Effective-Mass Theory of Electron Correlations in Band Structure of Semiconducting Carbon Nanotubes

Hideaki SAkAI, Hidekatsu SUZUURA and Tsuneya ANDO

Institute for Solid State Physics, University of Tokyo
5–1–5 Kashiwanoha, Kashiwa, Chiba 277-8581
1 Department of Physics, Tokyo Institute of Technology
2–12–1 Ookayama, Meguro-ku, Tokyo 152-8551

The band gap, the single-particle energy, and the effective mass are calculated for semiconducting carbon nanotubes in a random-phase approximation within a $k \cdot p$ scheme. The energy gaps are shown to be strongly enhanced due to the Coulomb interaction, while effects on the effective mass along the axis direction are small. For realistic values of the interaction parameter, effects of the dynamical screening are sufficiently weak, and the conventional screened Hartree-Fock approximation is shown to work quite well. Further, the band gap contains a term with a residual logarithmic dependence on the tube diameter $d$ after being scaled by $1/d$.

Keywords: graphite, carbon nanotube, electron-electron interaction, dynamical RPA, band gap, single-particle energy, effective-mass theory

§1. Introduction

A carbon nanotube (CN) was first discovered by Iijima in 1991. It 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 by the band-structure calculation in a tight-binding model and successfully reproduced in a $k \cdot p$ scheme or an effective-mass approximation. The purpose of this work is to study effects of the mutual Coulomb interaction on the band structure within such a $k \cdot p$ scheme.

Effects of the Coulomb interaction on the band structure were evaluated within a conventional screened Hartree-Fock approximation. The results show that the band gap is considerably enhanced by the Coulomb interaction. In this approximation the dielectric function appearing in the self-energy is replaced by the static interaction. In this paper, we shall calculate the single-particle energy and the effective mass in semiconducting carbon nanotubes in a random-phase approximation within a

\[ F^K(r + L) = F^K(r) \exp\left(- \frac{2\pi i \nu}{3}\right). \]

The integer $\nu$ is 0 or ±1, determined by $n_a + n_b = 3M + \nu$ with integer $M$, where $L = n_a a + n_b b$ is the chiral vector in the circumference direction and $a$ and $b$ are the primitive translation vectors of a 2D graphite.

Around the K point, the wave function and the energy bands are given by

\[ F^{K}_{nsk}(r) = \frac{1}{\sqrt{AL}} F^{\nu K}_{nsk} \exp\left[i\kappa(n)x + iky\right], \]

with

\[ F^{\nu K}_{nsk} = \frac{1}{\sqrt{2}} \left( b_{\nu}(n, k) + s \right), \]

\[ b_{\nu}(n, k) = \frac{\kappa_{\nu}(n) - ik}{\sqrt{\kappa_{\nu}(n)^2 + k^2}}, \]

\[ \kappa_{\nu}(n) = \frac{2\pi}{L} \left( n - \frac{\nu}{3} \right), \]

where $L = |L|,$ $A$ is the length of a CN, the $x$ axis is chosen along the circumference direction, and the $y$ axis

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is parallel to the tube axis. Further, n is an integer, k
the wave vector in the axis direction, and s the band
index (s = ±1 for the conduction band and s = −1 for the
valence band). Equations for the K’ point are the same
as those for the K point except that σ_y is replaced by
−σ_y and ν by −ν.

2.2 Coulomb interaction

The Coulomb potential between two electrons on the
cylindrical surface at \( r = (x, y) \) and \( r' = (x', y') \) is
written as

\[
v(x-x',y-y') = \sum_q \exp \left[ i q(y-y') \right] \frac{2 e^2}{\kappa A} K_0 \left( \frac{L|q|}{2\pi} \left| 2 \sin \left( \frac{\pi(x-x')}{L} \right) \right| \right),
\]

