Bulletin of Pure and Applied Science
Physics, Vol.43D No.2,
July-December 2024 P.90-95
Original Research Article

Print version ISSN 0970 6569
Online version ISSN 2320 3218
Available online at www.bpasjournals.com

Effect of Electron-Phonon Interactions against Electron-Electron Interactions in Carbon Nanotubes

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Received on 20.05.2024, Revised on 21.09.2024, Accepted on 09.10.2024

ABSTRACT

We have studied the effect of electron-phonon interactions against electron-electron interactions in carbon nanotubes. For this purpose we have used renormalization group method combined with a two cut off scaling scheme. This method allowed for low temperature phases without bias. We have studied on metallic single wall nanotubes with short range interactions and their wrapping were armchair or zigzag. We have studied the influence of electron-phonon coupling on low temperature phases of metallic single wall carbon nanotubes. In armchair carbon nanotube we have found that the phases induced by short range electronic correlations turned into a Peierls insulator by electron-phonon coupling. We have presented that the intraband scattering modes caused the softening and the radial breathing mode or the transverse optical mode was soften. In the case of zigzag carbon nanotubes no Peierls instability was found. This indicated that D-Mott phase or charge density wave appeared in zigzag carbon nanotubes. The effect of electron-phonon coupliong in zigzag carbon nanotubes do not produce a phonon softening instability and coupling is significant in this case. The phase diagrams of metallic armchair and zigzag carbon nanotubes are similar in the absence of electron-phonon coupling. We have also studied the behaviors of nanotubes based on renormalization equations became simple for carbon nanotubes. The obtained results were found in good agreement with previous obtained results.

KEYWORDS

Phonon Interaction, Renormalization, Wrapping, Intraband, Peierl Instability, D-Mott Phase, Electron-Phonon Coupling, Phase Diagram.

How to cite this article: Raj H. and Kumar A. (2024). Effect of Electron-Phonon Interactions against Electron-Electron Interactions in Carbon Nanotubes. *Bulletin of Pure and Applied Sciences- Physics,* 43D (2), 90-95.

INTRODUCTION

The effects of electron-phonon interactions for long range and short range carbon nanotubes have studied [1-5] and various phases have been presented, e.g. Mott insulators, D-wave superconductivity and Luttinger liquids. Kamida et al. [6], Barnett e al. [7] and Iyakutti et al. [8] studied and found that electron-phonon interactions are not negligible but leaded to different low temperature phases such as S-wave super conductivity, Peierls

instability [9-13] or Wentzel-Bardeen Singurality [14]. Laird et al. [15] studied and found that carbon nanotubes are quasi onedimensional system with variety of electronic states emerged at low temperatures. They are superconductivity in nano tubes embedded in a Zeolite Matrix [16-19]. A Mott insulatoring state in ultraclean nanotubes [20] and Wigner crystals in semiconducting nanotubes [21]. Varsano et al. [22] studied long range coulomb interaction for an excitonic insulator phase. It was found that by hybridization of nanotube and substrate electrons did not appear and the surface states of the substrate were away from the Fermi energy of the nanotubes. The critical temperatures of the ordered phases were found below and decreased due to the finite lifetimes of quasi particles. Edward Liu et al. [23] studied that conducting steady states of doped bilayer graphene produced non-zero sublattice pseudopin polarization. The electron-electron interactions renormalized this polarization even at zero temperature, when the phase space for electron-electron scattering vanished. It was presented that because of the strength of interlayer tunneling electron-electron interactions produced a negligible influence on the conductivity, which vanished as the carrier number density went to zero. The influence of interactions was weaker than in the comparable cases of single graphene or topological insulators, because the momentum space layer pseudo spin vorticity was 2 rather than one. Ihnatsenka and Kirczennow [24] studied the effect of edge reconstruction and electron-electron interactions on quantum transport in graphene nanoribbons. It was presented that numerical studied of conduction in graphene nanoribbons with constructed edges based on the standard tight binding model of the graphene and the extended Huckel model of the reconstructed defects. It was performed the atomic defects using density functional theory and then explicitly calculated the tight binding parameters used to model electron transport in graphene with reconstructed edges. Hawkins et al. [25] studied defect topologies for armchair and zigzag graphene nanoribbons. It was reported that pentagon and heptagon edge reconstructed to have little effect on the ribbon conductance near the Diracpoint. The role in the conductance quantization was found in experimental observation [26-28] on graphene nanostructures despite the presence of edge imperfections. Dhall et al. [29] studied the electron-phonon interactions in ultraclean suspended nanotubes. It was reported the pronounced electron-phonon interactions in suspended, nearly defect free metallic carbon nanotubes observed through a Kohn anomaly of greater strength than theoretically predicted values. It was found that the regime that did not exhibit a nonadiabatic Kohn anomaly was clearly observed and a regime where the non-adiabatic Kohn anomaly was absent. The enhancement of Raman intensity with gating was observed. Louis et al. [30] studied the universal properties of quantum transport in graphene nanowires that engender subtle universal conductance and its effects. The results showed for three models that described the sublattice of graphene and generated chiral universal symmetries. In nanotechnology it has been allowed the production and control of graphene monolayers with carbon atoms distributed in honey comb lattice [31-32]. Graphene nanotubes have received both experimental and theoretical explanation due to its special electronic transport properties [33-35]. Melnikov et al. [36] studied the influence of the coupling between the tubes and interactions on the localization for Plasmon resonance in them. The physical mechanisms is responsible for the electromagnetic interaction between crossing tubes with zero and non-zero intertube contact conductnces.

