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Superconductivity in Transition Metal Doped Nanotubes

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Abstract*— Carbon Nanotubes (CNT's) have attracted a lot of attention of various scientists from all over the world because of its nano size and amazing properties in the various fields of interest. These tubes usually manifest superconductivity at 15 K and 20K but doped with other atoms/ions are showing the transition temperature as high as room temperature. The calculations indicate that smaller the tube diameter, the higher the superconducting temperature. This is due to the greater curvature of the tube, which increases the interaction between electrons and lattice vibrations known as phonons--a property essential for superconductivity. An overview of the problem of the superconductivity in CNT's is discussed in this paper. We have considered a model system Hamiltonian consisting of usual electron (hole) phonon interaction, an interaction between neighbouring titanium (Ti) atoms and an interaction which involves the scattering of cooper pairs with delocalized electrons of Ti atoms. By using Quantum field theory green function formalism, we have obtained the expressions for superconducting order parameter (∆) and transition temperature which shows the strong presence of superconductivity in CNT's.

***Index Terms*—Carbon Nano tubes, Superconductivity, Cooper pair, Meissner Effect, Super Current.**

I. INTRODUCTION

Following the recent discovery [1] of superconductivity in Titanium adsorbed CNT's impressed us to study the phenomenon in detail.Sasaki and his colleagues presented [2] superconductivity in metallic zig zag CNT's where superconducting states are developed locally at both ends of tubes and a normal metal exists in the middle. Ferrier [3] and his co-workershave also shown the evidence of intrinsic superconductivity in suspended ropes of nanotubes where the presence of attractive interactions overcome coulomb repulsion at low temperature and enable investigation of superconductivity in a 1D limit. J.Gonzalez have shown [4] that the interaction among a large number of metallic nanotubes favours the appearance of a metallic phase in the ropes, intermediate between respective phases with spin-density-wave and superconducting correlations.

In particular, the Superconductivity in CNT's, which is a rolled-up graphene sheet and a typical one-dimensional (1D) carbon conductor, is attracting considerable attention [5, 6, and 7] for the following reasons: (1) The curvature resulting from a small diameter (~1 nm) can lead to formation of sp3 hybrid orbitals and σ-π mixed bands. Coupling of these σ-π electrons with radial breathing mode of [8] phonon might bring high Tc .(2) The alignment of the Fermi level (EF) to a van Hove singularity (VHS) can also lead to high Tc due to the presence of an extremely large density [9] of states (DOS). (3) It can provide an insight into the 1D electron correlation.

In the present work, an attempt is made to develop the microscopic theory of carbon nanotube superconductors. We have proposed the model of one-dimensional interacting electron systems for the superconductivity observed in CNT's. We have suppressed the single-particle hopping between neighboring nanotubes in a disordered rope of CNT and conclude that the tunneling takes place in pairs of electrons, which are formed within each nanotube due to the existence of large superconducting correlations.

II. MODEL HAMILITONIAN

The model Hamiltonian of the system has attractive electron-electron interactions, singlet Cooper pair interactions and the enhanced coupling between phonons and electrons of Ti doped CNT's.

$$H = \sum_{q\sigma} \xi_q b^+_{q\sigma} b_{q\sigma} - V \sum_{qq'} b^+_{q\uparrow} b^+_{-q\downarrow} b_{-q'\downarrow} b_{q'\uparrow} + \sum_{\substack{l\,n \\ \sigma\sigma'}} M_{\ln} b^+_{l\sigma} b^+_{n\sigma'} b_{l\sigma'} b_{n\sigma} + \sum_{\substack{\ln\sigma \\ q}} \eta^{\ln}_q \left(b^+_{l\sigma} b_{l\sigma} b_{-q\downarrow} b_{q\uparrow} + h.c. \right) \quad (1)$$

Where $b^+_{q\sigma}\left(b_{q\sigma}\right)$ and denote creation (annihilation) operators for conduction and localized electrons respectively. V is the usual electron phonon interaction. ξ_q denotes the single particle energy ,$M_{\ln}$ is the

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exchange interaction between localized electrons and the last term is an interaction involving scattering of Cooper pairs by delocalized electrons of titanium atoms.