(2.5)

where \( K_0(t) \) is the modified Bessel function of the second
kind and \( \kappa \) is a static dielectric constant representing
effects of the polarization of electrons in core states, filled
bands, and also occupied π bands away from the K
and K’ points. In the effective-mass approximation, this
potential appears only in the diagonal part of the matrix
\( k \cdot p \) Hamiltonian, and the Coulomb matrix elements are given by

\[
\langle \alpha, k, K; \beta', k'+q, K|v|\beta, k+q, K; \alpha', k', K \rangle
\]

\[
= \frac{1}{A} \delta_{n-n',m-m'} \left( F^{\nu K}_{\alpha \beta} \cdot F^{\nu K}_{\beta \beta'} \right) \left( F^{\nu K*}_{\beta' \beta} \cdot F^{\nu K*}_{\alpha' \alpha} \right) v_{n-m}(q),
\]

(2.6)

with

\[
v_{n-m}(q) = \frac{2 e^2}{\kappa} I_{|n-m|} \left( \frac{L|q|}{2\pi} \right) K_{|n-m|} \left( \frac{L|q|}{2\pi} \right),
\]

(2.7)

where \( I_n(t) \) is the modified Bessel function of the first
kind and \( \alpha = (n, \pm) \), \( \beta = (m, \pm) \), etc. Note that matrix elements corresponding to the scattering of an electron from the K point to the K’ point and vice versa are safely neglected in the effective-mass approximation.

In RPA, the Coulomb interaction is screened by the
dynamical dielectric function \( \varepsilon_{n-m}(q, \omega) \), given by

\[
\varepsilon_{n-m}(q, \omega) = 1 + v_{n-m}(q) P_{n-m}(q, \omega).
\]

(2.8)

The polarization function \( P_{n-m}(q, \omega) \) is expressed as

\[
P_{n-m}(q, \omega) = -\frac{2}{A} \sum_{K,K'} \sum_{m,m'} \sum_{k,k'} \delta_{n,m,n'-m'}
\]

\[
\times F^{\nu G}_{m+m',k,k'+q,k'} g_0 \left[ \varepsilon^G_{n-m}(k') \right] g_0 \left[ \varepsilon^G_{n-m'}(k'+q) \right]
\]

\[
\times \left[ \frac{1}{\omega - \varepsilon^G_{m+m'}(k') + \varepsilon^G_{n-n'}(k'+q) + i\delta} - \frac{1}{\omega + \varepsilon^G_{m+m'}(k') - \varepsilon^G_{n-n'}(k'+q) - i\delta} \right],
\]

(2.9)

with \( \delta \) being a positive infinitesimal,

\[
F^{\nu G}_{\alpha \beta \beta' \beta'; k, k+q} = \left( F^{\nu G}_{\alpha \beta} \cdot F^{\nu G}_{\beta \beta'} \right)^2
\]

\[= \frac{1}{2} \left( 1 + \frac{s_\alpha s_\beta s_\beta' s_\beta'' [\varepsilon_\nu(n) \varepsilon_\nu(m) + k(k+q)]}{\sqrt{\varepsilon_\nu(n)^2 + k^2} \sqrt{\varepsilon_\nu(m)^2 + (k+q)^2}} \right),
\]

(2.10)

and

\[
s_\alpha = \begin{cases} +1 & (\alpha = n+), \\ -1 & (\alpha = n-), \end{cases}
\]

(2.11)

where \( G \) takes the K and K’ point. The cutoff function
\( g_0(\varepsilon) \) is given by

\[
g_0(\varepsilon) = \frac{\varepsilon^\alpha}{|\varepsilon^\alpha + e^\alpha|},
\]

(2.12)

which contains two parameters \( \alpha \) and \( \varepsilon^\alpha \) so as to take only the contributions from states in the vicinity of the Fermi level into consideration. The introduction of \( g_0(\varepsilon) \) makes numerical calculations easy, but actually is not necessary in the polarization function because the summation in eq. (2.9) converges even for \( \varepsilon^\alpha \to \infty \). Obviously, the dielectric function satisfies

\[
\varepsilon_{n-m}(q, \omega) = \varepsilon_{n-m}(q, -\omega).
\]

(2.13)

2.3 Self-energy

Formally, the effective interaction gives the self-
energy for electrons in the dynamical RPA including the
cutoff function as

\[
\Sigma^K_{\alpha}(k, \omega) = \frac{i}{2\pi A} \int d\omega' \sum_{\beta,q} G^K_{\alpha,\beta,k,k+q} F^{\nu K}_{\alpha \beta \beta \beta'+q} v_{n-m}(q, \omega') \delta(\omega - \omega' + \varepsilon^K_{\beta'}(k+q)),
\]

(2.14)

where \( G^K_{\alpha}(k, \omega) \) is the non-interacting Green’s function written as

\[
G^K_{\alpha}(k, \omega) = \frac{1}{\omega - \varepsilon^K_{\alpha}(q) + i\sigma \delta}.
\]

(2.15)

Equation (2.14) is represented in terms of Feynman
diagrams shown in Fig. 1.

