Non-damped Acoustic Plasmon and Superconductivity in Single Wall Carbon Nanotubes

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We show that non-damped acoustic plasmons exist in single wall carbon nanotubes (SWCNT) and propose that the non-damped acoustic plasmons may mediate electron-electron attraction and result in superconductivity in the SWCNT. The superconducting transition temperature $T_c$ for the SWCNT (3.3) obtained by this mechanism agrees with the recent experimental result (Z. K. Tang et al, Science \textbf{292}, 2462(2001)). We also show that it is possible to get higher $T_c$ up to 99 K by doping the SWCNT (5.5).

PACS numbers: 74.20.Mn, 73.20.Mf, 74.70.Wz

As a novel and potential carbon material, carbon nanotubes (CNTs) have received a great deal of attention, and many of their unique properties have been found\textsuperscript{1} since they were first discovered\textsuperscript{2}. The possibility of superconductivity in CNTs has been discussed based on BCS theory (phonon-mediated)\textsuperscript{3,4}. The theoretical prediction given in Ref.\textsuperscript{3} about the superconductivity in the smallest SWCNTs\textsuperscript{5,6} showed that $T_c$ can be up to of 15 K\textsuperscript{7}. This important experimental finding requires us to explore a new mechanism for the superconductivity in the SWCNTs. In this Letter we suggest that the non-Landau damped acoustic plasmons (NDAPs) is responsible for the appearance of the superconductivity in the SWCNTs.

The plasmon mediated mechanism for High-$T_c$ superconductivity has attracted much attention\textsuperscript{8,11}. Compared to the original BCS phonon mechanism, a two dimensional (2D) plasmon with high frequency is favored by the ion-electron mass ratio $M/m^*$, as well as by a greater energy range, to mediate the electron-electron attraction. The possibility of high-$T_c$ superconductivity in the thin wires and quasi-1D organic materials based on the NDAP\textsuperscript{3,4} mechanism was predicted ten years ago\textsuperscript{4,5}. The acoustic plasmons in cylindrical quantum-well wires and in CNTs have also been discussed in Refs.\textsuperscript{6,8}.

The acoustic plasmon is the resonant excitation between two kinds of different charge carrier\textsuperscript{9}. The smallness of the radius of SWCNT gives rise to widely separation of transverse single-particle energy levels. An electron in particular transverse energy level $E_n$ will have a corresponding effective longitudinal Fermi momentum $\hbar k_n = \sqrt{2m(E_F - E_n)}$ within the total energy limited by the Fermi energy $E_F$, where $m$ is the mass of electron. The number of the effective longitudinal Fermi levels, corresponding to the number of kinds of the conductive electrons, is equal to the number of transverse energy levels below Fermi energy. A longitudinal disturbance with wavevector $q$ will transfer a momentum $\hbar q$ to each electron. Only those electrons within $\hbar q$ neighborhood of the 1D effective Fermi surface $k_n$ are allowed to have a real transition, with each of them gaining an energy between $\hbar^2 q^2/2m (k_n - q/2)$ and $\hbar^2 q^2/2m (k_n + q/2)$. In the limit of $q \ll k_n - k_{n+1}$, if the disturbance has a frequency $\omega \sim \hbar q k_n/m$, all these electrons within $\hbar q$ neighborhood of the 1D effective Fermi surface $k_n$ will be resonantly excited. If we denote the polarizability of system by $\chi^{(0)}(q,\omega)$, the charge density induced by perturbing external potential $\phi_{ex}(q,\omega)$ is

$$\rho_{in}(q,\omega) = -q^2 \chi^{(0)}(q,\omega) \phi_{ex}(q,\omega)/\varepsilon(q,\omega).$$

The resonance is determined by zero of the dielectric function $\varepsilon(q,\omega) = 1 + 4\pi \chi^{(0)}(q,\omega)$. The mode is obviously dominated by the interplay of the transverse energy levels labeled by $n$ and $n+1$. The effective perturbing field will cause a parallel polarization in the longitudinally oscillating particles with a higher characteristic frequency $\hbar q^2 m/(k_n - q/2)$ at the $n$ Fermi surface but antiparallel polarization in those with a lower characteristic frequency $\hbar q^2 m/(k_{n+1} + q/2)$ at the $(n+1)$ Fermi surface. Thus

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the oscillating particles in level \( n \) and \( n+1 \) will vibrate against each other in the \( n \)th resonating mode, resulting in the formation of NDAPs. The wider of separation of transverse levels, the more electron within the neighborhood of the effective 1D Fermi surface participate in resonant excitation and result in the higher frequency of the NDAP. Thus the SWCNTs, being a 1D system, is a good candidate for existence of the NDAPs.