Using Green Functions the following equations of motion are obtained.

$$\left(\omega-\tilde{\xi}_{q_1}\right)\left\langle\left\langle b_{q_1\uparrow}\middle|b^{+}_{q_1\uparrow}\right\rangle\right\rangle_{\omega}=\frac{1}{2\pi}-\Delta\left\langle\left\langle b^{+}_{-q_1\downarrow}\middle|b^{+}_{q_1\uparrow}\right\rangle\right\rangle_{\omega}+U\left\langle\left\langle b^{+}_{-q_1\downarrow}\middle|b^{+}_{q_1\uparrow}\right\rangle\right\rangle_{\omega} \quad (2)$$

$$\left(\omega+\tilde{\xi}_{q_1}\right)\left\langle\left\langle b^{+}_{-q_1\downarrow}\middle|b^{+}_{q_1\uparrow}\right\rangle\right\rangle_{\omega}=-\left(\Delta-U\right)\left\langle\left\langle b_{q_1\uparrow}\middle|b^{+}_{q_1\uparrow}\right\rangle\right\rangle_{\omega} \quad (3)$$

Where

$$\tilde{\xi}_{q_1}=\xi_q V\langle\ n_{q\downarrow}\ \rangle \quad (4)$$

$$\Delta=V\sum_{q'}\ \left\langle b_{-q'\downarrow}\,b_{q'\uparrow}\right\rangle=V\sum_{q'}\ \left\langle b^{+}_{q'\uparrow}\,b^{+}_{-q'\downarrow}\right\rangle \quad (5)$$

$$U=\sum_{\ln}\ \eta^{\ln}_{q}\left\langle b_{n\sigma}\,b_{l\sigma}\right\rangle=\sum_{\ln}\ \eta^{\ln}_{q}\left\langle\ b^{+}_{l\sigma}\,b^{+}_{n\sigma}\right\rangle \quad (6)$$

$$\langle\ n_{q\downarrow}\ \rangle=\left\langle b_{-q\downarrow}\,b_{q\downarrow}\right\rangle$$

Using equations (2) & (3) the superconducting order parameter can be obtained as:

$$\Delta\ =\ \mathrm{V}\sum_{\mathrm{q}}\ \left\langle b^{+}_{q_1\uparrow}\,b^{+}_{-q_1\downarrow}\right\rangle \quad (7)$$

And to evaluate the superconducting order parameter for the finite temperature case, we continue the Green's function of pure imaginary frequencies i ω_{n} i.e. $\omega=\mathrm{i}\,\omega_{\mathrm{n}}$

Thus, on using Poisson summation formulas [10] and contour integration over ω_{β}, Δ can be written as:

$$\Delta=\ N(o)\ V\int_0^{\hbar\omega_{\beta}}\left(\Delta-U\right)\frac{\tanh\ \frac{\beta}{2}\sqrt{\tilde{\xi}_q^2+\left(\Delta-U\right)^2}}{\sqrt{\tilde{\xi}_q^2+\left(\Delta-U\right)^2}}\,d\tilde{\xi}_q \quad (8)$$

Or

$$\frac{1}{N(o)V}=\int_0^{\hbar\omega_B}\frac{\tan h\frac{\beta}{2}\sqrt{\tilde{\xi}_q^2+(\Delta-U)^2}}{\sqrt{\tilde{\xi}_q^2+(\Delta-U)^2}}\,d\tilde{\xi}_q$$

As T $\rightarrow$T$_c$, $\Delta\rightarrow$ 0 we get

$$\frac{1}{N(o)V}=\int_0^{\hbar\omega_B}\frac{\tan h\frac{\beta}{2}\sqrt{\tilde{\xi}_q^2+U^2}}{\sqrt{\tilde{\xi}_q^2+U^2}}\,d\tilde{\xi}_q \quad (9)$$

On integration one gets in the weak coupling limit

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K_B (10)

Where,

ω = average boson (phonon) energy

N (o) = density of states at the fermi level

V = effective pairing potential

λ= N (o) V = electron phonon (boson) coupling constant

For solving the Superconducting transition temperature in Ti adsorbed CNT's, we have used the McMillan formula [11] and calculated the values of T_c for different values of Debye temperatur (θ_D).

Mc-Millan formula:

$T_C =$ (11)

Where θ_D is Debye temperature, λ is the EP coupling constant and μ^* is the coulomb psuedopotential.

