Bound states in the continuum in graphene quantum dot structures

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received 24 August 2010; accepted in final form 9 September 2010
published online 23 September 2010

PACS 61.46.-w – Structure of nanoscale materials
PACS 73.22.-f – Electronic structure of nanoscale materials and related systems
PACS 73.63.-b – Electronic transport in nanoscale materials and structures

Abstract – The existence of bound states in the continuum was predicted at the dawn of quantum mechanics by von Neumann and Wigner. In this work we discuss the mechanism of formation of these exotic states and the feasibility to observe them experimentally in symmetrical heterostructures composed by segments of graphene ribbons with different widths forming a graphene quantum dot. We identify the existence of bound states in the continuum in these graphene quantum dot systems by means of local density of states and electronic conductance calculations.

The new material denominated graphene is a single layer of carbon atoms which can be fabricated by different methods like mechanical peeling or epitaxial growth [1–3]. Nanoribbons are stripes of graphene which can be obtained through high-resolution lithography [4], by controlled cutting processes [5] or by unzipping multi-walled carbon nanotubes [6]. The electronic behavior of all these nanostructures is mainly determined by their geometric confinement which allows the observation of quantum effects such as quantum interference effects, resonant tunneling and localization effects. The possibility to control these quantum effects, by applying external perturbations to the nanostructures or by modifying the geometrical confinement, could be used to develop new technological applications, such as graphene-based composite materials [7], molecular sensor devices [8,9] and nanotransistors [10].

An interesting feature exhibited by certain confined nanostructures, such as quantum dots systems, is the presence of bound states in the continuum (BICs). Their existence was predicted at the dawn of quantum mechanics by von Neumann and Wigner [11] for certain spatially oscillating attractive potentials, for a one-particle Schrödinger equation. Much later, Stillinger and Herrick [12] generalized von Neumann’s work by analyzing a two-electron problem, they found BICs were formed despite the interaction between electrons. The occurrence of BICs was discussed in a system of coupled Coulombic channels and, in particular, in a hydrogen atom in a uniform magnetic field [13]. BICs have also shown to be present in the electronic transport in mesoscopic structures [14–19]. More recently, exploiting the analogy between electronics and photonics, Marinica et al. [20], Bulgakov and Sadreev [21] and Prodanović et al. [22] reported the presence of BICs in photonic systems. Several mechanisms of formation of BICs in open quantum dots (QDs) have been reported in the literature. The simplest one is based on the symmetry of the systems and, as a consequence, in the difference of parity between the QD eigenstates and the continuum spectrum [23]. Another mechanism takes into account a nonzero coupling between bound states in the QD and the continuum spectra. The formation of BICs would be the result of a destructive interference process of these resonances, for certain variations of the physical parameters of the QD [24–26]. A third mechanism for the BICs formation in optics, is associated with the Fabry-Pérot interferometer [27].

Until nowadays, there is only one experimental work, reported by Capasso and co-workers [28], in which BICs were measured in semiconductor heterostructures grown by molecular beam epitaxy. Thereby, the search of new systems which could be able to reveal the existence of

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EPL, 91 (2010) 66001
doi: 10.1209/0295-5075/91/66001
BICs, with the possibility to be measured, is a very interesting and relevant field of research. The experimental feasibility exhibits by graphene-based systems and the great advances in the controlled manipulation and measurements reported in graphene, together with the possibility of modifying their electronic properties by applying external potentials, suggests that BICs could be observable in graphene quantum dots heterostructures.

In this work we study the formation of BICs in quantum-dot–like structures, formed by segments of graphene ribbons with different widths connected with each other [29]. We identify the presence of BICs in these symmetrical graphene quantum dots (GQDs) and we discuss the mechanism for their formation. We found that the GQD local density of states as a function of the energy shows the presence of a variety of sharp peaks that we demonstrate to be BICs. The linear conductance also shows the presence of resonant states which contribute to the electronic transmission. By changing the geometrical parameters of the structure, it is possible to control the number and position of these resonances as a function of the Fermi energy.

