Effective-Mass Approach to Interaction Effects on Electronic Structure in Carbon Nanotubes

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Abstract

Effects of Coulomb interaction on the band structure are studied for carbon nanotubes in a random-phase approximation within a $\mathbf{k} \cdot \mathbf{p}$ scheme. The energy gaps are strongly enhanced due to the interaction, while effects on the effective mass along the axis direction are small. For realistic values of the interaction parameter, the conventional screened Hartree-Fock approximation works quite well.

Key words: graphite, carbon nanotube, electron-electron interaction, random phase approximation, band gap, single-particle energy, effective-mass theory, GW approximation
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1. Introduction

A carbon nanotube (CN) consists of coaxially rolled two-dimensional (2D) graphite sheets and its electronic states change critically from metallic to semiconducting depending on its tubular circumferential vector. The characteristic properties were first predicted in a tight-binding model [1,2] and successfully reproduced in a $\mathbf{k} \cdot \mathbf{p}$ scheme or an effective-mass approximation [3,4]. The purpose of this work is to study effects of mutual Coulomb interaction on the band structure within a $\mathbf{k}\cdot\mathbf{p}$ scheme.

Effects of the Coulomb interaction on the band structure were evaluated within a screened Hartree-Fock approximation [5]. The results show that the band gap is considerably enhanced by the interaction. In this approximation the dielectric function appearing in the self-energy is replaced by the static one and therefore dynamical effects such as coupling with charge density excitations are not taken into consideration explicitly.

In this paper, we calculate the electronic states using a full dynamical random-phase approximation (RPA), which is often called the GW approximation [6]. The same method was used previously for semiconducting CN's [7] and the present work discusses mainly metallic CN's.

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2. Effective-Mass Scheme

In the effective-mass approximation, electronic states of a 2D graphite near the K point are described by the $\mathbf{k} \cdot \mathbf{p}$ equation as [8]

$$\gamma(\boldsymbol{\sigma} \cdot \hat{\mathbf{k}}) \mathbf{F}(\mathbf{r}) = \varepsilon \mathbf{F}(\mathbf{r}), \qquad (1)$$

with γ being the band parameter without interaction, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ the Pauli spin matrices, and $\hat{\mathbf{k}} = (\hat{k}_x, \hat{k}_y)$ a wave vector operator. For a CN, its electronic states are obtained by imposing the boundary conditions in the circumference direction $\mathbf{F}(\mathbf{r}+\mathbf{L}) = \mathbf{F}(\mathbf{r}) \exp(-2\pi i \nu/3)$. The integer ν is 0 or ± 1, determined by $n_a + n_b = 3M + \nu$ with integer M, where $\mathbf{L} = n_a \mathbf{a} + n_b \mathbf{b}$ is the chiral vector in the circumference direction and $\mathbf{a}$ and $\mathbf{b}$ are the primitive translation vectors of a 2D graphite. The energy bands are given by

$$\varepsilon_{ns}(k) = s\gamma\sqrt{\kappa_\nu(n)^2 + k^2}, \qquad (2)$$

where n is an integer, $s = +1$ and -1 for the conduction and valence band, respectively, and $\kappa_\nu(n) = (2\pi/L)(n-\nu/3)$, with $L = |\mathbf{L}|$.

The method of the calculation was discussed in detail previously [7] and therefore will be discussed only briefly in the following. In RPA, the Coulomb interaction appearing in the self-energy diagram $\Sigma_{ns}(k, \varepsilon)$ is screened by the dynamical dielectric function $\varepsilon_{n-m}(q, \omega)$. The self-energy diverges logarithmically and therefore a cutoff function $g_0(\varepsilon) = \varepsilon_c^{\alpha_c}/(|\varepsilon|^{\alpha_c} + \varepsilon_c^{\alpha_c})$ is introduced so as to exclude contributions from states far away from the Fermi level. The cutoff energy ε_c is of the order of the width of the π bands in 2D graphite.

The single-particle energy $E_{ns}(k)$ is calculated by $E_{ns}(k) = \varepsilon_{ns}(k) + \Sigma_{ns}(k, \varepsilon_{ns}(k))$. Originally, it is determined by the equation obtained from the above by the replacement of $\Sigma_{ns}(k, \varepsilon_{ns}(k))$ by $\Sigma_{ns}(k, E_{ns}(k))$. However, the present procedure is known to give more accurate results if the self-energy is calculated only in the lowest order as in the present case [9,10].

Using the single-particle energy, we evaluate the band gap Δ_n which is defined by the energy difference at $k = 0$ between conduction and valence bands of the same index n as $\Delta_n = E_{n+}(0) - E_{n-}(0)$. The effective mass m_{ns}^* for each band with Coulomb interaction can also be estimated from the single-particle energy $E_{ns}(k)$ as $1/m_{ns}^* = (1/\hbar^2)(\partial^2 E_{ns}(k)/\partial k^2)|_{k=0}$.

