Andreev reflection in a proximity junction of graphene: Influence of a naturally formed $pn$ junction

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Abstract. We theoretically study the electron transport in a proximity junction made by partially covering a graphene sheet with a bulk superconductor. Such a system serves as a normal conductor–superconductor (NS) junction and its electron transport properties are mainly governed by Andreev reflection (AR). In this NS junction, the charge neutrality point (CNP) of graphene must spatially vary as a result of the penetration of excess carriers induced from the superconductor. By taking this into account in the electron-doped case, we calculate the differential conductance $G_{NS}$ of the graphene NS junction. Owing to the variation of the CNP in the uncovered region, a smooth $pn$ junction is naturally formed at the point where the Fermi energy crosses the CNP. The resulting $pn$ junction causes unusual behavior of $G_{NS}$. For example, a resonant peak structure appears in $G_{NS}$ reflecting the fact that quasi-bound states are created by the $pn$ junction.

1. Introduction

Andreev reflection (AR) is a scattering process in which an electron (hole) is reflected back as a hole (electron) [1]. This typically takes place at the interface between a normal conductor (N) and a superconductor (S). An anomalous feature of the AR is that a reflected particle traces back the path of an incident particle. This is referred to as retroreflection. As the AR process accompanies the transfer of two electrons across the interface, it greatly affects the conductance of an NS junction. Since nearly a decade ago, experimentalists have intensively studied the NS junction made by partially covering a graphene sheet with a superconductor [2, 3, 4, 5, 6, 7, 8, 9]. It has been theoretically predicted that, in the graphene NS junction, an incident electron can be reflected back as a hole in a specular manner [10].

In the graphene NS junction, the charge neutrality point (CNP) of graphene must spatially vary as a result of the penetration of excess carriers induced from the superconductor. Previous theoretical studies on the AR have assumed that the CNP uniformly shifts only in the covered region (i.e., S electrode) [10, 11, 12]. However, in actual situations, the CNP should vary even in the uncovered region (i.e., N electrode) over a screening length $\lambda$ from the NS interface [13]. By taking this into account in the electron-doped case, the present authors have studied the AR process in an NS junction of bilayer graphene [14]. It should be noted that, in the presence of the spatial variation of the CNP in the uncovered region, a smooth $pn$ junction [15, 16] is naturally formed at the point where the Fermi energy $E_F$ crosses the CNP [see Fig. 1(a)]. This
shows that quasi-bound states created by the *pn* junction give rise to resonant peaks in $G_{\text{NS}}$.

![Figure 1](image.png)

**Figure 1.** (a) Profile of the potential (the broken line) in a graphene NS junction. (b) Hexagonal lattice for a monolayer graphene sheet.

It is probable that these features of $G_{\text{NS}}$ are observed in a monolayer graphene system as well because a smooth *pn* junction can also be formed. However, it is unclear how they appear in a monolayer system as the transport properties of a *pn* junction are qualitatively different between the bilayer and monolayer cases. In this paper, we calculate $G_{\text{NS}}$ in the graphene NS junction and study how its features resemble or differ from between the bilayer and monolayer cases. We set $\hbar = 1$ hereafter.

### 2. Model

Let us introduce a graphene sheet of width $W$ infinitely long in the $x$-direction, where the region of $x > L$ is covered with a bulk superconductor. We assume that the potential $U(x)$ [see Fig. 1(a)], which determines the location of the CNP, is given by

$$
U(x) = \begin{cases}
-U_0 e^{(x-L)/\lambda} & \text{if } x \leq L, \\
-U_0 & \text{if } x > L,
\end{cases}
$$

where $U(x)$ vanishes in the asymptotic region of $x \leq 0$ if $L \gg \lambda$. The pair potential induced in a graphene sheet is assumed as $\Delta(x) = 0$ if $x \leq L$ and $\Delta(x) = \Delta_0$ if $x > L$. Quasiparticles are described by a tight-binding model [17, 18] on a hexagonal lattice [see Fig. 1(b)], in which the transfer integral between nearest neighbor sites is denoted by $\gamma_0$. By using the Bogoliubov–de Gennes equation in a tight-binding form [14], we consider the scattering problem for an electron with energy $E$ measured from $E_F$ incident to the NS interface from the asymptotic region. Imposing the periodic boundary condition in the $y$-direction, we specify the $y$ dependence of a wave function with a transverse wave number $q$. For any $q$, the number of conducting channels in the asymptotic region is 2 as there are two energy valleys. Using a recursive Green’s function technique, we can numerically determine the $2 \times 2$ Andreev reflection amplitude $r_A(E_F + E)$ and the $2 \times 2$ normal reflection amplitude $r_N(E_F + E)$. The differential conductance as a function of bias voltage $V$ is given by the Blonder–Tinkham–Klapwijk formula as [19, 20]

$$
G_{\text{NS}}(E_F + eV) = \frac{2e^2}{\pi \hbar} \frac{W}{a} g_{\text{NS}}(E_F + eV),
$$