A schematic view of the considered systems is presented in fig. 1. The conductor is formed by two symmetric crossbar junctions of widths \(N_B = 9\) and length \(L_B = 17\), and a central region that separates the junctions, of width \(N_C = 5\) and length \(L_C = 3\). Two semi-infinite leads of width \(N_L = N_C\) are connected to the ends of the central conductor. We studied the different electronic states manifested in the system as a function of the geometrical parameters of the GQD structure.

Systems are described by using a single \(\pi\)-band tight-binding Hamiltonian, taking into account first nearest neighbor interactions with a hopping parameter \(\gamma_0\). We consider hydrogen passivation by setting a different hopping parameter for the carbon dimers at the ribbons edge [30], \(\gamma_{edge} = 1.12\gamma_0\). To calculate electronic properties of the system we adopt the surface Green’s functions matching formalism [9,31]. In this scheme, we divide the heterostructure into three parts, two leads composed by semi-infinite pristine graphene nanoribbons, and the conductor region composed by two nanoribbon crossbar junctions, as it is shown in fig. 1.

In the linear response approach, the electronic conductance is calculated by the Landauer formula. In terms of the conductor Green’s functions, it can be written as [32]

\[
G = \frac{2e^2}{h} T(E) = \frac{2e^2}{h} \text{Tr}[\Gamma_L G^R_C \Gamma_R G^A_L],
\]

where \(T(E)\) is the transmission function of an electron crossing the conductor region, \(\Gamma_{L/R} = i[\Sigma_{L/R} - \Sigma_{L/R}^\dagger]\) is the coupling between the conductor and the respective leads, given in terms of the self-energy of each lead: \(\Sigma_{L/R} V_{C,L/R} g_{L/R} V_{L/R,C}\). Here, \(V_{C,L/R}\) are the coupling matrix elements and \(g_{L/R}\) is the surface Green’s function of the corresponding lead [9]. The retarded (advanced) conductor Green’s functions are determined by [32]:

\[
G^{R,A}_C = [E - H_C - \Sigma^{R,A}_L - \Sigma^{R,A}_R]^{-1},
\]

where \(H_C\) is the Hamiltonian of the conductor.

Figure 2 displays results of the local density of states (LDOS) (upper panel) and the linear conductance (lower panel) for a GQD structure formed by two armchair nanoribbons leads of width \(N_L = 5\) and a conductor region composed by two symmetric crossbar junctions of width \(N_B = 17\), length \(L_B = 3\) and relative distances between the junctions \(L_C = 5\). The conductance of a pristine \(N_L = 5\) armchair nanoribbon has been included for comparison (light green dotted line).

It can be observed in the LDOS and in the conductance curves a series of peaks at determined energies. This resonant behavior of the electronic conductance arises from the interference of the electronic wave functions inside the structure, which travel forth and back forming stationary states in the conductor region (well-like states).

We start our analysis focusing on the sharp states present in the LDOS displayed in this figure. We have

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**Fig. 1:** Schematic view of a GQD structure with leads of width \(N_L = 9\), a conductor region composed by two symmetrical junctions of width \(N_B = 21\) and length \(L_B = 3\) separated by a central structure of length \(L_C = 4\) and width \(N_C = 9\).**

**Fig. 2:** (Colour on-line) LDOS (upper panel) and conductance (lower panel) as a function of the Fermi energy for a GQD structure based on leads of width \(N_L = 5\), two symmetric crossbar junctions of width \(N_B = 17\) and \(L_B = 3\). The central region has a width \(N_C = 5\) and length \(L_C = 5\). Marks (a), (b) and (c) denote position of peaks in the LDOS which are absent in the conductance. These states are identified as BICs.
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Fig. 3: (Colour on-line) Corresponding contour plots of some sharp LDOS resonances marked in fig. 2 LDOS (upper panel).