The original \( k \cdot p \) Hamiltonian has the particle-hole
symmetry about \( \varepsilon = 0 \). It leads to

\[
G^K_{\alpha}(q, -\omega) = -G^K_{\alpha}(q, \omega),
\]

(2.16)

\[
F^{\nu K}_{\alpha \beta \beta \beta'+q} = F^{\nu K*}_{\alpha \beta \beta' \beta; k, k+q},
\]

(2.17)

where \( \alpha \) means a state with energy opposite to state \( \alpha \), i.e., \( \alpha = n- \) for \( \alpha = n+ \), \( \alpha = n+ \) for \( \alpha = n- \), etc. It should also lead to the symmetry of the band structure in the presence of interactions if the energy is measured from the Fermi level.

The self-energy can be separated into

\[
\Sigma^K_{\alpha}(k, \omega) = \Sigma^K_{\alpha}(k, \omega)^X + \Sigma^K_{\alpha}(k, \omega)^C,
\]

(2.18)

where the exchange or Hartree-Fock term \( \Sigma^K_{\alpha}(k, \omega)^X \) and the correlation term \( \Sigma^K_{\alpha}(k, \omega)^C \) are defined by

\[
\Sigma^K_{\alpha}(k, \omega)^X = \frac{i}{2\pi A} \int d\omega' \sum_{\beta,q} G^K_{\alpha,\beta,k+q} F^{\nu K}_{\alpha \beta \beta \beta'; k, k+q} \delta(\varepsilon^K_{\beta'}(k+q)),
\]

(2.19)

and

\[
\Sigma^K_{\alpha}(k, \omega)^C = \frac{i}{2\pi A} \int d\omega' \sum_{\beta,q} G^K_{\alpha,\beta,k+q} F^{\nu K}_{\alpha \beta \beta \beta'; k, k+q} \delta(\varepsilon^K_{\beta'}(k+q)),
\]

(2.20)

respectively. Because the integrand of eq. (2.20) decays faster than \( 1/\omega' \) for large \( |\omega'| \), the convergence factor
\[ e^{i\omega'} \] has been omitted in the expression of the correlation part. Then, the symmetry relations (2.16) and (2.17) together with eq. (2.13) immediately lead to the electron-hole symmetry for the correlation part, i.e.,

\[ \tilde{\Sigma}_\alpha(k, -\omega)^C = -\tilde{\Sigma}_\alpha(k, \omega)^C. \quad (2.21) \]

On the other hand, the contribution from the Hartree-Fock term can be evaluated with ease by closing the more simplified approximations as the static RPA and eq. (2.14) is neglected and \( \varepsilon \) has been used in a previous work.

The integral of \( \tilde{\Sigma}_\alpha(k, -\omega) \) is given by \( \Sigma^K_{n\pm}(k, -\omega) \) by \( \Sigma^K_{n\pm}(k, E^K_{n\pm}(k)) \) by \( \Sigma^K_{n\pm}(k, E^K_{n\pm}(k)) \). However, eq. (2.25) is known to give more accurate results if the self-energy is calculated only in the lowest order as in the present case.28,29

Using the above single-particle energy, we evaluate the band gap \( \Delta^K_n \) which is defined by the energy difference at \( k = 0 \) between conduction and valence bands of the same index \( n \) associated with the K point for a semiconducting CN (\( \nu = 1 \)) as

\[ \Delta^K_n = E^K_{n\pm}(0) - E^K_{n\mp}(0). \quad (2.26) \]