The effective strength of the Coulomb interaction is specified by the ratio between the effective Coulomb en-
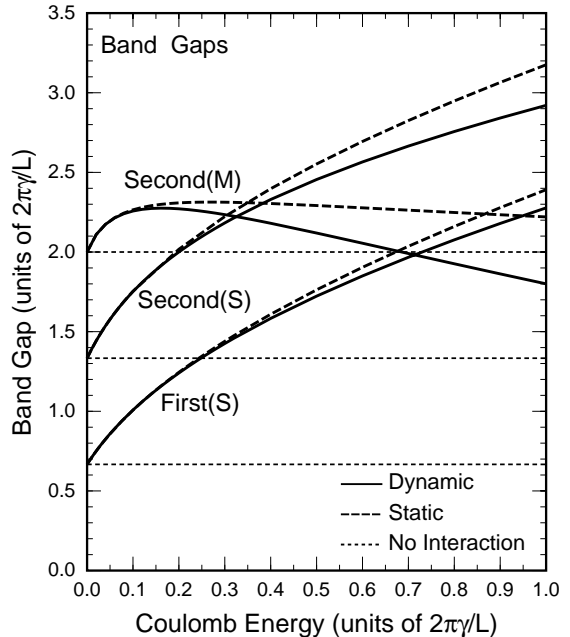

Fig. 1. Calculated gap of a parabolic bands ($n = \pm 1$) in a metallic CN (M) and first and second gaps of a semiconducting CN (S) versus the effective strength of the Coulomb interaction.

ergy $e^2/\kappa L$ and the typical kinetic energy $2\pi\gamma/L$, i.e., $(e^2/\kappa L)/(2\pi\gamma/L)$, which is independent of L. In actual nanotubes, the interaction parameter is estimated as $(e^2/\kappa L)/(2\pi\gamma/L) \sim 0.35/\kappa$. In the following we shall perform calculations for much wider parameter range, $(e^2/\kappa L)/(2\pi\gamma/L) < 1$, in order to make the dependence on the interaction strength clearer. The cutoff parameters are chosen as $\varepsilon_c/(2\pi\gamma/L) = 5$ and $\alpha_c = 4$.

3. Interaction Effects on Band Structure

Figure 1 gives the gap of the first parabolic band in a metallic CN and the first and second band gap for a semiconducting CN. In the regime of very weak interaction $(e^2/\kappa L)/(2\pi\gamma/L) < 0.05$, the band gap increases with the interaction strength in both metallic and semiconducting CN's. With the further increase of the interaction, however, the gap in a metallic CN starts to decease after taking a maximum at around $(e^2/\kappa L)/(2\pi\gamma/L) \approx 0.15$, while that in a semiconducting CN continues to increase.
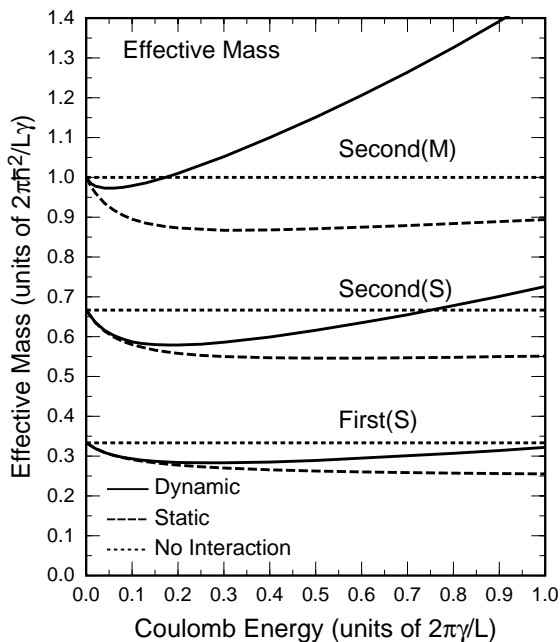
Fig. 2. The effective mass of the parabolic band in a metallic CN (M) and those of first and second bands in a semiconducting CN (S) as a function of the effective strength of the Coulomb interaction.

In the weak interaction regime $(e^2/\kappa L)/(2\pi\gamma/L) < 0.2$, dynamical effects on the band gap are small and the static RPA works well. When the interaction is stronger, the difference between the dynamical and static RPA becomes larger in a metallic CN than in a semiconducting CN. The shift in the gaps of a semiconducting CN is nearly independent of the band. This shows that the interaction effects cannot be absorbed into a simple renormalization of the band parameter γ.

Figure 2 shows the effective mass m^*. In metallic CN's, dynamical effects on m^* are much pronounced even when the interaction parameter $(e^2/\kappa L)/(2\pi\gamma/L)$ is small. In fact, the difference is apparent even for the interaction strength as small as $(e^2/\kappa L)/(2\pi\gamma/L) \sim 0.05$ and m^* in the dynamical RPA becomes larger than the mass without interaction at around $(e^2/\kappa L)/(2\pi\gamma/L) \sim 0.2$, while the effective mass in the static RPA stays smaller (about 90 %) in the whole range of the interaction strength.

