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Magnetic field effects on charge structure factors of gapped graphene structure

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ABSTRACT

We present the behaviors of dynamical and static charge susceptibilities of undoped gapped graphene using the Green's function approach in the context of tight binding model Hamiltonian. Specially, the effects of magnetic field on the plasmon modes of gapped graphene structure are investigated via calculating correlation function of charge density operators. Our results show the increase of magnetic field leads to disappear high frequency plasmon mode for gapped case. We also show that low frequency plasmon mode has not affected by increase of magnetic field and chemical potential. Finally the temperature dependence of static charge structure factor of gapp graphene structure is studied. The effects of both magnetic field and gap parameter on the static structure factor are discusses in details.

1. Introduction

Graphene is a two-dimensional crystal of carbon atoms has been recently discovered [1,2]. This stable crystal has attracted considerable attention because of its unusual effective many-body properties has attracted a great deal of interest and acts as new material for electronic technology [3,4]. Graphene consists of a single atomic layer of graphite, which can also be viewed as a sheet of unrolled carbon nanotube. Several anomalous phenomena ranging from half integer quantum Hall effect, nonzero Berry's phase [5], to minimum conductivity [2] have been observed in experiments. The discovery of graphene in 2004 [2], and its fabrication into a field-effect transistor [2], has opened up a new field of physics and offers exciting prospects for new electronic devices and apprantly possible to come over those aforementioned limitations. Graphene is itself a good thermal conductor such that graphene's thermal conductivity is about 5.3×10^3 W/mK at room temperature which is greater than the thermal conductivity of carbon nanotubes [6]. Interstingly, the mobility of carriers in graphene is quite high and it is about 10^5 cm^2/Vs at room temperature [7]. Providing capability to control a type and density of charge carriers by gate voltage or by the chemical doping made graphene instructive for novel nano-electronic devices. However, a gapped semiconducting behavior would be more suitable for electronic applications. There have been some proposed in literature for a gap generation in graphene due to breaking of sublattice symmetry by some substrates [8], to adsorbe some molecules [9], spin-orbit interaction and finite size effect [10]. Finite size effect by using graphene nanoribbons give rise to constriction of the electrons in the ribbon and it depends on the detailed structure of ribbon edges. Importantly, edge effects plays a crucial role in transport properties. The gap engineering can be also achieved through doping the graphene with chemical species [3].

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Another scenario is graphene by placing it on top of an appropriate substrate which breaks the graphene sublattice symmetry and, therefore generates an intrinsic Dirac mass for the charge carriers [8]. The gap can be generated dynamically by applying a magnetic field [11]. Moreover, when both mono and bilayer graphene material are covered with water and ammonia molecules, a gap induce in the spectrum [9].

In order to study electronic properties of electron gas in the nano structures and graphene, the dynamical polarizability whereby the screening effects have been found is required [12,13]. The static structure factor at fermi wave vactor that gives the Thomas-Fermi screening length is important for transport properties of two dimensional graphene [14,15]. The dynamical polarizability renormalizing the phononic Green's function can explain the phonon softening and Kohn anomlay phenomenon [16] at the Γ point. So far, the extensive studies have been performed on the charge response function of monolayer Graphene in the Dirac cone approximation so that the energy dispersion of the hexagonal lattice is considered to be linear form in terms of electronic wave vector. The chirality and a Berry phase of π at the two Dirac points provide an environment for highly unconventional and fascinating two-dimensional electronic properties such as the absence of backward scattering [17,18], Klein tunneling [4] and the π phase shift of the shubinkov-de Haas oscillations [19].

A semi-analytical expression for the dynamical density-density linear response function of doped graphene sheet within Dirac approximation at finite temperature has been performed [20]. Their results demonstrated the fluctuations of density in bilayer case can present either single-component massive-chiral character or standard two layer character, depending on energy and doping. In the calculation of high energy corrections to the charge and spin response, both inter and intraband transitions contribute to the frequency behavior of dynamical polarizability. Recently a theoretical work provides a study of both imaginary and real part of non-interacting polarizability of graphene within an analytical approach [21]. The authors found there is no noticeable angle dependence for imaginary part of polarizbility around the van Hove singularity, i.e, $\hbar\omega/t = 2.0$ where t implies nearest neighbor hopping integral. Also it has been shown the Dirac approximation has a good agreement with the analytical expression for imaginary part of charge response in low frequency region [21]. In a theoretical work, the paramagnetic susceptibility of zigzag graphene nanoribbons has been calculated [22]. Because the edge states lead to a sharp peak in the density of states at the Fermi level, the graphite ribbons with zigzag edges show Curie-like temperature dependence of the Pauli paramagnetic susceptibility [22].

The goal of this work is to study the effects of magnetic field and gap parameter on plasmon frequencies of undoped graphene sheet at finite temperature. In order to obtain these collective modes, we study the magnetic field and gap parameter dependence of dynamical charge susceptibility as a function of frequency in the context of tight binding model Hamiltonian. The frequency positions of sharp peak in dynamical charge susceptibility introduces the plasmonic oscillations of the mentioned nanostructure. Furthermore the temperature dependence of static charge susceptibility of gapped graphene due to variation of magnetic field has been studied. Green's function approach has been implemented to calculate the charge susceptibility, i.e. the time ordered charge density correlation. In the last section we discuss and analyze our results to show how external magnetic field and gap parameter affect the frequency of collective modes. Also we study the effect of chemical potential associated with electronic concentration on the frequency behavior of dynamical charge susceptibility. Moreover temperature dependence of static structure factor has been analyzed due to chemical potential variations.

2. Theoretical formalism

The honeycomb lattice structure consists two types of sublattices A and B as shown in Fig. 1. The unit cell contains A-type atoms and B-type atoms. This model has been successfully used for the calculation of electronic states of fullerene molecules, carbon nanotubes, and other carbon-related materials. In the absence of magnetic field, the dynamics of noninteracting π electrons with spin σ on the honeycomb lattice as gapped graphene structure can be described by the following tight binding model

$$H = -t\sum_{\langle ij\rangle,\sigma}\left(a^{\dagger}_{i,\sigma}b_{j,\sigma} + b^{\dagger}_{i,\sigma}a_{j,\sigma}\right) + \Delta\sum_{i,\sigma}a^{\dagger}_{i,\sigma}a_{i,\sigma} - \Delta\sum_{i,\sigma}b^{\dagger}_{i,\sigma}b_{i,\sigma}. \tag{1}$$

$a_{i,\sigma}(b_{i,\sigma})$ annihilates an electron with spin σ on sublattice A(B) of unit cell i and $t \approx 2.9eV$ implies the nearest neighbor hopping integral. The sum $\langle i,j\rangle$ in Eq. (1) runs over distinct nearest neighbors. The band gap, 2Δ has a nonzero value as a result of breaks the symmetry between sublattices, A and B. According to Fig. 1 the lattice structure of graphene is shown and the primitive unit cell vectors are given by

$$\mathbf{a}_1 = a/2\left(\mathbf{j} + \sqrt{3}\,\mathbf{i}\right), \mathbf{a}_2 = a/2\left(-\mathbf{j} + \sqrt{3}\,\mathbf{i}\right), \tag{2}$$

where a is the length of lattice translational vector. We consider unit vector $\mathbf{j}$ along armchair direction. In terms of Fourier transformation of electronic operators, the hamiltonian in Eq. (1) gets the following form within nearest neighbor approximation