where $a$ is the lattice constant and $g_{\text{NS}}$ is the dimensionless conductance per unit width:

$$
g_{\text{NS}}(E_F + eV) = \frac{k_F(E_F + eV) a}{2} \int_0^\pi d\phi \cos \phi \, \text{tr} \left\{ J_{12} + r_N^+ r_N + r_A^+ r_A \right\} \bigg|_{E_F + eV}.
$$
Here, $1_{2\times 2}$ is the $2 \times 2$ unit matrix, $k_F(E_F + eV)$ is the Fermi wave number, and $\phi = \arccos(q/k_F)$ is the angle of incidence. Details of numerical methods are given in Ref. [14] for the bilayer case.

3. Numerical results

We present the numerical results of $g_{NS}$ as a function of $eV$ for $E_F/\Delta_0 = 0.25$ and $-5.0$. The other parameters are $\gamma_0 = 3.16$ eV, $\Delta_0 = 1.2$ meV, $U_0 = 1.0$ eV, and $\lambda = 100$ or 400 nm. In the bilayer case, the interlayer transfer integral $\gamma_1$ is set equal to 0.39 eV.

Figure 2. $eV$ dependence of $g_{NS}(E_F + eV)$ at $E_F/\Delta_0 = 0.25$ with $\lambda = 100$ nm in the cases of (a) bilayer graphene and (b) monolayer graphene.

Figure 3. Trajectories of an incident electron and a reflected hole in the cases of (a) retroreflection ($E_F > eV \geq 0$) and (b) specular-reflection ($\Delta_0 > eV > E_F$). In the specular case, the reflected hole is diffracted by the $pn$ junction.

Figure 2 shows $g_{NS}(E_F + eV)$ in the bilayer and monolayer cases for $E_F/\Delta_0 = 0.25$ with $\lambda = 100$ nm. In Fig. 2(a) for the bilayer case, we observe that $g_{NS}$ shows an unusual asymmetric behavior [i.e., $g_{NS}(E_F + e|V|) \gg g_{NS}(E_F - e|V|)$] in the above gap region of $e|V| > \Delta_0$ [14]. This is caused by a naturally formed $pn$ junction, which reduces the transmission of an electron only when its energy (i.e., $E_F + eV$) is less than zero. Though this asymmetry is also observed in Fig. 2(b) for the monolayer case, it is weaker than that in the bilayer case. The reason for this is that, roughly speaking, the transmission probability of an electron through a $pn$ junction is larger in the monolayer case than in the bilayer case. Let us turn to the subgap region of $\Delta_0 > e|V|$, where retro AR takes place when $E_F > e|V| \geq 0$, while specular AR is expected to appear when $\Delta_0 > e|V| > E_F$ (see Fig. 3) [14]. In the bilayer case, $g_{NS}$ is much larger in the retroreflection regime than in the specular-reflection regime. This is simply explained by the fact that neither incident nor reflected particle passes through the $pn$ junction in the retroreflection regime, while one of them passes through it in the specular-reflection regime, resulting in the reduction of the AR probability. In Fig. 2(b) for the monolayer case, we do not observe clear difference of $g_{NS}$ between the retroreflection and specular-reflection regimes. This should be attributed to the nature of a $pn$ junction in the monolayer case that the transmission probability is not significantly reduced when the angle of incidence is small.

Figures 4 and 5 respectively show $g_{NS}(E_F + eV)$ in the bilayer and monolayer cases for $E_F/\Delta_0 = -5.0$. We observe that resonant peaks appear in $g_{NS}$ in both the bilayer and monolayer cases. These peaks directly reflect the appearance of quasi-bound states, which are created by
Figure 4. $eV$ dependence of $g_{NS}(E_F + eV)$ in the bilayer case for $E_F/\Delta_0 = -5.0$ with (a) $\lambda = 100$ nm and (b) 400 nm.

Figure 5. $eV$ dependence of $g_{NS}(E_F + eV)$ in the monolayer case for $E_F/\Delta_0 = -5.0$ with (a) $\lambda = 100$ nm and (b) 400 nm.

weak confinement potential due to the smooth $pn$ junction (see Fig. 6). As this potential depends on the details of junction parameters, the profile of resonant peaks significantly differs in each case.

Figure 6. Quasi-bound states are created between the $pn$ junction at $x = x_{pn}$ and the NS interface at $x = L$.

4. Summary
We studied the behavior of $G_{NS}$ in a graphene NS junction in the bilayer and monolayer cases by taking account of a naturally formed $pn$ junction. It was shown that, in the bilayer case, $G_{NS}$ is significantly reduced in the specular-reflection regime while such behavior does not appear in the monolayer case. It was also shown that $G_{NS}$ shows a resonant peak structure in both the bilayer and monolayer cases reflecting the appearance of quasi-bound states created by the $pn$ junction.
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