Physica E 61 (2014) 48–52

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

The effect of local electronic interaction on the optical properties of boron–nitride nanotubes

H. Rezania *

Department of Physics, Razi University, Kermanshah, Iran

AUTHOR-HIGHLIGHTS

- Theoretical calculation of optical conductivity of boron nitride nanotubes in the context of Hubbard model.
- The investigation of frequency dependent on optical conductivity versus electron electron coupling strengths.
- The investigation of optical conductivity for different values of chemical potential.

ARTICLE INFO

Article history:
Received 17 November 2013
Received in revised form
27 January 2014
Accepted 13 March 2014
Available online 21 March 2014

Keywords:
Boron–nitride
Optical conductivity
Hubbard model
Green's function

ABSTRACT

We investigate the behavior of optical absorption of boron–nitride nanotubes (6,0) in the context of Hubbard model at the paramagnetic sector. GW approximation has been implemented in order to make self-energy matrix of electronic system. Afterwards, the real and imaginary parts of transverse dielectric functions have been obtained using linear response theory. The results show that the frequency gap in the optical absorption decreases with Coulomb repulsion strength. Moreover the results show that the local Coulomb interaction leads to the appearance of the excitonic effects in the optical spectrum. Finally the effects of electronic concentration on the frequency behavior of imaginary part of dielectric function have been investigated.

1. Introduction

Briefly after the discovery of carbon nanotubes (CNTs) [1,2], and based on the similarities among graphite and other sp^2-like bonded materials, the existence of boron–nitride nanotubes (BNNTs) was theoretically predicted [3,4] and experimentally realized in the following year [5]. BNNTs are structurally similar to carbon nanotubes, thus they exhibit extraordinary mechanical properties like CNTs [6,7]. In contrast to the CNTs, the electronic properties of BNNTs are nearly independent of the tube diameter, chirality and whether the nanotube is single-walled, multi-walled or packed in bundles [3,4]. The theoretical calculations have predicted the band gap of BNNTs around ≈ 5 eV and can be eliminated by transverse electric fields through the giant DC stark effect [8].

The interesting mechanical, thermal and optical properties lead to apply the BNNTs in nanotechnology extensively. The elastic properties of an individual BNNT have been carefully studied by thermal vibration method [9]. Also various calculation approaches, including tight binding method, density functional theory, have been predicted such that BNNTs would have a larger low-temperature thermal conductivity than CNTs given that BNNTs have the same phonon mean free path as CNT [10,11]. Optical spectroscopies such as photon absorption and reflectance measurements are widely used for nanomaterial characterization. The photoelectric effect is one of the interesting cases of optical properties. This effect appears when unpolarized light can induce a shift current in BNNTs with a direction along the tube axis [12]. Local density approximation has shown that the optical band gap is independent of the chirality like the density of states case [13]. Nowadays, the synthesis and characterization of two dimensional materials with finite energy gap has been performed in order to use in optoelectronic devices [14,15]. Among these nanoscale systems that present interesting optoelectronic properties, one can point to the systems with electronic energy gap. The optical properties of hexagonal boron nitride have been investigated experimentally [16] and theoretically within random phase approximation(RPA) [17]. 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. An efficient implementation of the

* Tel./fax: +98 831 427 4556.
E-mail address: rezania.hamed@gmail.com

http://dx.doi.org/10.1016/j.physe.2014.03.014
1386-9477/

Bethe–Salpeter equation in the projector augmented wave method GAPW for optical properties of hexagonal BN has been applied [19]. For the two dimensional systems of graphene and hexagonal BN (h-BN), this method show that the results of optical gap of h-BN are in good agreement with the other many body approaches.