Table 1: Superconducting transition temperature (T_C)as a function of Debye temperature (θ_D)

Debye temperature (θ_D)	Superconducting transition temperature (T_C)
200	16.89
400	33.78
600	50.67
800	67.56
1000	84.45
1200	101.3
1400	120
1600	135
1800	154
2000	168
2200	185
2400	206
2600	233
2800	240
3000	257

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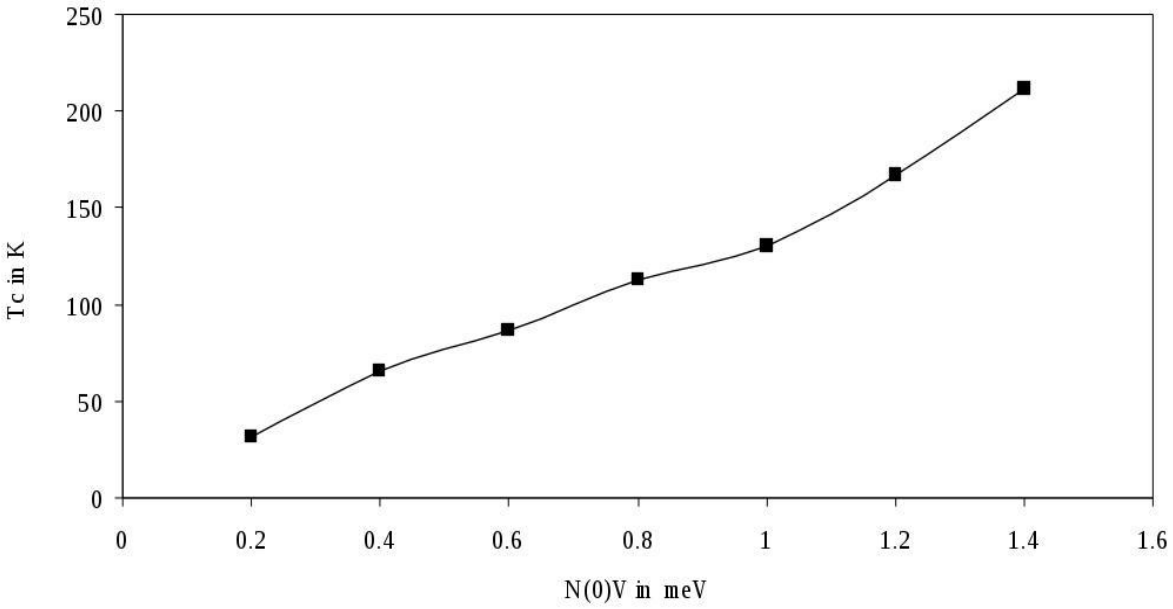
Fig(1): Variation of Transition temperature (Tc) with Density of states (N(0)V)



III. RESULTS & CONCLUSION

We have developed the Bardeen–Cooper–Schrieffer (BCS) formalism for the superconductivity in Ti adsorbed CNT's and have calculated the superconducting transition temperature(T_c) and order parameter by considering a pairing Hamiltonian having interaction describing the scattering of carriers (holes and/or electrons) by delocalized electrons of Ti atoms. The figure (1) shows that value of T_c goes on increasing with increase of N(0)V near the Fermi level which can further be enhanced to room temperature by increasing N(0)V and other parameters responsible of high values of T_c. It is found experimentally that T_c of single-walled CNT's increases [12] exponentially with the increase of the tube diameter because the densities of states near the Fermi energy is inversely proportional to the tube diameter. For the multi-walled CNT's, the Cooper pair hopping between layers enhances the superconducting correlation and increases the superconducting transition temperature, which is consistent with the experimental observation. Moreover the strong hybridization of delocalized electrons of Ti atoms with the atoms of carbon increases the interaction between electrons and excitations responsible for Cooper pairing in Ti doped CNT's and hence increase the transition temperature.

We know that electron-electron correlation via phonons is responsible in forming the cooper pair in conventional superconductors while in high TcCuprates, the elementary excitations magnons,polarons ,excitons etc. are thought to be responsible for Cooper pairing **but** there is no single consensus about pairing mechanism in Ti adsorbed CNT's. Due to which we have used Mc-Millan's formula to calculate the critical temperature in Ti doped CNT's.This research is still unbeatable due to absence of exact pairing mechanism forming the cooper pairs. It is theoretically found in this paper that the transition temperature as high as 270 K can be reached which essentially means that the room temperature superconductivity can be realized with doped CNTs : the dream of every condensed matter physicist.

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