The effective mass \( m^{K\pm}_{n\pm} \) for each band with Coulomb interaction can also be estimated from the single-particle energy \( E^K_{n\pm}(k) \), i.e.,

\[ \frac{1}{m^{K\pm}_{n\pm}} = \frac{1}{h^2} \frac{\partial^2 E^K_{n\pm}(k)}{\partial k^2} \bigg|_{k = 0}. \quad (2.27) \]

In general, the imaginary part of the self-energy comes solely from \( \Sigma^K_n(k, \omega)^C \) in the dynamical RPA since \( \Sigma^K_n(k, \omega)^R \) is real. In semiconducting CN’s at zero temperature, however, the imaginary part of \( \Sigma^K_n(k, \varepsilon \tilde{\Sigma}(k)^C) \) is actually zero and the self-energy then has only the real part. This result reflects the fact that the momentum and energy conservation prevents a single particle-hole pair excitation in the present system with a gap.

§3. Results

3.1 Numerical calculations

The effective strength of the Coulomb interaction is specified by the ratio between the effective Coulomb energy \( e^2/\kappa L \) and the typical kinetic energy \( 2\pi\gamma/L \), i.e., \( (e^2/\kappa L)/(2\pi\gamma/L) \), which is independent of the circumference length \( L \). In actual nanotubes, the interaction parameter is estimated as \( (e^2/\kappa L)/(2\pi\gamma/L) = (e^2/\kappa a)/\gamma_0 \) for \( \gamma = \sqrt{3} \pi \gamma_0/2 \) where \( \gamma_0 \) is the transfer integral between the nearest neighbor carbon atoms in a simplest tight-binding model and \( a \) is the lattice constant.

For \( \gamma_0 \sim 3 \text{ eV} \) and \( a = 2.46 \text{ Å} \), this gives \( (e^2/\kappa L)/(2\pi\gamma/L) \sim 0.35/\kappa < 0.35 \) because it is expected that \( \kappa > 1 \). In the following, however, we shall treat the above quantity as the interaction parameter and perform calculations for \( 0 < (e^2/\kappa L)/(2\pi\gamma/L) < 1 \) in order to make the dependence on the interaction strength clear. The cutoff parameters are chosen as \( \varepsilon_c/(2\pi\gamma/L) = 5 \) and \( \alpha_c = 4 \) in most of the cases and the cutoff dependence is studied also.

Poles of \( \varepsilon_n-m(q, \omega)^{-1} \) along the real axis make it quite difficult to calculate \( \tilde{\Sigma}_n^{K\pm}(k, \omega)^C \). In performing the integral of \( \omega' \) in eq. (2.14), therefore, we rotate the integration path along the real axis into the imaginary axis counter-clockwise to avoid such poles considering an infinitesimal imaginary part in the non-interacting Green’s function.28,14 Then, we must remember to add contributions from a finite number of poles of the Green’s function. The details of the calculations are shown in Appendix A.

The actual numerical calculation of the self-energy requires vast computational time. First, the polarization function given by eq. (2.9) involves the summation and
integration over wave vectors in the circumference $n'$ and axis direction $k'$, respectively, for all values of $q$ and $\omega$. Further, the self-energy requires the summation and integration over wave vectors $(n', q)$ and the integration over $\omega'$. Thus, the actual calculation of each self-energy requires double summations over the wave vector in the circumference direction and triple integrations over the wave vector in the axis direction and the frequency. The integration over $q$ and $\omega'$ should actually be performed very carefully because the integrand has singularities at different points with various degrees.

Actually, only the use of eq. (2.25) makes the explicit determination of interaction effects on the band structure feasible. A self-consistent determination of the Green’s function and the corresponding quasi-particle energy requires the calculation of the self-energy for all $(k, \omega)$ many times and is practically impossible for the present system without introducing further approximations. Besides, a self-consistent determination does not necessarily give more accurate results because corresponding vertex corrections should usually be considered for the consistency of the approximation.

