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Optical properties of gapped graphene structure driven by electron electron interaction

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AUTHOR-HIGHLIGHTS

- Theoretical calculation of density of states of boron nitride monolayer in the context of Holstein model.
- The investigation of density of states versus electron–electron interaction.
- The investigation of optical conductivity versus photon energy.

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ABSTRACT

We analyze the effects of on-site electronic coulomb repulsion U on the optical absorption and density of states of a graphene like structure with two different sublattice on-site energies in the context of Hubbard model. Mean field approximation has been implemented in order to find excitation spectrum of electronic system. Antiferromagnetic long range ordering has been considered as the ground state of model Hamiltonian. We find that the band gap in both optical conductivity and density of states decreases with strength of coulombic interaction. The absorption spectra of the graphene like structure as a nanoscale system exhibit the prominent peaks, mainly owing to the divergent density of states and excitonic effects.

1. Introduction

The interest in strongly correlated frustrated lattices has increased recently because of the possible realization of exotic magnetic states [1], spin and charge separation in two dimensions [2], and the discovery of superconductivity [3]. The honeycomb lattice, which is made of two interpenetrating triangular lattices, has been shown to stage many different types of exotic physical behaviors in magnetism and the growing experimental evidence of non-Fermi liquid behavior in graphene like structure has led to the study of electron–electron correlations and quasiparticle lifetimes in graphite [4]. Graphene [12] is a semimetal with a linear crossing of the π and π* bands at the K-point of the Brillouin zone. Among these nanoscale systems that present interesting optoelectronic properties, one can point to the systems with electronic energy gap. The role of coulomb interactions in graphene and related materials can be expected to be a significant factor in appearance of magnetic ordering [5,6]. From the theoretical side, an antiferromagnetic insulating ground state has been obtained for the local coulomb interactions exceeding a critical values $U_{AF} > (4.5 \pm 0.5)t$ within quantum Monte Carlo calculations [7] and $U_{AF} > (2.2)t$ in Hartree–Fock theory [8] where t is the nearest neighbor hopping parameter. In other hands, the electronic spectrum of tight binding model Hamiltonian on the honeycomb lattice can be modified via many perturbations [9]. From applications point of view, it is important to open up a gap in the spectrum by lowering the symmetry of the nearest neighbor tight binding Hamiltonian. For example the substrate can induce a sublattice symmetry breaking, e.g. by considering an difference between two on-site energy sublattices. This difference leads to a charge gap in the spectrum of single-particle excitations. Also *ab-initio* estimates of the strength of the Hubbard U in graphene suggest that the on-site coulomb repulsion is quite remarkable, ≈ 10 eV [10]. Therefore it is important to consider both the single particle gap parameter and the Hubbard parameter U on the electronic and optical properties of graphene like structure. Dynamical mean field approach has been employed to study the effect of on-site electron correlation on the gapped graphene structure[11]. For a fixed gap parameter, the charge gap in the

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spectrum closes beyond a critical value U_{c1}. Further increasing U beyond U_{c2}, another phase transition to the Mott insulating state takes place. In the other theoretical work, the magnetic phases of the Hubbard model on the honeycomb lattice have been studied [22]. The critical lines associated with instabilities of the paramagnetic phase are obtained in the interaction and particle density plane. The optical properties of related materials to the graphene structure such as hexagonal boron nitride (BN) monolayer have been investigated experimentally [13] and theoretically within random phase approximation (RPA) [14]. Moreover, BN monolayer has regained interest due to the discovery of BN-nanotubes [15,16] which can be constructed by rolling a single layer of BN onto itself. The RPA optical absorption spectra for two dimensional single sheet are very similar to that for the quasi one dimensional tubes [17]. This result has been obtained for light polarization parallel to the layer plane and tube axis. Also optical absorption of BN ribbons and nanotubes has been discussed within gradient approximation of tight binding model [18]. It has been shown that the number of absorption peaks and the excitation energies strongly depend on the geometry structure. GW approximation and Bethe–Salpeter calculations as many quantum particle approaches has been implemented in order to explain the nature of the electronic energy gap and optical absorption spectrum of carbon BN monolayers [19]. An efficient implementation of the Bethe–Salpeter equation in the projector augmented wave method GAPW for optical properties of hexagonal BN has been applied [20]. In this work, the effect of intersite coulombic repulsion between electrons on the band gap and optical absorption spectra for electrons on the honeycomb lattice is studied in a pure theoretical frame. In order to study problem generally, a difference between on-site energy for two different sublattice sites has been considered. Mean field approximation has been implemented to obtain electronic excitation spectrum at low values for local coulomb interaction (U). The sublattice antiferromagnetic long range ordering is considered as the ground state of model Hamiltonian. We find that the increase of local Hubbard interaction between electrons leads to decrease of the width of optical and band gaps of the structure. The height of the peaks in optical spectrum decreases with Hubbard coulomb interaction parameter. On the other hand, the existence of two peaks in the optical spectrum structure is of novel properties of our results. Based on the quantum many particle methods, theses two peaks of optical spectrum are related to the excitonic effects [13].

