Fano effect on dynamical conductivity for perpendicular polarization in double-wall carbon nanotubes

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Abstract. The dynamical conductivity of double-wall carbon nanotubes for perpendicularly polarized light to the tube axis is studied by taking into account screening effects, exciton effects and depolarization effects within an effective-mass theory. The exciton peak of the semiconducting inner tube has an asymmetric line shape due to the coupling with a continuum state of the outer tube, indicating the Fano effect. The Fano coupling strength can be tuned by varying the inter-wall distance.

1. Introduction
A carbon nanotube is a quasi-one-dimensional system and thus has characteristic optical properties such as the strong enhancement of exciton effects arising from the electron-hole Coulomb interaction. In fact, exciton effects play a crucial role for absorption of light polarized parallel to the tube axis [1]. For single-wall carbon nanotubes, it is known that the dynamical conductivity for perpendicularly polarized light is reduced considerably by a depolarization effect in comparison with that for parallel polarized light, but still exhibits prominent exciton peaks in semiconducting nanotubes due to the strong Coulomb interaction [2, 3, 4].

For double-wall carbon nanotubes, the Coulomb interaction is suppressed by not only intra-wall screening effects but also inter-wall screening effects. This leads to the reduction of exciton binding energies and band gaps [5]. In this paper, we theoretically clarify perpendicularly polarized optical absorption of double-wall carbon nanotubes by taking into account both exciton effects and depolarization effects within an effective-mass approximation.

2. Model
We consider a double-wall nanotube consisting of an inner tube with radius $R$ and an outer tube with radius $R'$. In usual multi-wall nanotubes where the lattice structure of adjacent walls is incommensurate, inter-wall charge transfer is negligibly small due to cancellation of inter-wall coupling at different sites in the absence of disorder [6, 7]. This fact allows us to discuss screening effects without consideration of inter-wall charge transfer. In the static screened Hartree-Fock
absorption spectra for double-wall nanotubes consisting of (a) semiconducting inner and outer

Figure 1 shows the dynamical conductivity \( \bar{\sigma}_R(\omega) \) describing the perpendicularly polarized absorption spectra for double-wall nanotubes consisting of (a) semiconducting inner and outer
Figure 1. Calculated absorption spectra of double-wall carbon nanotubes consisting of a semiconducting inner tube and (a) semiconducting outer tube, and (b) metallic outer tube. The dashed (dotted) curves denote the contribution from the inner (outer) tube.

We find some features of depolarization effects peculiarly in double-wall nanotubes: (i) The inner tube gives a negative absorption in the lower energy region. This means that the direction of the electric field (or induced current) in the inner tube is nearly opposite to that of an external field. (ii) The exciton peak of the inner tube has an asymmetric line shape or even a dip structure due to the coupling with a continuum state of the outer tube, indicating the Fano effect.

The Fano behavior of the exciton peak can be understood qualitatively by a simple model consisting of a single level and a continuum with a constant density of states:

\[
\sigma_R^j(\omega) = \frac{\kappa R \omega}{2\pi i} \frac{(\hbar \omega_p)^2}{E_R^2 - (\hbar \omega)^2}, \quad \sigma_R^l(\omega) = 0,
\]

where \((\hbar \omega_p)^2 = 8\hbar^2 e^2 |\langle u, l; R|v_g|g\rangle|^2/(\kappa AR^2 E_R^2)\). The zero point of \(\epsilon_R^j(\omega)\) is given by

\[
(h\omega_0)^2 = E_R^2 \left[ 1 - \frac{(R/R')^2(\kappa - 1)}{\kappa^2 - (R/R')^2(\kappa - 1)^2} \right] (\hbar \omega_p)^2,
\]

which is smaller than (and is, for \(R/R' = 0\), reduced to) the zero point of \(\epsilon_R^l(\omega)\) in single-wall nanotubes, \((h\omega_0)^2 = E_R^2 + (\hbar \omega_p)^2\).
Figure 2. Model calculations of absorption spectra for (a) $W_c/(e^2/h) = 1.5$ and (b) $W_c/(e^2/h) = 4$. The dashed curves denote $\tilde{\sigma}_R(\omega)$ in eq. (6) and $\hbar\omega_0$ is given by eq. (7).

Figure 2 shows some examples of absorption spectra $\tilde{\sigma}(\omega)$ calculated from the model (6) for various values of $R^*/R$. In Fig. 2(a) for a small $W_c$ corresponding to the semiconducting outer tube, the exciton peak maintains its peak structure but becomes asymmetric with decreasing $R^*/R$. In Fig. 2(b) for a large $W_c$ corresponding to the metallic outer tube, the exciton peak almost vanishes, while a dip structure appears, exhibiting a crossover from peak- to dip-behavior with decreasing $R^*/R$. These describe well the spectra near the exciton peak of the inner tube in Fig. 1. It is clearly reproduced that the Fano line shape is determined by the inter-wall distance and by the intensity of the continuum state of the outer tube. Consequently, the inter-wall distance can change the Fano coupling strength.

In summary, we have found that the Fano effect emerges in dynamical conductivity for perpendicular polarization in double-wall carbon nanotubes. The exciton peak of the semiconducting inner tube becomes asymmetric or changes into a dip structure depending on the coupling with a continuum state of the outer tube. The Fano coupling strength can be tuned by varying the inter-wall distance.

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