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Inter-band and intra-band reflections in graphene–insulator–superconductor junctions with zigzag or armchair edge

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ABSTRACT

We analyze electron–electron and Andreev reflections (**AR**) for a graphene–insulator–superconductor junction for *zigzag* and *armchair* edges, where the insulator is modeled as a potential barrier characterized by a strength. We calculate the reflection probabilities and differential conductance using the Bogoliubov–de Gennes–Dirac (BdGD) equations. For low doping values and *zigzag* edge the reflection coefficients have the same behavior that in a graphene–superconductor junction. However for high doping values the reflection probabilities have a periodicity of $\pi$with the strength barrier values. For high doping values and *armchair* edge the electron–electron reflections associated to $\mathbf{K}'$ valley increase and **AR** associated to **K** valley decrease. We compare our results with the differential conductance obtained by the Green formalism. We show that the effect of barrier strength for high doping resembles the behavior when a hopping between graphene and superconductor interfaces is considered.

1. Introduction

The graphene is a two-dimensional material recently discovered [1]. The graphene is made out of carbon atoms arranged in a hexagonal structure [2]. This material presents two types of edges, *zigzag* or *armchair*. These edges have been observed by using the scanning tunneling microscope (STM) technique [3]. One interesting feature of graphene is its electronic behavior, since it depends on the type of edge [2,4,5]. For instance, in the *zigzag* edges this material has surface states that are not present in the *armchair* edge [6]. Another feature of graphene is that it shows a conical spectrum without gap. Also, due to its particularities, this material has exhibited phenomena which have not been observed in the conventional condensed matter systems. One particular example is the Klein paradox, where the charge carriers can be transmitted with probability 1 through a barrier. This phenomenon has been studied across junctions based on graphene [7–9]. The signatures of Klein paradox were observed experimentally at a graphene heterojunction [10] via the conductance oscillations.

For this reason, such properties have been the subject of a number of works [4,10–13]. In particular, studies on the electric transport in **GS** junctions (**G**: graphene at state normal and **S**: graphene at state superconductor) have found specular Andreev reflections (Inter-band reflections) in contrast with Andreev retroreflection (Intra-band reflections) in conventional systems [14,15]. The Andreev reflections (**AR**) at an interface are fundamental quantum transport phenomena. For instance, they have been used to study the electric transport in other types of junctions such as **SGS** [16], **GIS** (**I**: insulator) [17,18] and **FIS** (**F**: ferromagnet) [19].

The works on transport in **GS** and **SGS** junctions considered a *zigzag* edge at the interface. In this paper we study the effect on differential conductance at a **GIS** junction with an insulating barrier. The insulating barrier is modeled by a Dirac delta function or as a finite potential barrier. We analyze different edges, *armchair* and *zigzag*, and show how the differential conductance depends on the edge and insulating barrier parameters. We compare the results obtained by means of Bogoliubov–de Gennes–Dirac (BdGD) equations and by Green's functions formalism.

2. Solutions for graphene

The Brillouin zone of graphene is a hexagonal structure, where in its spectrum can be distinguished two inequivalent corners **K** and $\mathbf{K}'$ [4]. The charge carriers in the vicinity of this corners obey the Dirac equation $H_\eta \psi^\eta = E\psi^\eta$, where $H_\eta = \vec{\sigma}_\eta \cdot \vec{p}_\eta$, with $\vec{\sigma}_\eta = (\eta\sigma_x, \sigma_y)$ where $\eta = \pm$ denote the $\mathbf{K}(\mathbf{K}')$ valley, $\sigma_{x(y)}$ are the

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Pauli matrices and $\vec{p}_\eta$ the momentum. In fact, the wave function $\psi^{\eta\dagger} = (\psi_A^\eta, \psi_B^\eta)^\dagger$ is a two-component spinor in the A–B space.

