

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

Hideaki Sakai¹, Hidekatsu Suzuura² and Tsuneya Ando²

¹ *Institute for Solid State Physics, University of Tokyo
5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581*

² *Department of Physics, Tokyo Institute of Technology
2-12-1 Ookayama, Meguro-ku, Tokyo 152-8551*

We study effects of the Coulomb interaction on the band structure of carbon nanotubes (CN's) within an effective-mass theory, using a full dynamical random-phase approximation (RPA). It is shown that the band gap is strongly modified by interactions, while effects on the effective mass remain small. Further, interactions give rise to a term dependent on the tube diameter logarithmically.

Figure 1 shows schematically the band structure in semiconducting and metallic nanotubes in the absence of interactions. The typical kinetic energy is given by $2\pi\gamma/L$, where γ the band parameter and L the circumference length of the tube. We are interested in effects of interactions on the band gaps and the effective mass at band edges. The effective interaction strength is specified by the ratio between the effective Coulomb energy and the typical kinetic energy, i.e., $(e^2/\kappa L)/(2\pi\gamma/L)$, where κ is a static dielectric constant including the effects of the polarization of the valence-band states away from the Fermi level.

Figure 2 gives the calculated energy gaps for the parabolic bands obtained in the dynamical RPA, static RPA, and Hartree-Fock approximation (HFA). For semiconducting CN's, both first and second band gaps are strongly enhanced due to the interaction even when the interaction is not strong. For metallic CN's, on the other hand, the enhancement of the second band gap saturates and the gap starts to decrease with increase of the interaction strength, and finally, becomes smaller than those in semiconducting CN's. When the interaction strength is small ($(e^2/\kappa L)/(2\pi\gamma/L) \lesssim 0.2$), dynamical screening effects on band gaps are small and the static RPA used previously [1] works well.

Figure 3 shows the effective mass. The effective-mass shift is rather small when the interaction is weak, in contrast to that of the band gap. This fact indicates that there exists a large difference in the interaction effects on the band gap and effective mass, showing that the Coulomb interaction effects cannot be absorbed into a renormalization of the single band parameter γ .

For actual calculations of the self-energy, we need cutoff energy ε_c of the order of the π -band width, i.e., $\varepsilon_c \sim 2\pi\gamma/a$ with a the lattice constant. Figure 4 shows the cutoff dependence of the band gaps in semiconducting CN's. The band gaps with interaction contain a term that shows a logarithmic dependence on the diameter L/π , such as $\propto (2\pi\gamma/L) \ln(L/\pi a)$. A similar correction can be found in the second band of metallic CN's.

Because the first bands in metallic CN's form gapless linear bands, there can be no well-defined quasi-particle states associated with these bands. In fact, the straightforward application of RPA gives a charge-spin separation expected in a Tomonaga-Luttinger liquid.

References

- [1] T. Ando: J. Phys. Soc. Jpn. **66** (1997) 1066.

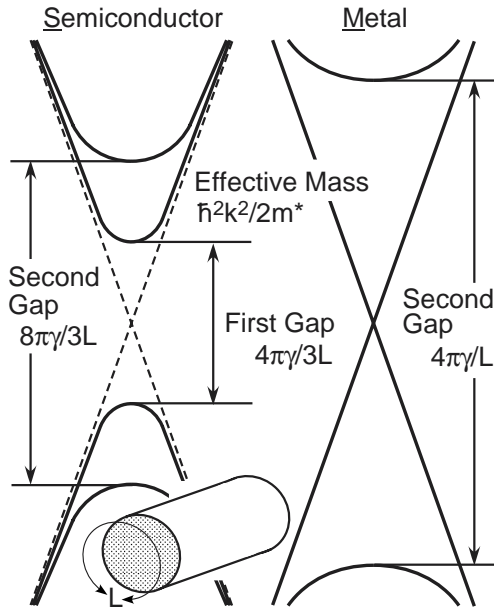


Fig. 1 (Left) A schematic illustration of the band structure in semiconducting and metallic CN's in the absence of interaction.

