to radial and polar angle variables separation, ξ is defined as a difference of the energy and the value of the confining potential being a constant 0 or V_0 in two regions $r<r_0$, $r>r_0$). The Bessel functions behave as sine and cosine functions at large values of their argument. It means non-normalization of the solutions in a whole space and, accordingly, the absence of the bound states in such a model system. We construct eigenstates for this problem of circular GQD with a step-like potential by matching the wave functions on the boundary of the quantum dot. Inside GQD we choose a non-zero coefficient $c_{1,in}$ at first kind Bessel function and $c_{2,in}$ equal to zero at second kind Bessel function (because this function is singular in the origin) in the linear combination. Outside the dot the coefficients are chosen from the condition of the continuity of the both component of the spinor wave function. This condition determines unknown coefficients $c_{1,in}$ $c_{1,out}$, $c_{2,out}$ up to a common factor as it should be for linear equations. The solution exists for real energies (real eigenvalues) and corresponds to a scattering state (see Figure 1).

Figure 1. Upper and lower components of the spinor eigenfunction for the case $m=0$, $\varepsilon=0.09$, $V_0=3$.

III. RESULTS AND DISCUSSION

We have shown that there is no resonant condition (associated with appearance of quasi-bound state) as it was erroneously stated in [4]. The origin of the mistake in [4] was an assumption on the value for the phase of the wave function at infinity that led to additional condition between $c_{1,out}$, $c_{2,out}$ besides the matching ones. The last made the linear system to be overcomplete and, as a result, inconsistent for all real energies except $\varepsilon=V_0$ (state at the edge of the well). We also reproduce the appropriate theoretical derivation for the scattering problem (when one assumes the plane wave incidence on the GQD) and demonstrate explicitly that the resonance condition found in [5] corresponds to the inconsistent system of linear equations obtained from the spinor wave function matching conditions on the boundary of a quantum dot. , or (in the above mentioned special case $\varepsilon=V_0$) directly to a regime of a total wave reflection from a quantum dot rather than to a some kind of temporal trap regime that could be associated with quasi-bound states. The results of our consideration can be stated as the necessity of alternative approaches to the GQD theoretical description.

In our recent publication [10] it has been demonstrated that electronic properties of such electrically confined GQDs can be described by application of the concept of pseudo-potential together with the usage of the quasi-relativistic graphene model developed earlier in [11] (see also references in [10]). GQD in this consideration is represented as a supercell with a definite type of boundary conditions. These boundaries are connected with two topologies of the GQDs: 2D-sphere and 2D-torus. On the basis of this model it has been demonstrated a nice correspondence between our theoretical and experimental results [8,9] on quasi-zero energy part of GQD spectra of a system under consideration contrary to existing toy models (see [4-6] and the references therein).

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REFERENCES

[1] Jia Zhang, Shu-Hong Yu, Carbon dots: large-scale synthesis, sensing and bioimaging. Materials Today. Vol. 19, p.382, 2016.

[2] N.M. Freitag et al. Electrostatically Confined Monolayer Graphene Quantum Dots with Orbital and Valley Splittings. Nano Lett. Vol 16, p.5798, 2016.

[3] A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov, A.K.Geim. The electronic properties of graphene. Rev. Mod. Phys. Vol. 81, p.109, 2009.

[4] P. Hewageegana and V. Apalkov Trapping of an electron in coupled quantum dots in graphene Phys. Rev. B Vol. 79 p115418, 2009.

[5] A. Matulis and F. M. Peeters, Quasibound states of quantum dots in single and bilayer graphene Phys. Rev.B Vol. 77, p.115423, 2008.

[6] T D Linh Dinh et al. Quasibound states in single-layer graphene quantum rings, J. Phys.: Condens. Matter Vol. 30, p.315501, 2018.

[7] M. Grujic, M.Zarenia, A. Chaves, M.Tadic, G.A. Farias, F.M. Peeters. Electronic and optical properties of a circular graphene quantum dot in a magnetic field: Influence of the boundary conditions. Phys. Rev. B Vol. 84, p.205441, 2011.

[8] Y. Jiang et.al Tuning a circular p-n junction in graphene from quantum confinement to optical guiding. Nat. NanotechnologyVol. 12, p.1045, 2017.

[9] J. Lee et al. Imaging electrostatically confined Dirac fermions in graphene quantum dots. Nature Physics. Vol. 12, p.1032, 2016.

[10] H. V. Grushevskaya et al. Electronic properties and quasi-zero-energy states of graphene quantum dots Phys. Rev. B Vol. 103, p.235102, 2021.

[11] H. V. Grushevskaya et al. Electronic Structure and Transport in Graphene: Quasi Relativistic Dirac-Hartree-Fock Self-Consistent Field Approximation. // In: Graphene Science Handbook: Electrical and Optical Properties. Vol. 3. Eds. M. Aliofkhazraei, N. Ali, W.I. Milne, C.S. Ozkan, S. Mitura, J.L. Gervasoni. (Taylor and Francis Group, CRC Press, USA, UK, 2016). pp. 117-132.