Figure 3 shows the band gap for a metallic CN for different cutoffs, $\varepsilon_c/(2\pi\gamma/L) = 2.5$, 5.0, and 10. The band gap scaled by $2\pi\gamma/L$ increases logarithmically with the
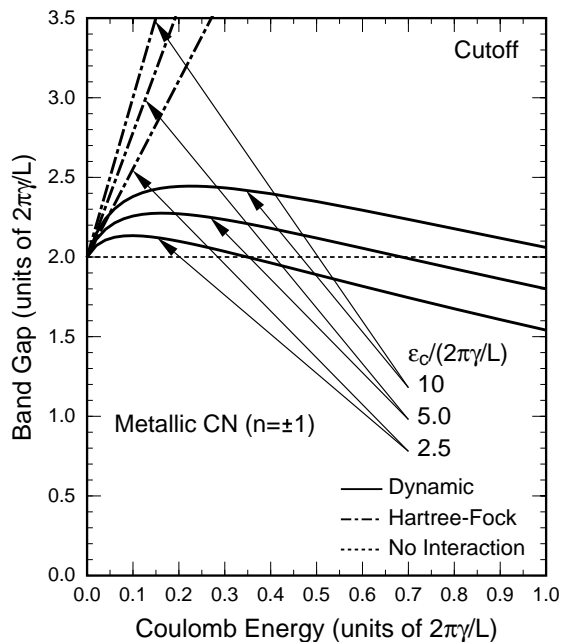

Fig. 3. The cutoff-energy dependence of the gap of the parabolic band ($n = \pm 1$) in a metallic CN.

increase of the cutoff energy. The same is applicable in a semiconducting CN [7]. This logarithmic cutoff dependence means that the band-gap enhancement increases slightly (logarithmically) with the increase of the CN diameter if being scaled by $2\pi\gamma/L$. Unfortunately, experimental measurements of band gaps have not been accurate enough to make detailed comparison possible so far.

4. Discussion

If we employ the same scheme, we can calculate the self-energy for the linear bands with $n = 0$ in metallic CN's, giving a gapless linear band with a renormalized velocity. In fact, although each term of perturbation expansion of the self-energy is known to exhibit a divergence, the RPA self-energy itself does not diverge because of the cancellation of divergent polarization function. This result is in clear contradiction with the fact that only a charge-density and a spin-density excitation can exist and there are no well-defined quasiparticle excitations in systems with a linear dispersion [11,12], leading to the breakdown of the Fermi liquid
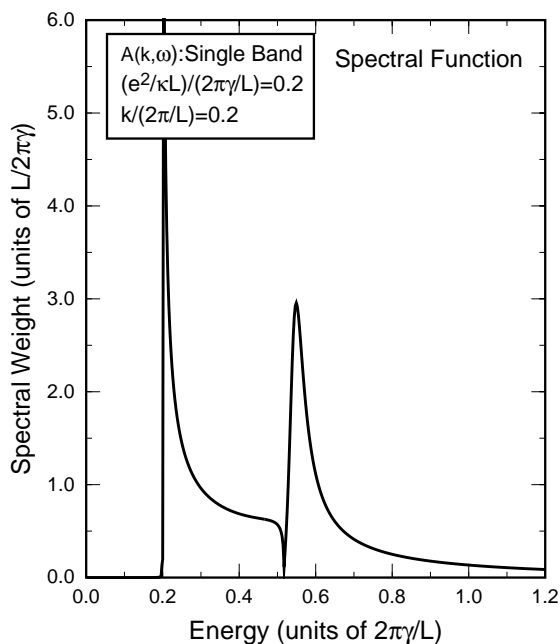
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Fig. 4. An example of the spectral function in a single linear-band model calculated in RPA. The energy of the first peak corresponds well to the spin-density excitation and the second to the charge-density excitation.

picture.

This apparent inconsistency arises from the way of determining the quasi-particle energy from the self-energy. Even in RPA, the spectral function (the imaginary part of the Green's function) exhibits double sharp peaks in a system with only metallic linear bands as shown in Fig. 4. This peak splitting, into charge-density and spin-density excitations presumably, is a result of the divergent behavior of the polarization function and qualitatively in agreement with that of the spectral function for a Tomonaga-Luttinger liquid reported in refs. [13] and [14]. For the parabolic bands both in semiconducting and metallic CN's, no singular behavior appears in the polarization function and therefore quasi-particle states are expected to give a good picture of their low-energy excitations.

In summary, we have studied effects of the Coulomb interaction on the bands with parabolic dispersion using a full dynamical random-phase approximation within an effective-mass scheme. For the interaction parameter $(e^2/\kappa L)/(2\pi\gamma/L)$ appropriate in actual systems ($\lesssim 0.1$ [15]), the screened Hartree-Fock ap-

proximation has been shown to work sufficiently well. The band gaps are strongly enhanced but effects on the effective mass are much smaller, showing that interaction effects cannot be absorbed into a renormalization of a single band parameter γ.

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