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The effects of impurity doping on the optical properties of biased bilayer graphene

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ABSTRACT

We address the optical conductivity of doped AA-stacked bilayer graphene in the presence of a finite bias voltage at finite temperature. The effect of scattering by dilute charged impurities is discussed in terms of the self-consistent Born approximation. Green's function approach has been implemented to find the behavior of optical conductivity of bilayer graphene within linear response theory. We have found the frequency dependence of optical conductivity for different values of concentration and scattering strength of dopant impurity. Also the dependence of optical conductivity on the impurity concentration and bias voltage has been investigated in details. A peak appears in the plot of optical conductivity versus impurity concentration for different values of chemical potential. Furthermore we find optical conductivity reduces with frequency for any impurity concentration and scattering strength.

1. Introduction

Graphene is a subject of numerous investigations motivated by its unique electronic and lattice properties interesting both conceptually and for applications [1–3]. Single layer graphene is two-dimensional crystalline form of carbon with a linear electronic spectrum and chiral symmetry, whose extraordinary electron mobility and other unique features hold great promise for nano-scale electronics and photonics.

Initial studies of graphene were limited to realm of theory where the low energy linear dispersion and chiral nature of the honeycomb carbon lattice were shown to result from a simple the nearest neighbor hopping tight binding hamiltonian which at low energy maps on to a Dirac Hamiltonian for massless fermions with Fermi velocity v_F.

With the experimental realization of grapehen [4], a considerable literature has now accumulated which has uncovered a variety of exotic effects, such as an unusual quantum Hall effect [5] giant faraday rotations [6], plasmarons, and so on, some of which has been summarized in reviews [7].

Bilayer graphene, which are made out of two graphene planes, has also been produced by the mechanical friction and motivated a lot of researches on their transport properties [8–10].

In contrast to the case of single-layer graphene (SLG) low energy excitations of the bilayer graphene has parabolic spectrum, although, the chiral form of the effective 2-band hamiltonian persists because the sublattice pseudospin is still a relevant degree of freedom. The low energy approximation in bilayer graphene is valid only for small doping $n < 10^{12}\ cm^{-2}$, while experimentally doping can obtain 10 times larger densities. For such a large doping, the 4-band model [11] should be used instead of the low energy effective 2-band model. Furthermore, an electronic band gap can be introduced in a dual gate bilayer graphene [10,11], and it makes BLG very appealing from the point of view of applications. It was shown theoretically [11,12] and demonstrated experimentally [13,14] that a graphene bilayer is the only material with semiconducting properties that can be controlled by electric field effect [15]. The size of the gap between conduction and valence bands is proportional to the voltage drop between the two graphene planes and can be as large as 0.1–0.3 e, allowing for novel terahertz devices [14] and carbon based quantum dots [16] and transistors [17]. Nevertheless, just as single layer graphene [18], bilayer graphene is also sensitive to the unavoidable disorder generated by the environment of the SiO_2 substrate: adatoms, ionized impurities, etc. Disorder generates a scattering rate τ and hence a characteristic energy scale $\hbar/\tau$ which is the order of the Fermi energy $E_F = \hbar v_F k_F$ ($k_F \propto \sqrt{n}$ is the Fermi momentum and n is the planar density of electrons) when the chemical potential is close to the Dirac point ($n \to 0$). Thus, one expects disorder to have a strong effect in the physical properties of graphene. Indeed, theoretical studies of the effect of disorder in unbiased [19]

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and biased [20] graphene bilayer show that disorder leads to strong modifications of its transport and spectroscopic properties. The understanding of the effects of disorder in this new class of materials is fundamental for any future technological applications.

The optical properties of graphene are of considerable importance for technological applications and all variants of graphene are also of potential interest and should be examined. The dynamical conductivity of graphene has been extensively studied theoretically [21] and experiments have largely verified the expected behavior [22]. The conductivity for Bernal-stacked bilayer graphene has been studied theoretically [23] and observed [24]. Some preliminary work on the absorption coefficient of undoped AA-stacked graphene in zero magnetic field has been reported [25] however most materials naturally occur with charge doping where the Fermi level is away from charge neutrality. Furthermore, the interesting feature for practical applications is the variation of optical properties with doping, usually achieved through a field effect transistor structure. The optical conductivity of a few-layer epitaxial graphite [26] and oriented pyrolytic graphite [27] in finite external magnetic field has been reported recently, as well as for graphene [28]. There have also been theoretical studies [29,30] of the conductivity, including discussions of optical sum rules [31] which continue to provide useful information on the electron dynamics. In the other theoretical work, frequency dependence of dynamical conductivity of AA-stacked bilayer graphene in the presence of electron doping has been calculated within Dirac approximation [32]. For in-plane response, AA-stacked graphene shows a Drude weight at charge neutrality along with Pauli blocking at low frequencies below the onset of a flat interband absorption.

In an experimental work the effects of both bias voltage and impurity doping on Raman spectrum and electrical resistivity have been studied [33]. In this experimental study the transport results presents a variable range hopping conduction near the charge neutrality point at low temperatures. Such results provide evidence for the impurity level inside the gap. Also magnetoresistance of biased bilayer graphene as a function of magnetic field has been studied. The electron-impurity scattering rate as a function of quasi particle energy for doped bilayer graphene has been theoretically calculated [34]. The results show that scattering rate for bilayer graphene enhance on increasing impurity concentrations. Also electron impurity scattering rate of bilayer graphene goes to a constant value for zero limit of quasi particle energy. The other theoretical works study the impurity levels and the effects of impurity doping on the local density of states in the gapped doped bilayer graphene [19,35–37].