The graphene is not a natural superconductor. However, current measurements of the Josephson effect showed graphene at state superconductor via a proximity effect [20]. This state consists of Cooper pairs, therefore the dynamics of quasiparticles in this system can be described via the Bogoliubov–de Gennes–Dirac (BdGD) [14] equations with excitation energy E as

$$\begin{pmatrix} H_\eta - E_{FS} & \mathbf{\Delta} \\ \mathbf{\Delta}^* & E_{FS} - \tilde{H}_\eta \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = E \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}, \tag{1}$$

where $\mathbf{u}$ and $\mathbf{v}$ are the electron-like and hole-like quasiparticle amplitudes in the Nambu space, respectively. E_{FS} is the Fermi energy and $\tilde{H}_\eta = \tilde{\mathfrak{T}} H_\eta \tilde{\mathfrak{T}}^{-1}$ with $\tilde{\mathfrak{T}}$ being the time-reversal operator [14,15]. The pair potential $\mathbf{\Delta}$ couples electron and hole states in the same valley.[1]

We obtain graphene at normal state when the pair potential vanishes $\Delta = 0$. The solutions ψ in the x direction of the quasiparticles are

$$\mathbf{u} = \psi^e_{>(<)} \propto \begin{pmatrix} 1 \\ (-)e^{(-)i\alpha_e} \end{pmatrix} e^{\pm i k_e x},$$
$$\mathbf{v} = \psi^h_{<(>)} \propto \begin{pmatrix} 1 \\ (-)e^{(-)i\alpha_h} \end{pmatrix} e^{\pm i k_h x}, \tag{2}$$

where the subscript $e(h)$ denotes electron (hole), $>(<)$ denote quasiparticles with positive (negative) group velocity. $e^{i\alpha_{e(h)}} \equiv \hbar v_F (k_{e(h)} + iq)/E \pm E_F$, with $k_{e(h)} = (((E \pm E_F)/\hbar v_F)^2 - q^2)^{1/2}$, i.e., the energy has been measured with respect to Fermi level E_F in the graphene. We assume that $\psi(x,y) = e^{iqy}\psi(x)$.

The relation between *armchair* and *zigzag* edges is a rotation of 90° [21]. Therefore, the solution at $\mathbf{K}'$ valley is obtained with the relation k and q as

$$\begin{aligned} &Armchair \;\Rightarrow\; \{k \to -k \therefore e^{i\alpha} \leftrightarrow -e^{-i\alpha}, \\ &Zigzag \;\Rightarrow\; \{q \to -q \therefore e^{i\alpha} \leftrightarrow e^{-i\alpha}, \end{aligned} \tag{3}$$

where k and q are the wave numbers in the x and y directions respectively.

The solution in homogeneous superconductor with $\Delta = \Delta_0$ can be written as

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}_{qe_{>(<)}} \propto \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \otimes \psi^{qe}_{>(<)},$$
$$\begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}_{qh_{<(>)}} \propto \begin{pmatrix} v_0 \\ u_0 \end{pmatrix} \otimes \psi^{qh}_{<(>)}, \tag{4}$$

where u_0, v_0 are the BCS factors. The subscript qe and qh denote the electron-like (hole-like) quasiparticle with $|\mathbf{k}| > (<) k_F$. The functions $\psi^{qe,qh}_{>(<)}$ are given at (2), with the substitution $e^{\pm i\alpha_{e(h)}} \to e^{\pm i\alpha_{qe(qh)}} \equiv \hbar v_F (k_{qe(qh)} \pm iq)/(E_{FS} \pm \Omega)$, with $k_{qe(qh)} = (((E_{FS} \pm \Omega)/\hbar v_F)^2 - q^2)^{1/2}$ and $\Omega \equiv (E^2 - |\Delta_0|^2)^{1/2}$. Therefore the wave function of the quasiparticles at $\mathbf{K}$ valley is given as the superposition of spinors as

$$\begin{aligned} \Phi_S(x) = \Bigg\{ &\begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \otimes \psi^{qe}_{>} + \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \otimes \psi^{qe}_{<} \\ &+ \begin{pmatrix} v_0 \\ u_0 \end{pmatrix} \otimes \psi^{qh}_{>} + \begin{pmatrix} v_0 \\ u_0 \end{pmatrix} \otimes \psi^{qh}_{<} \Bigg\}. \end{aligned} \tag{5}$$

[1] In the wave vector space the electron and hole components of the quasiparticle are in the same valley $\mathbf{K}(\mathbf{K}')$, but in the momentum space the electron is in the valley with momentum $\hbar\mathbf{K}$ and the hole is in $\hbar\mathbf{K}' = -\hbar\mathbf{K}$.