Because the frequency of the NDAPs is much higher than the phonon frequency and it is non Landau damped, it will be more suitable to mediate e-e attraction. In this Letter we introduce a simple potential to model the quasi-1D structure of the SWCNTs, and apply the random phase approximation (RPA) and the linear response theory to show the existence of NDAPs in SWCNT(3,3). Then we propose that the NDAPs may mediate e-e attraction and result in the superconductivity in the SWCNTs. The superconducting transition temperature \( T_c \) for SWCNT (3,3) based on this mechanism is calculated and compared with the recent experimental result \( [6] \). The possibility for obtaining high \( T_c \) for doped SWCNTs is also suggested.

The model used is as follows. The electrons are totally confined in an effective potential with cylindrical surface of radius \( \rho_0 \) of a SWCNT and are free to move along the axis of the SWCNT which we assume to be the \( z \) axis. The single particle Schrödinger equation reads

\[
\begin{align*}
-\frac{\hbar^2}{2m} \left[ \frac{\partial^2}{\partial z^2} + \frac{1}{\rho_0^2} \frac{\partial^2}{\partial \varphi^2} \right] \Psi(\rho_0, \varphi, z) &= E \Psi(\rho_0, \varphi, z), \quad (1)
\end{align*}
\]

where \((\rho_0, \varphi, z)\) are cylindrical coordinates. The corresponding energy eigenvalue is given by

\[
E_n(k_z) = \frac{\hbar^2 k_z^2}{2m} + E_n,
\]

where \( E_n = \frac{n^2 \hbar^2}{2m \rho_0^2} \) is the transverse energy level, \( n \) is an integer.

We now consider the NDAPs as in Refs. \( [12, 13] \). The Hamiltonian of the electron gas confined on the surface of cylinder is

\[
H = -\sum_{j=1}^{N} \frac{\hbar^2 \nabla_j^2}{2m} + \frac{1}{2} \sum_{j \neq k} \frac{e^2}{|\mathbf{r}_j - \mathbf{r}_k|} + H_+,
\]

where the second term is the Coulomb interaction between electrons and the last term is the contribution from the uniformly distributed positive charge background. By the RPA and the linear response theory, we get a dielectric function as follows \( [13] \)

\[
\varepsilon(q, \omega) = 1 + v(q) \sum_K u_k (E_{k+q} - E_k - (\hbar \omega + i\eta))^{-1}
+ (E_{k+q} - E_k + (\hbar \omega + i\eta))^{-1},
\]

where \( \eta = 0^+ \), and

\[
v(q) = \frac{e^2}{2\pi L} \int_0^{2\pi} d\phi \int_{-\infty}^{+\infty} dz \frac{e^{iqz}}{\sqrt{z^2 + 2\rho_0^2(1 - \cos\phi)}},
= \frac{2e^2}{L} K_0(\sqrt{2}\rho_0 q), \quad (5)
\]

where \( L \) is the length of the tube and \( K_0(x) \) is the second class zero-th Bessel function. The form of this \( \varepsilon(q, \omega) \) is the same as in 3D system except the difference in \( v(q) \).

Under zero temperature approximation, we obtain that

\[
\varepsilon_1 = 1 + \frac{2K_0(\sqrt{2}q_0 a)}{\pi q a_0} \sum_{E_n < E_F} \ln \left| \frac{s^2 - u_n^+ - u_n^-}{2s^2} \right|,
\]

and an imaginary part

\[
\varepsilon_2 = \begin{cases} \frac{2K_0(\sqrt{2}q_0 a)}{\pi q a_0} \sum_{n \ if \ s \ lies \ between \ u_n^+ \ and \ u_n^-} 1 & \text{if } s \ lies \ between \ u_n^+ \ and \ u_n^- \\ 0 & \text{otherwise} \end{cases},
\]

where \( s = \omega/q, a_0 \) is the Bohr radius and \( u_n^\pm = u_n \pm \frac{\hbar}{2m} \), \( u_n = [E_F - E_n]/m \]1/2.