In the present paper, we study the effects of site dilution or unitary scattering and bias voltage on the optical conductivity of AA-stacked graphene bilayer within the well-known self-consistent Born approximation(SCBA) [38–40]. This approximation allows for analytical results of electronic self-energies, allowing us to compute physical quantities such as spectral functions measured by angle resolved photoemission ARPES [41,8], and density of states scanning tunneling microscopy STM [42,43], besides standard transport properties such as the DC and AC conductivities. To ensure the applicability of SCBA, we restrict our calculations to relatively clean systems with low impurity concentrations. Optical conductivity of AA-stacked bilayer graphene as a function of impurity concentrations is calculated for different bias voltage and scattering potential strengths. We also study effects of impurity concentration and scattering potential strengths on the frequency behavior of optical conductivity.

2. Theoretical model and method

A bilayer graphene composed of two graphene single layers arranged in the simple stacking [17] has been considered. The optical properties of AA-stacked bilayer graphene have been calculated using the band structure and the electronic Green's function. For the case of AA-stacking, an A (B) atom in the upper layer is stacked directly above A(B) atom in the lower layer. An on-site potential energy difference between the two layers is included to model the effect of an external voltage. In the presence of impurity, the Hamiltonian consists of two parts: $H = H_0 + H_{imp}$. Without of magnetic field or magnetic impurities, the two spin flavors are degenerate. For AA-stacking and under the nearest neighbor approximation, the single spin free part of model hamiltonian is given by Ref. [44,45].

$$H = \sum_{\mathbf{k}} \phi^{\dagger}_{\mathbf{k}} H_0(\mathbf{k}) \phi_{\mathbf{k}}, \tag{1}$$

in which the vector of fermion creation operators is defined as $\phi^{\dagger}_{\mathbf{k}} = (a^{\dagger}_{1,\mathbf{k}}, b^{\dagger}_{2,\mathbf{k}}, a^{\dagger}_{2,\mathbf{k}}, b^{\dagger}_{1,\mathbf{k}})$. $a^{\dagger}_{l,\mathbf{k}}$, $b^{\dagger}_{l,\mathbf{k}}$ create l layer states with wave vector $\mathbf{k}$ on the A and B sublattice, respectively. The nearest neighbor approximation gives us the following matrix form for $H_0(\mathbf{k})$ as

$$H_0(\mathbf{k}) = \begin{pmatrix} V/2 & 0 & t_{\perp} & f(\mathbf{k}) \\ 0 & V/2 & f^*(\mathbf{k}) & t_{\perp} \\ t_{\perp} & f(\mathbf{k}) & -V/2 & 0 \\ f^*(\mathbf{k}) & t_{\perp} & 0 & -V/2 \end{pmatrix}. \tag{2}$$

$f(\mathbf{k}) = -t_{\parallel}(1 + exp(i\mathbf{k}.\mathbf{a}_1) + exp(i\mathbf{k}.\mathbf{a}_2))$ describes the intralayer nearest neighbor hopping with strength $t_{\parallel}$. Furthermore the primitive vectors of the triangular sublattice presented in Fig. 1 have property $|\mathbf{a}_1| = |\mathbf{a}_2| = \sqrt{3}a_{cc}$ that $a_{cc} = |\mathbf{a}_{01}| = |\mathbf{a}_{02}| = |\mathbf{a}_{03}|$ is the nearest carbon–carbon distance. The hopping parameter between an A (B) site in one layer and the nearest A(B) site in the other layer is given by $t_{\perp}$ and is reported to be about 0.2 eV [46,47]. V is the potential energy difference between the first and second layers induced by a bias voltage. Since for every attainable carrier density, it is possible to find a bias voltage to make the potential difference between the two layers as V, we would not consider the Coulomb interaction between imbalanced electron densities of the two layers and also neglect the dependence of V on the carrier density n in this work.

Impurity scattering effects are included in the tight-binding description by the addition of a local energy term

$$H_{imp} = \sum_{\mathbf{q}} v_i \left(a^{\dagger}_{1,\mathbf{q}} a_{1,\mathbf{q}} + b^{\dagger}_{1,\mathbf{q}} b_{1,\mathbf{q}} + a^{\dagger}_{2,\mathbf{q}} a_{2,\mathbf{q}} + b^{\dagger}_{2,\mathbf{q}} b_{2,\mathbf{q}} \right), \tag{3}$$

where v_i is the electron-impurity potential at site $\mathbf{R}_i$. This term breaks the translational symmetry of crystal so that it introduces the scattering of electrons from impurities situated at randomly distributed but fixed positions. Under half filling constraint

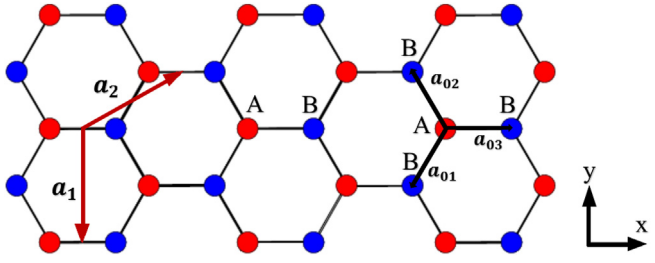

Fig. 1. The structure of honeycomb structure is shown. The light dashed lines denote the Bravais lattice unit cell. Each cell includes two nonequivalent sites, which are indicated by A and B. a_1 and a_2 are the primitive vectors of unit cell. a_{01}, a_{02} and a_{03} are three vectors that connect nearest neighbor sites.