Discrete and resonance states in graphene near the Dirac point

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Abstract. We consider the problem of impurity states in the vicinity of Dirac point in graphene taking into account the spin-orbit (SO) interaction. Two main contributions to the SO interaction, namely the internal and Rashba, are considered. Even though the internal SO interaction is relatively small, its effect is crucial because a very small perturbation potential can create both discrete and resonance impurity states located near the gap. In the case of strong Rashba SO interaction like in the case of graphene on a substrate, the resonance impurity states can be created producing some anomalies in transport properties.

1. Introduction

Electric and magnetic properties of graphene are mostly determined by the electronic states in the vicinity of Dirac points [1, 2, 3, 4, 5]. If the spin-orbit (SO) interaction is neglected [7, 8, 9, 10], the energy spectrum in these points is degenerate, and the elementary excitations belong to the linear spectrum, which can be described by the two-dimensional relativistic Dirac model [6]. In reality, the SO interaction is not zero and, correspondingly, there is an energy gap [11]. However, it was found that in case of internal SO interaction the magnitude of SO gap is very small, and correspondingly it can be neglected [12, 13, 14, 15]. In this paper we demonstrate that even though the energy gap is really very small, the presence of SO interaction of any origin leads to formation of additional low-energy impurity states, which are absent if the SO interaction is neglected. Besides, we find that the impurity creating very small perturbation like, for example, some neutral adatoms or molecules, can be responsible for these states.

In the case of SO interaction related to the Rashba term, the magnitude of SO is not necessarily small, and the energy spectrum at low energies is completely different from the Dirac spectrum. In this case one can also study the problem of impurity states, which can be effectively controlled by electric gate, as it is known that the electric field of the gate modifies the magnitude of Rashba SO coupling.

2. Nonmagnetic impurity: the case of internal spin-orbit interaction

We start from considering the internal SO interaction in graphene, using the following Hamiltonian [11]

$$\hat{H}_0 = v \tau \cdot \mathbf{k} + \tau_z \sigma_z \Delta.$$  \hspace{1cm} (1)
Here the first term is the relativistic two-dimensional Dirac Hamiltonian for the $K$ point in the Brillouin zone of graphene, and the second term is due to the internal SO interaction. Hamiltonian (1) is $4 \times 4$ matrix, in which the Pauli matrices $\sigma$ and $\tau$ are acting in the sublattice and spin spaces, respectively. The constant $v$ is the velocity parameter and $\Delta$ is the constant of SO interaction. The energy spectrum consists of two bands, $\varepsilon = \pm \varepsilon_k$, and $\varepsilon_k \equiv (v^2k^2 + \Delta^2)^{1/2}$.

Let us consider now the impurity states created by a single nonmagnetic impurity which is described by a perturbation in the basis of eigenfunctions of the Hamiltonian without SO interaction (first term in Eq. (1)). For definiteness we assume that the impurity atom is located at the site of sublattice A. We also assume that the perturbation is strongly localized within the site, so that the matrix elements of the perturbation with the eigenfunctions of basis do not depend on electron momentum $k$ for the states in a vicinity of the single Dirac point, where the Hamiltonian (1) can be used. Thus, the matrix of perturbation in our model is

$$\hat{V}_{kk'} = \frac{1}{2} (1 + \tau_z) V_0 \equiv \hat{V}_0. \quad (2)$$

It should be noted that this model can be justified for relatively short range potential of neutral impurities. As we do not consider Umklapp scattering, then in this model, the matrix elements of perturbation with large transition of momentum are assumed to be strongly suppressed, which restricts the consideration of impurities of not too small potential range.

We use the $T$-matrix method [16], which accounts for the scattering in all orders of the impurity perturbation. The general equation for the $T$-matrix has the following form

$$\hat{T}_{kk'}(\varepsilon) = \hat{V}_{kk'} + \sum_{k_1} \hat{V}_{kk_1} \hat{G}_{k_1}(\varepsilon) \hat{T}_{k_1,k'}(\varepsilon), \quad (3)$$

where $\hat{G}_{k}(\varepsilon)$ is the electron Green’s function corresponding to Hamiltonian (1),

$$\hat{G}_{k}(\varepsilon) = (\varepsilon - \hat{H}_0)^{-1} = \frac{\varepsilon + \tau_z \sigma z \Delta + v \tau \cdot k}{\varepsilon^2 - \varepsilon_k^2}, \quad (4)$$

and we assume that the energy parameter $\varepsilon$ has a small imaginary part, $\varepsilon \to \varepsilon + i\delta$, where $\delta = 1/2\tau$ and $\tau$ is the momentum relaxation time. It corresponds to consideration of the retarded Green’s function.

Using (3) and (4) we calculate the $T$-matrix as $\hat{T}(\varepsilon) = [1 - \hat{V}_0 \hat{F}(\varepsilon)]^{-1} \hat{V}_0$ where the function $\hat{F}(\varepsilon) = \sum_k \hat{G}_{k}(\varepsilon)$. This function is diagonal in spin space, and we can find for the spin up state the real and imaginary parts (here we take the limit of $\delta \to 0$)

$$\text{Re} \hat{F}_{\uparrow}(\varepsilon) \simeq -\frac{\varepsilon + \tau_z \Delta}{4\pi v^2} \ln \left| \frac{v^2k_m^2}{(\Delta^2 - \varepsilon^2)} \right|, \quad (5)$$

$$\text{Im} \hat{F}_{\uparrow}(\varepsilon) \simeq \frac{\varepsilon + \tau_z \Delta}{4\pi v^2} \theta(\varepsilon^2 - \Delta^2), \quad (6)$$

where $\theta(\varepsilon)$ is the Heaviside step function. The location of impurity level is determined by the poles of $T$-matrix, and we can find for the spin up and spin down levels the following equations

$$\varepsilon_{1,1} = \mp \Delta - 4\pi v^2 \left( V_0 \ln \left| \frac{v^2k_m^2}{(\Delta^2 - \varepsilon_{1,1}^2)} \right| \right)^{-1}. \quad (7)$$

If the imaginary part of $\hat{F}(\varepsilon)$ for corresponding energy is nonzero, then we obtain the resonance state, and the width of resonance is proportional to $\text{Im} \hat{F}(\varepsilon)$. 