3. Conductance at interface GIS

We considered a system, contained in the x–y plane, which consists of graphene at normal state at $x < 0$, an insulator (region **I**) at $0 \le x \le d$ and graphene in the superconducting state at $x > d$. The insulator is modeled as a potential barrier of width $d \to \xi_0$ and height V_0, the barrier is characterized by a dimensionless strength $\chi \equiv V_0 d/\hbar v_F$. Let us consider an electron incoming at the $\mathbf{K}$ valley from the graphene at normal state. It can be scattered as electron or hole in the same valley or as electron or hole in the inequivalent valley. The general solution is

$$\begin{aligned} \Phi_G(x) = e^{i\mathbf{K}x} \Bigg[&\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \psi^{e,+}_{>} + U_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \psi^{e,+}_{<} \\ &+ V_+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \psi^{h,+}_{>} \Bigg] + e^{-i\mathbf{K}'x} \Bigg[U_- \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \psi^{e,-}_{<} \\ &+ V_- \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \psi^{h,-}_{<} \Bigg], \end{aligned} \tag{6}$$

with $U_\pm$ and $V_\pm$ being the probability amplitudes of electron or hole reflection, respectively in the $\mathbf{K}(\mathbf{K}')$ valley.

From the probability amplitudes the normal reflection coefficient R_{e-e} and the Andreev reflection coefficient R_{e-h} in each valley are

$$R^{\pm}_{e-e} = |U_\pm|^2, \tag{7}$$

$$R^{\pm}_{e-h} = |V_\pm|^2 \left| \frac{\cos(\alpha_h)}{\cos(\alpha_e)} \right|, \tag{8}$$

Fig. 1 shows the reflection coefficients for a low and high doping value for the graphene. In this case we consider *zigzag* edge where the valleys are uncoupled $U_- = V_- = 0$, the insulating barrier V_0 is high (in comparison with doping) and $d \ll; \xi_0$, with ξ_0 being the BCS coherence length.

The electron–hole reflection coefficient is null when the excitation energy is equal to doping. This behavior is presented only when doping of graphene at normal state is $|E_F| \le \Delta_0$. For a low doping value the intra-band reflections appear for $E < E_F$ and the intra-band reflections appear for $E > E_F$. Since $\hbar v_F q \ll V_0, E_{FS}$, the angle of incidence on the superconductor is near to zero and in this case the Klein tunneling probability on the insulating barrier is near to one. For the case of high doping graphene the incidence angle increases and the probability of transmission through the insulating barrier decreases and therefore, the **AR** decreases also. The reflection coefficients are oscillatory with the change of strength χ, since its values are repeated for strength barrier $\chi = 0, \pi$.

For the *armchair* edge the incident electron can be reflected in the other valley, so $U_-, V_- \ne 0$. The reflection coefficients are shown in Fig. 2. In this case we consider Dirac insulating barrier ($d \to 0$ and $V_0 \to \infty$).

The reflection coefficients in $\mathbf{K}'$ valley are null when the insulator is transparent. For any doping, the electron–electron reflection coefficient in $\mathbf{K}$ decreases when the insulator strength increases. Therefore, the effect of the insulator is to increase the electron–electron reflection in $\mathbf{K}'$. In the inset of Fig. 2 we show the transition from intra-band reflections to inter-band reflections. The **AR** reflection coefficient decreases with the barrier strength, since the electron–electron reflections increases.

The differential conductance for a **GIS** junction in terms of reflection coefficients [22] is

$$\frac{G(\mathrm{eV})}{G_0} = \int dq \left\{ 1 - (|U_+|^2 + |U_-|^2) + (|V_+|^2 + |V_-|^2) \cdot \left| \frac{\cos(\alpha_h)}{\cos(\alpha_e)} \right| \right\}, \tag{9}$$