Obviously, \( \varepsilon_1 \rightarrow \pm \infty \), as \( s \rightarrow u_n \). Here \( s \) lies between \( u_n^+ \) and \( u_n^- \) or between \( u_{n+1}^+ \) and \( u_{n-1}^- \). In each case, there always exists a point \( \varepsilon_1 = 0 \) between \( \varepsilon_1 = -\infty \) and \( \varepsilon_1 = +\infty \). In the former case, \( \varepsilon_2 \neq 0 \) which corresponds to a damped mode; but in the second case, the mode \( \varepsilon_2 = 0 \) is undamped. As \( q \) becomes sufficiently large the damping regions overlap, so all the acoustic plasmon will be damped, and there exists a maximum: \( q_{max} = m(u_n - u_{n+1})/\hbar \). The condition for the existence of NDAP is \( \hbar q/m \ll u_n - u_{n+1} \). This means that there are two or more transverse level below the Fermi energy of the system which must be sufficiently widely separated so that each level can house a large number of electrons with different \( k_z \), leading to the collective nature of the NDAP.

Substituting the radius of armchair SWCNT (3,3), \( \rho_0 = 2.1 \AA \), into expression of \( E_n \), we get \( E_0 = 0, E_1 = 0.858 \text{ ev}, E_2 = 3.43 \text{ ev}, E_3 = 7.72 \text{ ev} \). For a 1D system, if we denote the line density of the electrons in the system by \( n_1 \), then \( E_F = n_1^2 \omega_{NDAP}^2, \) \( \omega_{NDAP} = \frac{\hbar q_0}{m} \). If there are \( N \) electrons per cell, then \( n_1 = N/a, \) for SWCNT (3,3), \( a = 2.52\AA \). Taken \( N = 2 \), then we get that \( E_F = 5.88 \text{ ev} \). This means there are three transverse energy levels below the Fermi energy. Let \( \varepsilon_1 \) and \( \varepsilon_2 \) equal to zero, we can get the dispersion curves of NDAP as shown Fig. \( [5] \). From Fig. \( [5] \) we obtain the \( \omega_{NDAP} = 3.9 \times 10^{15} \text{ Hz} \), which is much higher than the frequency of phonon.
where changing the NDAPs, leading to electrons pairing. We superconducting transition temperature as the units of \( \lambda \), and \( (0) \).

Following the usual BCS theory \([20]\), we can get the
\[
3 = \frac{1}{2} \sum q \int dq \int dq' \frac{\omega}{\omega_{NDAP}}.
\]

For SWCNT(3,3), as shown above one has \( \omega_{NDAP} = 3.9 \times 10^{15} \text{ Hz} \) and hence we have \( \lambda = 0.171 \) and \( \mu^* = 0.036 \). Substituting them into to Eq. (7), we get \( T_c = 19 \text{ K} \), which agrees roughly with the experiment result \( T_c = 15 \text{ K} \) reported in Ref. [2].

We finally discuss how to get higher \( T_c \) in the SWCNTs. For SWCNT (5,5) with radius of 3.39 Å, the separation of transverse energy levels is not wide as SWCNT (3,3). Its transverse energy levels are \( E_0 = 0, E_1 = 0.329 \text{ ev}, E_2 = 1.32 \text{ ev}, E_3 = 2.96 \text{ ev}, E_4 = 5.26 \text{ ev}. \) Taking \( k_F = .831 \times 10^{10} \text{ m}^{-1} \) as in Ref. [3], we get \( E_F = 2.61 \text{ ev} \) under which there are three transverse energy levels. Substituting these parameters into the expression of \( \omega(q, \omega) \), we can obtain the dispersion curves of the NDAPs for SWCNT (5,5) as shown in Fig. 2 and \( \omega_{NDAP} = 1.5 \times 10^{15} \text{ Hz} \). Then we have \( \lambda = 0.148, \quad \mu^* = 0.039 \) and \( T_c = 1.3 \text{ K} \). Thus the value of \( T_c \) is only 1/15 of that of SWCNT(3,3). In fact, as the radius of SWCNT increases, the separation of transverse energy levels decreases, so that \( \omega_{NDAP} \) becomes lower and leads \( T_c \) lower. This conclusion is in agreement with that obtained in Ref. [2].