The results for the optical spectrum of single wall carbon and boron nitride nanotubes have been obtained by time dependent density functional theory [22]. The results of this method are relevant for the interpretation of data obtained by recent experimental tools for nanotube characterization such as optical and fluorescence spectroscopies. Going beyond the simplistic picture of independent electrons and using the techniques of many body perturbation theory, optical absorption is shown to be strongly dominated by excitonic effects. The influence of excitonic effects in CNTs was recently shown [23]. The effect of on-site Coulomb repulsion between electrons on the transition from insulator phase to correlated metallic leads to the appearance the excitonic effect in the optical spectrum of BNNTs. The *ab-initio* calculations predicted that the strength of the Hubbard U in graphene like structures such as BNNT is quite remarkable [24]. It is well known that many-body effects play a crucial role in low-dimensional nanostructures [23,25]. Both *ab initio* calculations and experiments have shown that excitonic effects due to electron–hole interaction dramatically alter the optical properties of low dimensional structures, such as carbon nanotubes [26] and boron nitride nanotubes [27]. The effects of intrinsic defects on the electronic density of states of BNNT have been investigated [28]. These defects or substitutional impurities lead to scattering of electrons. The results of the work for band structure of disordered BNNT show that the presence of such defects affects the band structure of the BNNT.

In the present work, the effect of Coulombic repulsion between electrons on the optical properties of zigzag BNNT (6,0) is studied in the context of Hubbard model. We have implemented Green's function approach to calculate optical absorption spectrum of zigzag BNNT (6,0). In order to correct electronic Green's function, self-energy is calculated within GW approximation [29]. Both real and imaginary parts of transverse dielectric function, as optical properties of the compound, have been obtained using linear response theory. Also, frequency behavior of optical absorption due to electron doping has been investigated.

2. Model Hamiltonian and Green's functions

In order to find the effect of Coulombic repulsion between electrons on the electronic properties of the BNNT, the dynamics of tight binding electrons on a honeycomb lattice as a bipartite case with two different sublattices A, B is discussed within Hubbard model as

$$H=(\epsilon_{0N}-\mu)\sum_{i,\sigma}c_{i,A}^{\sigma\dagger}c_{i,A}^{\sigma}+(\epsilon_{0B}-\mu)\sum_{i,\sigma}c_{i,B}^{\sigma\dagger}c_{i,B}^{\sigma} -t\sum_{i,j,\sigma,\alpha,\beta}(c_{i,\alpha}^{\sigma\dagger}c_{j,\beta}^{\sigma}+h.c.)+U\sum_{i}\rho_{i,\alpha}^{\uparrow}\rho_{i,\beta}^{\downarrow}, \quad (1)$$

where $c_{i,A(B)}^{\sigma}$ implies the annihilation operator of electrons with spin σ on ith unit cell at the sublattice sites $A(B)$ including nitrogen (boron) atoms. Also $a^{\dagger}(b^{\dagger})$ denotes the corresponding creation operators. Furthermore ϵ_{0N} and ϵ_{0B} denote the on-site energies of nitrogen and boron, respectively. Also U and t are the Hubbard repulsion and the nearest neighbor hopping integral, respectively. $\rho_{i,\alpha}^{\sigma}=c_{i,\alpha}^{\sigma\dagger}c_{i,\alpha}^{\sigma}$ is the density operator of electrons on the lattice unit cell i and sublattice α with spin σ. μ refers to the chemical potential of electronic system. In the half filling case, i.e. population of electrons on each site equals to one, chemical potential is chosen to be $U/2$. The crystal structure of honeycomb lattice with two different sublattices is shown in Fig. 1. The nearest neighbor unit cells are connected to each other via following vectors:

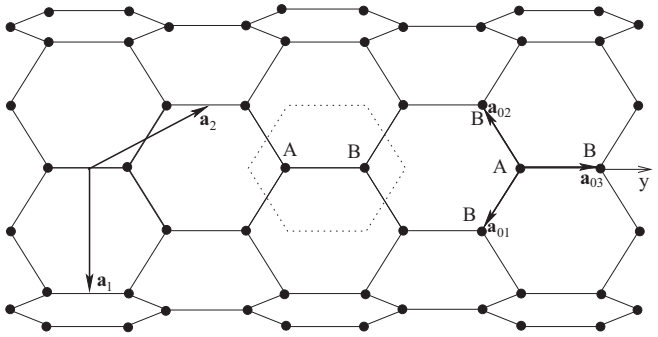

Fig. 1. The lattice structure of BN nanotube where nitrogen and boron sit on the sites A and B, respectively. The light dashed lines denote the Bravais lattice unit cell. Each cell includes two nonequivalent sites, which are indicated by A and B. $\mathbf{a}_1$ and $\mathbf{a}_2$ are the primitive vectors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

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

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 boron and nitrogen. Moreover $\mathbf{i}$ and $\mathbf{j}$ are unit vectors along x and y directions, respectively. According to Fig. 1, the direction of axes of zigzag CNT is assumed to be along axis y. Here, periodic boundary condition along circumference of BBNT, that is perpendicular to the BNNT axis, implies

$$e^{ik_xL}=1,\quad L=2\pi R, \quad (3)$$

where R is the BNNT radius. For a zigzag BNNT $(m,0)$, wave vector k_x is quantized as $k_x=2\pi l/am$, where a is the length of primitive vectors and l is the integer number. Since wave vector $\mathbf{k}$ belongs to the first Brillouin zone, l should be determined based on constraint $-4\pi/3<k_x<4\pi/3$. It is clear that, for each index m which is corresponding to BNNT radius, there are various l.

The Fourier transformation of annihilation operators for each sublattice is defined by

$$a_{i,\sigma}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{R}_i}a_{\mathbf{k},\sigma},\quad b_{i,\sigma}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{R}_i}b_{\mathbf{k},\sigma}, \quad (4)$$

where N denotes the number of unit cells. Using Eq. (4), the noninteracting part of model Hamiltonian gets the following form in terms of Fourier transformation of electronic operators:

$$H=\sum_{\mathbf{k},\sigma}((\epsilon_{0N}-\mu)a_{\mathbf{k},\sigma}^{\dagger}a_{\mathbf{k},\sigma}+(\epsilon_{0B}-\mu)b_{\mathbf{k},\sigma}^{\dagger}b_{\mathbf{k},\sigma} +\phi(\mathbf{k})a_{\mathbf{k},\sigma}^{\dagger}b_{\mathbf{k},\sigma}+\phi^{*}(\mathbf{k})a_{\mathbf{k},\sigma}^{\dagger}b_{\mathbf{k},\sigma}), \quad (5)$$

such that the off-diagonal element is given by

$$\phi(\mathbf{k})=1+\cos(k_x/2)e^{-ik_y\sqrt{3}/2}. \quad (6)$$

From now on, the spin index σ has not been shown at all spin dependent parameters. It is expected to be reasonable because of paramagnetic phase of BNNT. Because there are two sublattices, Matsubara Green's function is a 2×2 matrix whose each element is given by

$$G_{\alpha\beta}^{(0)}(k,i\omega_n)=-\int_0^{\beta}e^{i\omega_n\tau}\langle T_{\tau}(c_{\mathbf{k},\alpha}(\tau)c_{\mathbf{k},\beta}^{\dagger}(0))\rangle=\sum_{j=\pm}\frac{C_j^{\alpha\beta}(k)}{i\omega_n-E_j(k)+\mu},$$
$$E_{j=\pm}(k)=\frac{\epsilon_{0B}+\epsilon_{0N}}{2}\pm\sqrt{\left(\frac{\epsilon_{0B}-\epsilon_{0N}}{2}\right)^2+|\phi(\mathbf{k})|^2}, \quad (7)$$

where α,β refer to the each atomic basis of honeycomb lattice and $E_j(k)$ is the band structure of BNNT. $\omega_n=(2n+1)\pi/\beta$ denotes the fermionic Matsubara's frequency and β is the inverse of