3.2 Band gaps

Figure 2 gives the numerical results of the first and second band gaps for a semiconducting CN ($\nu = 1$) versus the effective strength of the Coulomb interaction. The first band means $n = 0$ in eq. (2.25) for the K and K’ point and the second $n = 1$ for the K point or $n = -1$ for the K’ point. When the Coulomb interaction is not strong, i.e., for $(e^2/\kappa L)/(2\pi\gamma/L) \lesssim 0.3$, the results in the static RPA are almost the same as those in the full dynamical approximation, showing that the static approximation is sufficient in this parameter range. Even in this weak coupling regime, the band gaps are considerably enhanced due to the Coulomb interaction. For $(e^2/\kappa L)/(2\pi\gamma/L) = 0.1$, for example, the first band gap with interaction is about 1.5 times as large as that without interaction. Furthermore, for $(e^2/\kappa L)/(2\pi\gamma/L) < 0.05$, the results in the Hartree-Fock approximation become equally valid.

3.3 Single-particle energy and effective mass

Figure 3 shows the dispersion relation of the single-particle energy of the first and second conduction bands measured from the Fermi level for the particle energy of the first and second conduction bands. The dynamical effect of the band gap as shown in Fig. 4. The dynamical effect on the effective mass along the axis direction is also quite small for $(e^2/\kappa L)/(2\pi\gamma/L) < 0.3$, while it becomes more apparent for $(e^2/\kappa L)/(2\pi\gamma/L) \sim 1$ than that on the band gaps. Away from weak-coupling regime, the dynamical RPA can cause positive shift to the effective mass, while the static RPA shows almost constant negative shift. This is always smaller than that in the dynamical case. In the Hartree-Fock approximation the mass is considerably reduced with the increase of the interaction strength.

3.4 Diameter dependence

So far, we have considered only the fixed value of the cutoff energy $\varepsilon_c/(2\pi\gamma/L) = 5$. In this case the interaction parameter is independent of the CN diameter and therefore the band gap is inversely proportional to the circumference length $L$ or the diameter $d = L/\pi$ even in the presence of interaction. Actually, however, a small dependence on the CN diameter $d$ can appear through the cutoff energy $\varepsilon_c$. In fact, the cutoff should be chosen as $\varepsilon_c \sim 3\gamma_0$ corresponding to the $\pi$ band width of the 2D graphite, giving $\varepsilon_c/(2\pi\gamma/L) \sim (\sqrt{3}/\pi)(L/a)$. Therefore, a dependence on the CN diameter $d$ appears through this cutoff energy.

The band gaps shown in Fig. 5 are calculated for $\varepsilon_c/(2\pi\gamma/L) = 2.5, 5,$ and 10 in the Hartree-Fock approximation and the dynamical RPA. We can see that the cut-off energy induces a small correction to the band gap that scales as $2\pi\gamma/L \propto 1/d$. The correction shows logarithmic increase with respect to $\varepsilon_c$, and this means that the band gap scaled by the inverse of the diameter contains a term that shows a logarithmic dependence on the diameter. In fact, as shown in Appendix B, it is analytically estimated that the band gaps have such a term as $\delta\Delta_n \propto (2\pi\gamma/L) \ln[\varepsilon_c/(2\pi\gamma/L)] \sim (2\pi\gamma/L) \ln(d/a)$ in both the Hartree-Fock approximation and the static RPA. The results given in Fig. 5 show the presence of such contributions in the dynamical RPA, too.

§4. Discussion

Figure 2 shows that the shift in the gap is almost independent of the band except in the Hartree-Fock approximation. Furthermore, the band gap is considerably enhanced due to the Coulomb interaction while the effective mass in the axis direction is slightly changed as shown in Figs. 2 and 4. Therefore, there exists a large difference in the interaction effect on the band gap and the effective mass. These facts show that the Coulomb interaction effects cannot be absorbed into a renormalization of the single band parameter $\gamma$. In the absence of interaction, the first and second band gaps become $4\pi\gamma/3L$ and $8\pi\gamma/3L$, respectively, and the corresponding effective masses are given by $2\pi\hbar^2/3L\gamma$ and $4\pi\hbar^2/3L\gamma$, respectively. Therefore, a renormalization of $\gamma$ should give the fact that the ratio between the first and second gaps should remain the same and that the effective mass should also be reduced by the same amount as that of the band-gap enhancement.