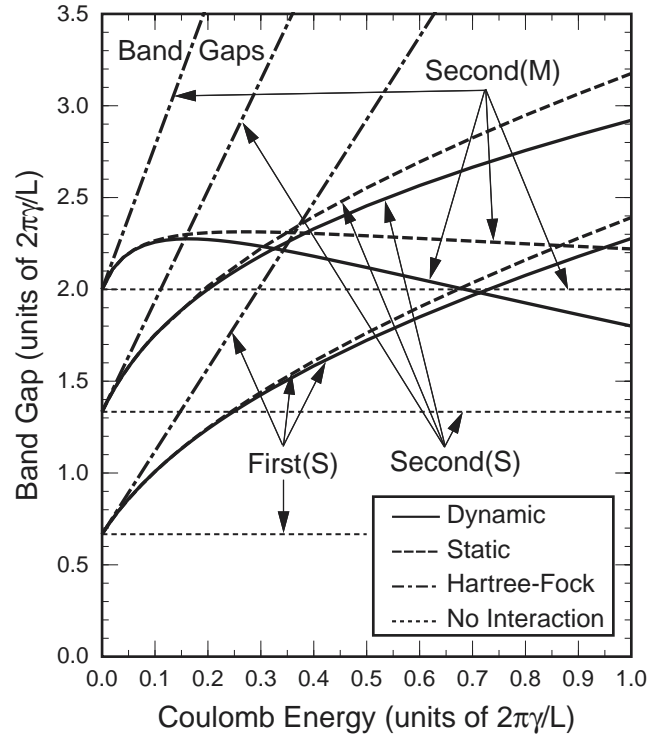


Fig. 2 (Right) The calculated band gaps for the parabolic bands in CN's versus the effective strength of the Coulomb interaction.

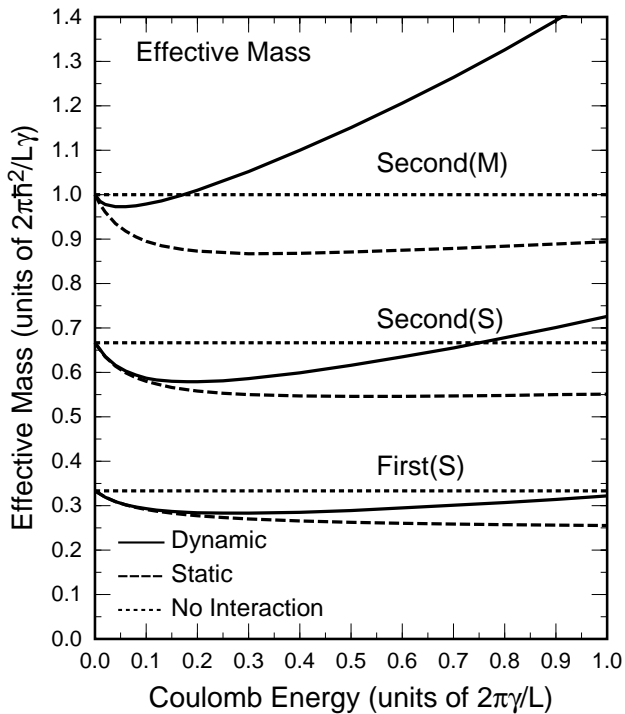


Fig. 3 (Left) The effective mass for the parabolic bands in CN's versus the effective strength of the Coulomb interaction, estimated from the single-particle energy of each band.

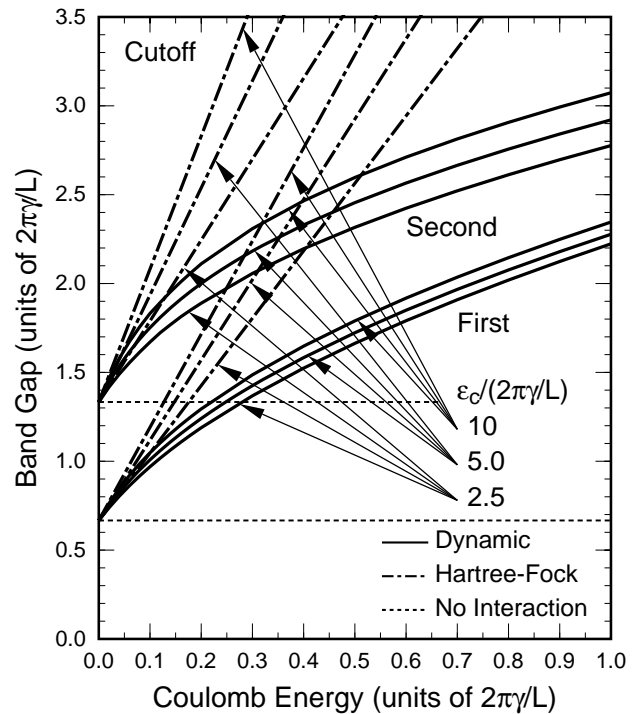


Fig. 4 (Right) The cutoff energy dependence of the first and second band gap in semiconducting CN's. The band gaps are calculated in the HFA and dynamical RPA for $\epsilon_c/(2\pi\gamma/L) = 2.5, 5, \text{ and } 10$.