2. Model Hamiltonian and density of states

In order to find the electronic properties of the honeycomb lattice due to coulombic repulsion between electrons, we consider Hubbard model to describe the dynamics of tight binding electrons on a bipartite lattice (sublattices A, B) as

$$H=(\epsilon_{0A}-\mu)\sum_{i,\sigma}a^{\dagger}_{i,\sigma}a_{i,\sigma}+(\epsilon_{0B}-\mu)\sum_{i,\sigma}b^{\dagger}_{i,\sigma}b_{i,\sigma}-t\sum_{i,j,\sigma}(a^{\dagger}_{i,\sigma}b_{j,\sigma}+h.c.)$$
$$+U\sum_{i}a^{\dagger}_{i,\uparrow}a_{i,\uparrow}a^{\dagger}_{i,\downarrow}a_{i,\downarrow}+U\sum_{i}b^{\dagger}_{i,\uparrow}b_{i,\uparrow}b^{\dagger}_{i,\downarrow}b_{i,\downarrow}, \quad (1)$$

where $a_{i,\sigma}(b_{i,\sigma})$ implies the annihilation operator of electrons with σ at ith unit cell at the sublattice sites $A(B)$. Also $a^{\dagger}(b^{\dagger})$ denotes the corresponding creation operators. Furthermore ϵ_{0A}, ϵ_{0B} are the on-site energies of two different sublattice atoms. U and t are the Hubbard repulsion and the nearest neighbor hopping integral, respectively. The chemical potential is chosen to be $\mu=U/2$, so that the average occupancy is $(\langle n_A\rangle+\langle n_B\rangle/2=1)$. Fig. 1 shows the crystal structure of honeycomb lattice with two different sublattices. According to Fig. 1, the primitive unit cell vectors of

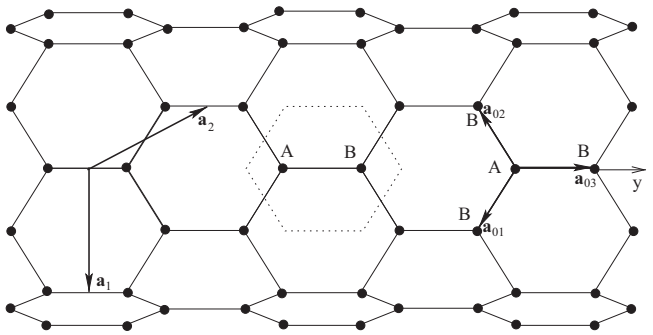

Fig. 1. The honeycomb lattice structure with two sublattices, A, B. The light dashed lines denote the Bravais lattice unit cell. Each cell includes two nonequivalent sites, which are indicated by A and B. $\mathbf{a}_1$ and $\mathbf{a}_2$ are the primitive vectors of unit cell. $\mathbf{a}_{01}$, $\mathbf{a}_{02}$ and $\mathbf{a}_{03}$ are three vectors that connect nearest neighbor sites.