The failure of the $\gamma$ renormalization is quite possible because the Coulomb interaction is weaker than the typical band energy, i.e., $e^2/\kappa L \ll 2\pi\gamma/L$. In the weak-coupling regime, the interaction effect on the band gap can vary from that on the dispersion relation because they are likely to involve different energy scales. If we consider the strong interaction regime, $e^2/\kappa L \gg 2\pi\gamma/L$, the treatment becomes intricate. However, it appears that the influence of the interaction is weakly dependent on $\gamma$. This is a typical feature of the weak-coupling regime which can be considered to be due to the small coupling parameter $\gamma$. Therefore, the strong interaction regime seems to be not very important for the present problem.
with a sufficiently large cutoff energy, the structure of the discrete energy bands will become less important. In this case electronic properties of the system will be similar to those in 2D graphite sheets and then interaction effects may be absorbed into a simple renormalization of $\gamma$. The present results are understood reasonably well in terms of a constant shift in the band gap together with a small renormalization of $\gamma$ due to interaction effects.

In actual nanotubes, the coupling strength $(e^2/\kappa L)/(2\pi\gamma/L)$ is at most 0.35 as mentioned in the previous section. From Figs. 2, 3(a), 3(b), and 4, we can safely conclude that the dynamical screening effects are sufficiently weak both for band gaps and for effective mass and, therefore, that the static approximation is really satisfactory.

The logarithmic cutoff dependence obtained in the previous section shows that the band-gap enhancement increases slightly (logarithmically) with the increase of the CN diameter $d$ if being scaled by $2\pi\gamma/L$. Previously, the diameter dependence of the band gap in a CN was investigated in various ways both from theoretical and experimental aspects.

Theoretically, for example, calculations of the band gaps were performed in a first-principles local-density approximation. In both refs. 15 and 16, the first band gaps measured for various CN’s are consistent with the $1/d$ dependence. However, large error bars prevent verification of the deviation from the $1/d$ dependence.

Optical absorption spectra were measured in thin films of single-wall nanotubes and the optical gap displays slightly more rapid decrease than the $1/d$ scaling with increase of the CN diameter from about 0.7–2.6 nm and we cannot be certain whether they have a logarithmic correction on their $1/d$ dependence. The logarithmic dependence on the CN diameter comes from the screened nonlocal exchange term as shown in Appendix B and therefore it is doubtful that a logarithmic correction can appear in the local-density approximation where interaction effects are incorporated only in the form of a local exchange-correlation potential.

Experimentally, the first band gap was directly measured by scanning tunneling microscopy and spectroscopy. In both refs. 15 and 16, the first band gaps measured for various CN’s are consistent with the $1/d$ dependence. However, large error bars prevent verification of the deviation from the $1/d$ dependence.

In this appendix, we shall briefly explain the method of calculating the correlation term in the self-energy. In evaluating the contribution from the correlation term, we should change the contour $C_1$ along the real axis into $C_2$ along the imaginary axis in the complex $\omega'$ plane in eq. (2.14) in order to avoid the poles of $\varepsilon_{n-m}(q, \omega').$ Figure 6 shows an example of singularities and two contours. The resulting self-energy consists of the contribution from the poles of the Green’s function and that of the integral along the imaginary axis, i.e.,

$$\Sigma_{n+}(k, \varepsilon_{n+}(k)) = \hat{\Sigma}_{n+}(k)_{\text{res}}^{\text{res}} + \hat{\Sigma}_{n+}(k)_{\text{line}}^{\text{line}}.$$  \hspace{1cm} (A1)

The former is given by

$$\hat{\Sigma}_{n+}(k)_{\text{res}}^{\text{res}} = \frac{1}{A} \sum_{m,q} \theta\left[\varepsilon_{n+}^K(k) - \varepsilon_{m+}^K(k+q)\right] F_{n+;m+;k+q;v_{n-m}}(q) \times \left(\frac{1}{\varepsilon_{n-m}[q, \varepsilon_{m+}^K(k+q) - \varepsilon_{n+}^K(k)]} - 1\right) g_0\left[\varepsilon_{m+}^K(k+q)\right].$$  \hspace{1cm} (A2)