![FIG. 1. The dispersion curves of NDAP for SWCNT (3,3) with radius of 2.1 Å, transverse energy levels \( E_0 = 0, E_1 = 0.858 \text{ ev}, E_2 = 3.43 \text{ ev} \) and \( E_F = 5.88 \text{ ev} \), where the units of \( \omega \) and \( q \) are \( 10^{15} \text{ Hz} \) and \( 10^{19} \text{ m}^{-1} \) respectively.](image)

![FIG. 2. The dispersion curves of NDAP for SWCNT (5,5) with radius of 3.39 Å, transverse energy levels \( E_0 = 0, E_1 = 0.329 \text{ ev}, E_2 = 1.32 \text{ ev}, E_3 = 2.96 \text{ ev} \) and \( E_F = 2.61 \text{ ev} \). The units of \( \omega \) and \( q \) are \( 10^{15} \text{ Hz} \) and \( 10^{19} \text{ m}^{-1} \) respectively.](image)

For 1D systems, \( g(0) = \sqrt{\frac{m_{e} k^2}{2 \hbar^2 \pi^2}} \). To estimate \( T_c \), we need to know the e-e attraction strength. Suppose that the strength is \( V_0 \) and zero in the effective attraction range \( l \) and outside respectively. Similar to the calculation for exchanging Pi meson between nucleons, we can get 
\[
\cot \left( \frac{m_{e} k^2}{2 \hbar^2 \pi^2} \right) = \frac{B}{V_0} \Rightarrow \lambda = g(0) V \zeta \omega_{NDAP}, \quad l \leq \frac{k_F}{V_0^2} \simeq \frac{\omega_{NDAP}}{\omega_{NDAP}}, \quad \text{where } \Delta p = \text{ change of electron momentum}.
\]

Finally, we obtain 
\[
\lambda = g(0)V \zeta \omega_{NDAP}.
\]

For SWCNT(3,3), as shown above one has \( \omega_{NDAP} = 3.9 \times 10^{15} \text{ Hz} \) and hence we have \( \lambda = 0.171 \) and \( \mu^* = 0.036 \). Substituting them in to 

Eq. (7), we get \( T_c = 19 \text{ K} \), which agrees roughly with the experiment result \( T_c = 15 \text{ K} \) reported in Ref. [2].

We finally discuss how to get higher \( T_c \) in the SWCNTs. For SWCNT (5,5) with radius of 3.39 Å, the separation of transverse energy levels is not wide as SWCNT (3,3). Its transverse energy levels are \( E_0 = 0, E_1 = 0.329 \text{ ev}, E_2 = 1.32 \text{ ev}, E_3 = 2.96 \text{ ev}, E_4 = 5.26 \text{ ev}. \) Taking \( k_F = .831 \times 10^{10} \text{ m}^{-1} \) as in Ref. [3], we get \( E_F = 2.61 \text{ ev} \) under which there are three transverse energy levels. Substituting these parameters into the expression of \( \omega(q, \omega) \), we can obtain the dispersion curves of the NDAPs for SWCNT (5,5) as shown in Fig. 2 and \( \omega_{NDAP} = 1.5 \times 10^{15} \text{ Hz} \). Then we have \( \lambda = 0.148, \quad \mu^* = 0.039 \) and \( T_c = 1.3 \text{ K} \). Thus the value of \( T_c \) is only 1/15 of that of SWCNT(3,3). In fact, as the radius of SWCNT increases, the separation of transverse energy levels decreases, so that \( \omega_{NDAP} \) becomes lower and leads \( T_c \) lower. This conclusion is in agreement with that obtained in Ref. [2].

However, if one fills the tube with some alkali metallic elements so that the electron can move freely not just on the tube surface but in the whole cylinder, the single particle Schrödinger equation reads

\[
H = H_1 + H_2 + H_3
\]

where \( H_1 = \sum_{k,\sigma} E_k C_{k,\sigma} C_{k,\sigma}^+ \) is the kinetic energy of electrons,

\[
H_2 = -\frac{1}{2} \sum_{q, k_1, k_2, \sigma} V_{NDAP}(q) C_{k_1+q, \sigma_1}^+ C_{k_2-q, \sigma_2}^+ C_{k_2, \sigma_2} C_{k_1, \sigma_1}
\]

is the e-e attraction by exchanging the NDAPs with

\[
V_{NDAP} = \begin{cases} \text{Const.} \frac{V}{\omega_{NDAP}} & \text{in the } 2\hbar\omega_{NDAP} \text{ energy shell} \\ 0 & \text{otherwise} \end{cases}
\]

and

\[
H_3 = \frac{1}{2} \sum_{q, k_1, k_2, \sigma_1, \sigma_2} V^c(q) C_{k_1+q, \sigma_1} C_{k_2-q, \sigma_2} C_{k_2, \sigma_2} C_{k_1+q, \sigma_1}
\]

is the coulomb interaction between electrons with

\[
V^c(q) = \begin{cases} 2c(q)/\omega(q, 0) & \text{if } E_{k_1}, E_{k_2} < E_F \\ 0 & \text{otherwise} \end{cases}
\]

where \( c(q) = 4\pi p_0 K_0(\sqrt{2}p_0 q) \) and \( \omega(q, 0) \) is the static dielectric function.