honeycomb lattice are given by

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

where $a\approx 1.42$ Å is the length of unit cell vector and is considered to be one. Moreover a_{01}, a_{02} and a_{03} are the bonding lengths of two nearest neighbor atoms. In an antiferromagnetic long range ordering as a broken state, we describe the average lattice site occupation as $\langle n_{i,\sigma}\rangle=(n\pm m\sigma)/2$, where the positive sign is regarded to sublattice A and negative one is related to sublattice B. Also n denotes the electron density and m is the staggered magnetization and $\sigma=\pm 1$. The Fourier transformation of field operators for each sublattice is defined by

$$a_{i,\sigma}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}e^{i\mathbf{k}.\mathbf{R}_i}a_{\mathbf{k},\sigma},\quad b_{i,\sigma}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}e^{i\mathbf{k}.\mathbf{R}_i}b_{\mathbf{k},\sigma}, \quad (3)$$

where N denotes the number of unit cells. Using mean field approximation or Hartree–Fock approach, two particle parts of model Hamiltonian are transformed as one particle operator. After replacing the Fourier transformation of each operator into Eq. (1) and implementing mean field theory, the final result for Hubbard model Hamiltonian is given by [22]

$$H=\sum_{\mathbf{k},\sigma}(\alpha_{\mathbf{k},\sigma}a^{\dagger}_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma}+\beta_{\mathbf{k},\sigma}b^{\dagger}_{\mathbf{k},\sigma}b_{\mathbf{k},\sigma}+\phi(\mathbf{k})a^{\dagger}_{\mathbf{k},\sigma}b_{\mathbf{k},\sigma}+\phi^{*}(\mathbf{k})a^{\dagger}_{\mathbf{k},\sigma}b_{\mathbf{k},\sigma}), \quad (4)$$

with coefficients given by

$$\alpha_{\mathbf{k},\sigma}=\epsilon_{0A}-\mu+U\frac{n-\sigma m}{2},\quad \beta_{\mathbf{k},\sigma}=\epsilon_{0B}-\mu+U\frac{n+\sigma m}{2}$$
$$\phi(\mathbf{k})=1+\cos(k_x/2)\exp(-ik_y\sqrt{3}/2). \quad (5)$$

Diagonalization of the model Hamiltonian introduced in Eq. (5) leads to the band spectrums for electrons with spin σ as

$$E_{n=-(+),\sigma}(\mathbf{k})=\frac{Un+\epsilon_{0B}+\epsilon_{0A}-2\mu}{2}(+)\sqrt{\left(\frac{mU\sigma+\epsilon_{0A}-\epsilon_{0B}}{2}\right)^2+|\phi(\mathbf{k})|^2}. \quad (6)$$

Also band wave functions for each spin σ are obtained by

$$\psi^{\sigma}_{n,\mathbf{k}}(\mathbf{r})=\frac{1}{\sqrt{N}}\sum_{\mathbf{R},\alpha=A,B}e^{i\mathbf{k}.\mathbf{R}}\mathcal{C}^{\sigma}_{n,\alpha}(\mathbf{k})\phi_{\alpha}(\mathbf{r}-\mathbf{R}), \quad (7)$$

where ϕ_{α} implies Wannier wave function of electron for the atom in the unit cell with position R and for sublattice $\alpha=A,B$. The expansion coefficients $\mathcal{C}^{\sigma}_{n,\alpha}$ are given by

$$\mathcal{C}^{\sigma}_{+(-),A}=\frac{1}{\sqrt{1+(\zeta^{\sigma}_{+(-)})^2}},\quad \mathcal{C}^{\sigma}_{+(-),B}=\frac{\zeta^{\sigma}_{+(-)}}{\sqrt{1+(\zeta^{\sigma}_{+(-)})^2}}$$
$$\zeta^{\sigma}_{+(-)}=\frac{-\phi^{*}_{\mathbf{k}}}{\frac{Um\sigma-\epsilon_{0B}+\epsilon_{0N}}{2}-(+)\sqrt{\left(\frac{mU\sigma+\epsilon_{0N}-\epsilon_{0B}}{2}\right)^2+|\phi_k|^2}}. \quad (8)$$

The density of states for honeycomb lattice due to magnetic long