where $\theta(t)$ is the step function defined by $\theta(t) = 1$ for
\[ t > 0 \text{ and } \theta (t) = 0 \text{ for } t < 0. \text{ The latter is given by} \]
\[ \hat{\Sigma}_{n+}^{K} (k) = \frac{1}{2\pi \alpha} \int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} \omega^{2} \sum_{\beta, q} \frac{\varepsilon_{\beta}^{K} (k) - \varepsilon_{\beta}^{K} (k + q)}{2 \varepsilon_{\beta}^{K} (k) - \varepsilon_{\beta}^{K} (k + q)} \]
\[ \times F_{n+}^{K, \beta, q} v_{n-m} (q) \left( \frac{1}{\varepsilon_{n-m} (q, \omega)} - 1 \right) g_{0} \left[ \varepsilon_{\beta}^{K} (k + q) \right]. \]

\[ \text{(A3)} \]

The integration of \( \omega \) in eq. (A3) has a singularity at \( \varepsilon_{\beta}^{K} (k) - \varepsilon_{\beta}^{K} (k + q) = 0 \). We can avoid this singularity by replacing \( \omega \) with \( \omega' = \omega / (\varepsilon_{\beta}^{K} (k) - \varepsilon_{\beta}^{K} (k + q)) \).

**Appendix B: Cutoff Dependence**

Here, we shall discuss the dependence of the band gap \( \Delta_{K}^{n} \) on the cutoff energy \( \varepsilon_{c} \) in the Hartree-Fock approximation. From eqs. (2.22) and (2.26), the enhancement of the band gap due to the Coulomb interaction can be expressed in the Hartree-Fock approximation as

\[ \delta \Delta_{K}^{n} = \sum_{m, q} \frac{\text{sgn}(n-\nu/3) \nu_{m}(m)}{A \nu_{m}^{2} + q^{2}} v_{n-m}(q) g_{0} \left[ \gamma \sqrt{\nu_{m}(m^{2} + q^{2})} \right], \]

where \( \text{sgn}(t) = 1 \) for \( t > 0 \) and \( \text{sgn}(t) = -1 \) for \( t < 0 \). Since we consider the cutoff energy sufficiently large, we can replace the summation over \( m \) by an integral and have

\[ \delta \Delta_{K}^{n} \sim \int dm \int d\varepsilon \frac{e^{2}}{k \nu} \frac{\text{sgn}(n-\nu/3)}{m^{2} + q^{2}} v_{n-m}(q) g_{0} \left[ \frac{2 \gamma}{L} \sqrt{m^{2} + q^{2}} \right] \]

\[ \times \left[ \frac{2 \pi \nu \gamma}{L} \frac{m^{2}}{\sqrt{m^{2} + q^{2}}} g_{0} \left[ \frac{2 \pi \gamma}{L} \sqrt{m^{2} + q^{2}} \right] \right], \]

\[ \text{(B2)} \]

which is scaled by \( 2\pi / L \) and the summation can safely be replaced by the integral for large \( m \) and \( q \). Further, we have used \( v_{n-m}(q) \sim (e^{2}/\nu)(|m-n|^{2} + q^{2})^{-1/2} \), which is valid for large \( |n-m| \) and \( |q| \).

When \( n \) and \( \nu/3 \) are much smaller than \( m \) and \( q \), the above becomes

\[ \delta \Delta_{K}^{n} \sim \int dm \int d\varepsilon \frac{e^{2}}{k \nu} \frac{\text{sgn}(n-\nu/3)}{m^{2} + q^{2}} v_{n-m}(q) g_{0} \left[ \frac{2 \gamma}{L} \sqrt{m^{2} + q^{2}} \right] \]

\[ \times \left[ \frac{2 \pi \nu \gamma}{L} \frac{m^{2}}{\sqrt{m^{2} + q^{2}}} g_{0} \left[ \frac{2 \pi \gamma}{L} \sqrt{m^{2} + q^{2}} \right] \right], \]

\[ \text{(B3)} \]

where \( g_{0}(\varepsilon) = \partial g_{0}/\partial \varepsilon \). We can easily find that the second term including \( g_{0}(\varepsilon) \) in the bracket of the right hand side of eq. (B3) only gives contributions independent of \( \varepsilon_{c} \), which will be ignored completely in the following. By introducing the polar coordinate \( (\varepsilon, \theta) \) through \( m = \varepsilon \cos \theta \) and \( q = \varepsilon \sin \theta \), we have