Figure 1. The location of impurity levels as a function of the impurity strength parameter $V_0$ (a) and the schematic presentation of the impurity levels (b) in the case of non-magnetic impurity and internal SO interaction in graphene. In numerical calculations we use the units: $\varepsilon_c = \hbar^2/m_e a_0^2$ and $V_c = \varepsilon_c a_0^2$, where $m_e$ is the electron mass and $a_0$ is the lattice constant.

There is another nonequivalent Dirac point $K'$ in graphene, which can be also described by Hamiltonian (1) with the substitutions $k_x \rightarrow -k_x$ and $\Delta \rightarrow -\Delta$. We performed the analogous calculations for the $K'$ point, and the results of numerical calculations for both Dirac points are presented in Fig. 1. As we see, in the case of very small impurity potential $V_0$, there are impurity states located near the edge of the SO gap. In the absence of SO interaction, only very strong impurity potential leads to creation of the resonance state in the vicinity of Dirac point.

It should be noted that the spin degeneration in this figures is due to the levels related to different Dirac points. The most important is presence of impurity states in the vicinity of the SO gap. These states appear even for very weak impurity potential.

3. Nonmagnetic impurity: Rashba spin-orbit interaction

The Hamiltonian of low-energy excitations near the Dirac point, which takes into account the Rashba SO interaction has following form

$$H_0 = v\tau \cdot k + \lambda_R (\tau_x \sigma_y - \tau_y \sigma_x),$$

(8)

where $\lambda_R$ is the Rashba coupling constant. This type of SO interaction appear for the graphene on substrate, and the magnitude of the constant $\lambda_R$ depends strongly on the material of substrate. The energy spectrum corresponding to Hamiltonian (8) has four branches, and there is no gap in the energy spectrum at $k \rightarrow 0$, $E_{1,2}(k) = \lambda_R \pm \sqrt{\lambda_R^2 + v^2 k^2}$ and $E_{3,4}(k) = -\lambda_R \pm \sqrt{\lambda_R^2 + v^2 k^2}$.

We do not present the details of calculations in this case because they are quite similar to the ones presented before. The perturbation is assumed in the same form of Eq. (2) corresponding to short-range neutral impurities. The results of calculations of the location of impurity levels as a function of $V_0$ for the Dirac points $K$ and $K'$ are presented in Figs. 2 and 3, respectively. Here 1 and 2 label different impurity states, each of them being certain superposition of the spin up and down states belonging to different sublattices (i.e., superposition of spins and pseudospins).
As we see, the asymmetry with respect to reverse of sign of the perturbation, $V_0 \rightarrow -V_0$, is absent in each of the figures 2 and 3, but it is completely restored if we take into account both Dirac points. The location of the low-energy impurity states is determined by the magnitude of Rashba SO interaction.

4. Nonmagnetic impurity with strong SO interaction

Using the same formalism, one can consider the impurity, which locally enhances the internal SO interaction. Physically, it can be the case of heavy neutral atoms like, for example, gold or platinum. In this case the corresponding perturbation for the $K$ point has the form

$$\hat{V}_\Delta = \frac{\Delta_0}{2} (1 + \tau_z) \sigma_z,$$  \hspace{1cm} (9) 

where $\Delta_0$ is the constant of local SO perturbation. The perturbation for the $K'$ points differs from (9) by the sign of $\Delta_0$. It should be noted that both the spin and sublattice index are
the good quantum numbers in this case. Using again the $T$-matrix method and performing the calculations similar to presented above we come to the following equations determining the spin polarized states belonging to the Dirac points $K$ and $K'$

$$
\varepsilon^K_{1,1} = \mp \Delta \mp 4\pi v^2 \left( \Delta_0 \ln \frac{v^2 k_{m}^2}{|\Delta^2 - \varepsilon_{1,1}^2|} \right)^{-1},
$$

(10)

$$
\varepsilon^{K'}_{1,1} = \pm \Delta \pm 4\pi v^2 \left( \Delta_0 \ln \frac{v^2 k_{m}^2}{|\Delta^2 - \varepsilon_{1,1}^2|} \right)^{-1}.
$$

(11)

**Figure 4.** The same dependences as in Fig. 1 in the case of spin-orbit interaction on impurity.

The results are presented in Fig. 4 as a function of $\Delta_0$. Here the constant $\Delta$ refers to the internal SO interaction like in the case considered in Sec. 2. The important point is that each of the states for a given Dirac point is spin polarized, but the spin degeneration is restored for both Dirac points.

5. Discussion

Spin-orbit interaction in graphene can be responsible for creation of a number of additional impurity states near the Dirac point. As we see from the results of calculations, in many cases they are resonance states in the continuum, which can affect substantially the electronic and magnetic properties of graphene. In this paper we considered the case of nonmagnetic impurity. Correspondingly, there is no net magnetization on the site. However, spin degeneracy is related to the presence of two nonequivalent Dirac points. It means that for a single Dirac point the impurity can be magnetically polarized. It can be used in the "valley electronics" [17] exploring the difference between the properties related to separated valleys. As we see, in the case under consideration, the valley electronics has exactly the same meaning as spin electronics because the localized electron spin is related to the certain Dirac point.

Acknowledgments

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