METHOD

We have derived effective low energy models for metallic single wall carbon nanotubes from an extended Hubbad model in graphene. The renormalization group analysis with electron-phonon interactions was used for the study. We have analysed renormalization group equations and explained the consequences of the electron-phonon coupling on low temperature phase. We have taken weak short range electron-electron interactions, on site repulsive interactions$\cup$, and nearest neighbor interactions$V_{(1)}$. For free standing nanotubes, the long range coulomb interaction existed. Weak short range interactions were realized by screening the coulomb interaction, by putting single wall nanotubes on the substrate. The nearest neighbor interactions captured the essential physics induced by the long range

interaction. An excitonic insulator phase in model with the long range coulomb interaction appeared in our model. The substrate was chosen such that electrons not to occur, the surface states of the substrate were away from the Fermi energy of the nanotubes. The critical temperatures of the ordered phases were found below due to finite lifetime of quasiparticles. A graphene lattice consisted of two triangular sublattices, A and B sites with basis vectors $a_{\pm} = a\left(\pm\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$, where a is the distance between neighbor equivalent sites and the sublattice offset vector $d = a\left(0, -\frac{1}{\sqrt{3}}\right)$. The hopping Hamiltonian is given by

$$H_0 = -J_0 \sum_{r\in R,\alpha} \sum_{i=1}^{3} \left[c_{A\alpha}^{\dagger}(r) c_{B\alpha}(r+\delta_i) + H.c. \right]$$

.

Where $c_{m\alpha}^{(\dagger)}$ is the annihilation / creation operator of the fermion on sublattice m with spin α, and J_0 is the hopping energy between neighboring sites. The A sites are $R = n_+ a_+ + n\_a\_$ with integers $n_{\pm}$ and their neighboring B sites are at $R + \delta_i (i = 1,2,3)$ with

$\delta_1 = d, \delta_2 = a\_ + d, \delta_3 = a_+ + d$.

Fourier transforming the hopping Hamiltonian leaded to band dispersions $E_{\pm}(k) = \pm|h(k)|$ with

$$h(k) = 2J_0 \cos\left(k_x \frac{a}{2}\right) e^{ik, \frac{a}{2\sqrt{3}}} + J_0 e^{-i\frac{k_y}{\sqrt{3}}}$$

An undoped graphene sheet has point like Fermi surfaces at the Dirac points, where the band dispersion is linear. The on site interaction is

$$H_U = U \sum_{r\in R} \left[n_{A\uparrow}(r) n_{A\downarrow}(r) + n_{B\uparrow}(r+d) B\downarrow x(r+d) \right]$$

And the nearest neighbor interactions are

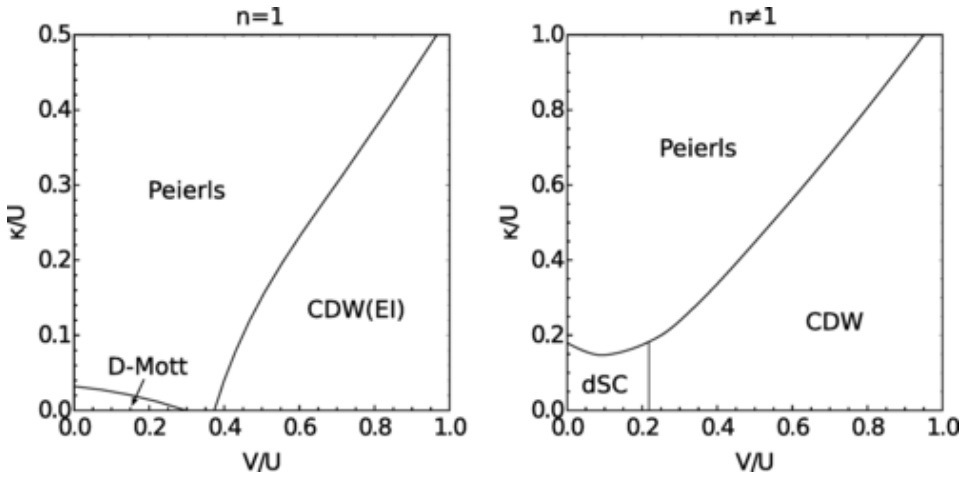
$$H_V = \sum_{r\in R,\alpha\beta} \left[V_{\perp} n_{A\alpha}(r) n_{B\beta}(r+\delta_1) + V \sum_{i=2.3} n_{A\alpha}(r) n_{B\beta}(r+\delta_i) \right]$$

We have assumed $|V|, |V_{\perp}| < U$.