Following the usual BCS theory \([20]\), we can get the superconducting transition temperature as

\[
k_B T_c = 1.13 \hbar \omega_{NDAP} \exp \left( \frac{-1}{\lambda - \mu^*} \right),
\]

where \( \lambda = g(0)V, \quad \mu^* = \frac{g(0) Y}{1 + \ln(E_F^*/\hbar \omega_{NDAP})}, \quad \mu = \frac{g(0)}{\pi} \int_0^{2k_F} V^c(q) dq \), \( g(0) \) is the electron state density on the Fermi surface.
\[
\frac{\hbar^2}{2m} \left[ \frac{\partial^2}{\partial z^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right] \Psi(\rho, \varphi, z) = E \Psi(\rho, \varphi, z).
\]  

We can also make a similar calculation as given above. For this situation the \( V^*(q) \) appearing in Eqs. (3) and (4) changes its form. Under such condition, for the doped SWCNT(5,5) with radius of 3.39 \( \text{Å} \), the lowest transverse energy levels are \( E_{01} = 1.904 \text{ ev}, \ E_{11} = 4.831 \text{ ev}, \ E_{21} = 8.678 \text{ ev}, \) where the subscript of \( E_{n,m} \) are the radial and angular quantum numbers respectively. If a suitable conductive electron number density is chosen, there will be two or more transverse energy levels under the Fermi level, e.g. \( E_F = 5.88 \text{ ev} \). Substituting this parameters into the expression of \( \varepsilon(q, \omega) \), we can obtain the dispersion curve of NDAP for doped SWCNT (5,5) and get \( \omega_{NDAP} = 4.45 \times 10^{15} \text{ Hz} \). Then we have \( \lambda = 0.195 \), \( \mu^* = 0.027 \) and hence \( T_c = 99 \text{ K} \). Its \( T_c \) is much higher that of undoped SWCNT(5,5). This means it is possible to raise the superconducting transition temperature \( T_c \) of the SWCNTs by doping with some alkali metallic elements.

To summarize, we have obtained the dispersion curves of the non damped acoustic plasmons in SWCNTs, and proposed a possible new mechanism for superconductivity in these SWCNTs in which the electron-electron attraction is mediated by the NDAPs. The smallness of the radius of SWCNT gives rise to widely separation of transverse single-particle energy levels. The wider separation of transverse level, the more electrons within the neighborhood of the effective 1D Fermi surface participate in resonant excitation and result the higher frequency of NDAPs. Moreover, if filling the SWCNTs with alkali metallic elements so that the electron can move freely in the whole cylinder, there is much wider separation of transverse level and leads much higher frequency of the NDAPs. However, if the transverse energy level separate too wide so that there is only one level under the Fermi surface, it will lose the NDAP.

Because the frequency of the NDAPs is much higher than the frequency of phonon, it is more suitable to mediate the e-e attraction. The superconducting transition temperature \( T_c \) for SWCNT(3,3) obtained by the NDAP mechanism is in agreement with the experimental result in Ref. [6]. We have also pointed out that the doped SWCNTs will have much higher transition temperature, if suitable doped materials are chosen so that there are two transverse energy levels just under the Fermi surface. The value of \( \omega_{NDAP} \) depends on transverse energy level structure below Fermi energy, but it is independent of the Fermi energy. However the coupling strength of electron pair is in inverse proportion to \( E_F \). So a quasi-1D system which exists two sufficient separated transverse energy levels under Fermi energy, but its Fermi energy is not very high, will have higher \( T_c \). For Example, taking \( E_F = 5.0 \text{ ev} \) for doped SWCNT(5,5), \( \omega_{NDAP} \) is still \( 4.45 \times 10^{15} \text{ Hz} \), but \( T_c \) is higher than 200 K.

The authors are grateful for hospitality and support of the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy, where this work was carried out. Sheng thanks Yu Lu, T. Xiang, and S.Y. Lou for useful discussion. The work is also supported in part by funds from Pandeng Project of China, NSFC and Zhejiang Provincial Natural Science Foundation of China.

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