Fig. 4: Scheme of side-coupled impurities attached to a perfect wire.

We introduce a simple model that captures the essence of the formation of BICs in our GQD structures. The model consists in two side-coupled impurities attached to a perfect quantum wire [34] as shown in fig. 4.

By using the Dyson equation \( G = g + g V G \) we calculate the Green’s function (\( G \)) in terms of the corresponding Green’s function of the isolate sub-systems (\( g \)), here \( V \) is the matrix coupling between the impurities and the wire (\( V_{0u} = V_{0d} = V_0 \)). To obtain the LDOS of each impurity, \( \rho_\alpha, (\alpha = u, d) \), we calculate the imaginary part of the diagonal elements of the Green’s functions, \( G_\alpha \). Setting the site energies as, \( \varepsilon_u = \varepsilon_0 + \delta \) and \( \varepsilon_d = \varepsilon_0 - \delta \), \( \gamma = \pi V_0^2 \rho(0) \), where \( \rho(0) \) corresponds to the LDOS in the site 0 of the wire without impurities, and taking \( \delta \ll \gamma \), the density of states of the entire system is obtained summing over \( \alpha \) and can be written approximately as

\[
\rho \approx \frac{1}{\pi} \frac{2 \gamma}{(\omega - \varepsilon_0)^2 + 4 \gamma^2} + \frac{1}{\pi} \frac{\delta^2/2 \gamma}{(\omega - \varepsilon_0)^2 + (\delta^2/2 \gamma)^2}. \tag{1}
\]

The density of states is then the sum of two Lorentzian shapes lines with widths \( \Gamma_+ = 2 \gamma \) and \( \Gamma_- = \delta^2/2 \gamma \), corresponding to those states strongly and weakly coupled to the continuum, respectively. In the limit of \( \delta \to 0 \), \( \Gamma_- \) vanishes and the state weakly coupled to the continuum becomes a bound state in the continuum. This state arises from the interference of the localized states in the impurities, through the continuum states of the wire. In this sense, this interference phenomenon is similar to phenomena like Fano and Aharonov-Bohm effects. If we denote as \( \psi_u \) and \( \psi_d \) the wave functions of the up and down impurity, respectively, it is straightforward to show that the antisymmetric state, \( (\psi_u - \psi_d) \), is an eigenstate of the complete system and therefore it is a bound state in the continuum. In analogy, in the GQD structure the formation of the BICs follows the same mechanism. According to it, if any infinitesimal small perturbation breaks the transversal symmetry, the BICs become resonant states with infinitesimal widths. The widths of these “quasi-BICs” can be controlled, for example, by tuning the asymmetry of the system through gate potentials. For instance, fig. 5 displays the LDOS and conductance as a function of the Fermi energy, for the same systems considered in fig. 2, but now taking into account a small up-down asymmetric gate potential applied to the edges of the GQD. Due to this external perturbation, it is possible to observe
In this sense, we expect that the study of this kind of states could have important applications in photonic crystals, so be used as a qubit for quantum information. Also, BICs on the other hand, the presence of two simultaneous BICs could open a potential, an efficient spin filter can be designed. On the one hand, the presence of two simultaneous BICs could be used as a qubit for quantum information. Also, BICs could have important applications in photonic crystals, so in this sense, we expect that the study of this kind of states in graphene nanoribbons quantum dots could open a new line of applied research.

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The authors acknowledge the financial support of CONICYT/Programa Bicentenario de Ciencia y Tecnología (CENAVA, grant ACT27), USM 110971 internal grant, FONDECYT program grants 11090212, 1100560 and 1100672. LR also acknowledges to PUCV-DII grant 123.707/2010.

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Fig. 5: (Colour on-line) LDOS (upper panel) and conductance (lower panel) as a function of the Fermi energy for a GQD structure composed by the same parameters of fig. 2, with an up-down asymmetric gate potential applied to the junction regions.
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