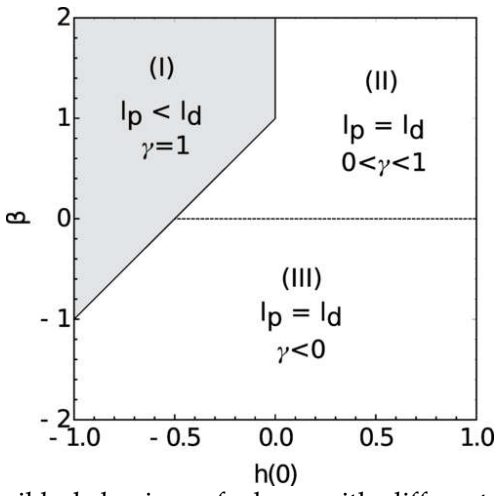
RESULTS AND DISCUSSION

Graph (1) shows the plot of phase diagrams of armchair carbon nanotubes with electron-phonon interactions and couplings. In this graph (1) we have considered $K_1 = K_2 = K$ and the phase in terms of K and $V = V_{\perp}$. The S-Mott Phase between D-Mott and Charge density wave phases immediately disappeared as K is turned on. We have found that when K becomes strong then $-\tilde{c}_{11}^{J}$ and $\tilde{u}_{12}^{+}$ flow to $+\infty$ or in other words $\kappa_1 \to \infty$. The intraband phonons were found soften. The phonon softening leaded to a Peierls lattice distortion with periodicity $\sim \frac{1}{2} k_F^0 \sim \frac{3a}{8\pi}$. k contains contribution of several phonon modes, the divergence of k did not show which of these modes often. Considering the coupling strength and the mode frequencies we have calculated radial acoustic mode, i.e., radial breathing mode is the one that softend for a relatively small radius nearly 4Å. Considering that the coupling strength of radial acoustic mode and its frequency scales as R_0^{-2} and R_0^{-1}. We have found transverse optical mode i.e. in plane optical mode became more dominant for larger radius carbon nanotubes. In case of doped carbon nanotubes the d-wave super conducting phae and the charge density wave phase turned into Peierls states as K becomes large, while they are more stable thant he corresponding phases at half filling. Graph (2) shows the plot of three regimes given by β_i and $h_i(0)$. In region first the standard coupling diverges faster than the instaneous coupling, i.e. $l_p < l_d$ with $Y = 1$. In region second the retarded coupling are divering at l_d but subdominant to the instantaneous ones since $o < y < 1$. In region III hi are irrelevant and renormalized to zero i.e., lp=ld with y<0. Case I gives the phonon driven phase. The phase boundary was affected by the initial part of the renormalization group flow, where the coupling constants do not follow the ansatz. In the case of undoped nanotubes the D-Mott phase, h_2 is always dominant, in case I, since $\beta_2 > 1$. In the charge density wave phase, k_1

are larger than a critical value for h_2 to be dominant since $-1 < \beta_2 < 1$. Since k_1 is responsible for the Peirls distortion this explains charge density wave phase in some more stable than the D-Mott Phase against the Peierls instability. In the case of dope nanotubes h_1 becomes dominant when k_1 is above a critical value since $-1 < B < 1$, while h_2 is again subdominant. The obtained results were compared with previously obtained results of theoretical and experimental research works and were found in good agreement.



Graph 1: Plot of phase diagram for armchair nanotubes vs with electron-phonon interaction and coupling.



Graph 2: Plot of three possible behaviors of phase with different parameter of dependence vs phonon phases driven due to asymptotic solution.

CONCLUSION

We have studied effect of electron-phonon interactions against electron-electron interactions in carbon nanotubes. We have also presented the effect of electron-phonon coupling on low temperature phases in metallic single wall carbon nanotubes. We have found the phase diagrams of armchair and zigzag carbon nanotubes with screened interactions with a weak coupling using renormalizations group method. It was found

that in the absence of electron-phonon coupling two types of carbon nanotubes have same phase diagram. We have derived effective low energy models for metallic single wall carbon nanotubes from an extended Hubbard model in graphene carbon nanotubes. We have utilized a renormalization group method combined with a cut off scaling scheme. We have found that in armchair carbon nanotubes the phase induced by short range electronic correlation, e.g., a D-Mott phase, d-wave and a charge density wave turned into a Peierls insulator by electron-phonon coupling. In the doped carbon nanotubes case more stable Peierls instability were found in comparision of undoped cases. The Peierls instability assisted by electronic scattering. For strong electron-phonon interactions, phonon softening was induced and a Peierls insulator phase appeared in armchair carbon nanotubes. This softening occurred for interaband scattering phonon mode. The obtained results were found in good agreement with previously obtained results of theoretical and experimental research works.

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