\[ \delta \Delta_{K}^{n} \sim \int_{0}^{\varepsilon_{c}} d\varepsilon \int_{0}^{2\pi} d\theta \frac{e^{2}}{k \nu} \frac{\text{sgn}(n-\nu/3)}{\varepsilon_{c}} \]

\[ \times \left( \frac{1}{\varepsilon_{c}} \right) \left[ n - \frac{\nu}{3} \right] \ln \frac{\varepsilon_{c}}{(2\pi \gamma / L) n_{min}}, \]

\[ \text{(B4)} \]

where we have introduced an infrared cutoff \( n_{min} \), which should be chosen in such a way that the above approximations are valid for \( m \) and \( q \) satisfying \( \varepsilon \equiv \sqrt{m^{2} + q^{2}} > n_{min} \). Thus, the exchange contribution to the band gap contains a term which shows a logarithmic dependence on the cutoff energy.

Similarly, we can estimate the cutoff dependence in the static RPA. In this case, we only have to replace \( v_{n-m}(q) \) by \( v_{n-m}(q)/\varepsilon_{n-m}(q, 0) \) in eq. (B1). Considering that static polarization function \( P_{n-m}(q, 0) \) can be approximated by that for a 2D graphite sheet for large \( m \) and \( q \) for \( \varepsilon > n_{min} \), we have \( P_{n-m}(q, 0) \sim (\pi/2\gamma) \sqrt{(n-m)^{2} + q^{2}} \). Apart from terms independent of \( \varepsilon_{c} \), the resulting band gap in the static RPA becomes

\[ \delta \Delta_{K}^{n} \sim \frac{\pi \varepsilon^{2}}{n_{min} \ln \frac{\varepsilon_{c}}{(2\pi \gamma / L) n_{min}}}, \]

\[ \text{(B5)} \]

which shows a similar logarithmic dependence although the coefficient is reduced by the screening effect.

**References**

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Figure Captions

Fig. 1 (a) The diagram of the self-energy in the random-phase approximation. (b) The diagram of the full polarization function.

Fig. 2 Calculated band gaps in a semiconducting CN as a function of the effective strength of the Coulomb interaction \((e^2/\kappa L)/(2\pi\gamma/L)\). The first band gap corresponds to that of \(n = 0\) for both K and K’ points and the second \(n = 1\) for the K point or \(n = −1\) for the K’ point.

Fig. 3 Calculated single-particle energy levels for the conduction band in a semiconducting CN. (a) \((e^2/\kappa L)/(2\pi\gamma/L) = 0.1\), (b) 0.2, and (c) 0.5.

Fig. 4 The effective mass for the first and second band in a semiconducting CN versus the effective strength of the Coulomb interaction, estimated from the single-particle energy of each band.

Fig. 5 The cutoff-energy dependence of the first and second band gap in a semiconducting CN. The band gaps are calculated for \(\varepsilon_c/(2\pi\gamma/L) = 2.5, 5, \text{ and } 10\).

Fig. 6 The contours \(C_1\) and \(C_2\) in the complex \(\omega'\) plane. The Green’s function in the integrand gives poles denoted by crosses and the dielectric function is singular along the dotted lines. The integral along \(C_1\) is equal to that along \(C_2\) plus the contribution of the pole at \(-\omega + \varepsilon_m + (k + q) - i\delta\).
\begin{align*}
W(\omega') = & \quad G(\omega + \omega') + G(\omega + \omega') + G(\omega + \omega') + \cdots \\
\mathbb{P}(\omega) = & \quad G(\omega + \omega')_{KK'}
\end{align*}

Fig. 1

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig2}
\caption{Fig. 2}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig3a}
\caption{Fig. 3 (a)}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig3b}
\caption{Fig. 3 (b)}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig3c}
\caption{Fig. 3 (c)}
\end{figure}
Electron Correlations in Band Structure of Semiconducting Carbon Nanotubes

Fig. 4

Fig. 5

Fig. 6