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Phonon-Raman Scattering in a Nested Fermi Liquid

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Abstract

The spectral density function for the $q = Q$ phonon besides the usual $q = 0$ Raman active phonon is calculated in a nested Fermi liquid theory. It has been shown that the phonon self-energy in the later case vanishes where as it gives rise to a finite contribution in the former which is manifested in the particle-hole polarisability. The Raman intensity is computed and compared with the experimentally observed spectrum which successfully explains the frequency softening of the $500cm^{-1}$ phonon in the deoxygenated sample of YBCO above the superconducting transition temperature.

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Raman scattering in high T_c oxides [1] shows several unusual features in the normal state as well as in the superconducting state. In the normal state, a rather large but constant background intensity which extends up to nearly 1 eV [2] has been observed. This could be attributed to the scattering of the charge carriers in the system [3]. Moreover, in the case of YBCO compound, some of the phonon peaks ride over the constant background intensity. These phonon peaks show Fano line shapes indicating a strong electron-phonon interaction in the system. Recently Altendorf et al [4] have studied the temperature dependence of $340cm^{-1}$ and $440cm^{-1}$, $500cm^{-1}$ phonons in different crystals of $YBa_2Cu_3O_\delta$ ($6.7 \leq \delta \leq 7.0$), which show unusual behaviour. Below the superconducting transition temperature (T_c), the $340cm^{-1}$ phonon shows softening where as the $440cm^{-1}$ and the $500cm^{-1}$ phonons harden in oxygenated samples. Furthermore, the later phonons show softening in the deoxygenated samples at temperatures which are well above their T_c's, i.e., in the normal state. From the measurement of the Raman shift, the line width and the Fano asymmetry parameter in different samples of YBCO, they observed that the above two sets of phonons show almost opposite behaviour to each other. This behaviour strongly depends on the doping concentration and hence it is argued [4] that the $440cm^{-1}$ and $500cm^{-1}$ phonons interact with a different set of electrons than does the $340cm^{-1}$ phonon.

A theoretical model for the normal state as well as the superconducting state is needed for an explanation of the Raman data. Unfortunately, at present time we are far away from the proper understanding of the high T_c superconductors even though many

theoretical models have been proposed [5]. However, due to the anomalous normal state properties, it is believed that the usual Fermi liquid may not be a good candidate to explain these materials. A specific model which accounts for the anomalies of the normal state such as the flat behaviour in ω and T of the Raman continuum [6], the resistivity [8] as well as the optical data [7] etc. assumes the electron-electron scattering in the substantial region of the Fermi surface where it allows nesting, i.e., the nested Fermi liquid (NFL) theory [8]. This is supported by the band theory calculations in the 123 compound [9]. The Hamiltonian which describes the nested Fermi liquid [8] is given by

$$H_e = \sum_{k,\sigma} \xi_k c^\dagger_{k,\sigma} c_{k,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

where $U > 0$, denotes the on site Coulomb repulsion, $c^\dagger_{k,\sigma}(c_{k,\sigma})$ are the creation (annihilation) operators for an itinerant electron or hole within a band ξ_k of width W and $\xi_k = \epsilon_k - \mu$.

In the case of quasi-particles on a Fermi surface that exibits nesting i.e., $\epsilon_k \pm \epsilon_{k+Q} \simeq 0$, there exists an extended region of the phase space which enhances the electron-electron cross section and also alters the constraints on the momentum integration, ultimately modifying the frequency and the temperature variation of quasi-particle life time. This is obvious from the polarisability in a nested Fermi liquid which has the same form as that of the marginal Fermi liquid proposed by Varma and his co-workers [3]. Deviations from perfectly parallel sections of the Fermi surface will yield a cross over temperature T^* below which ordinary Fermi liquid behaviour should set in, thus assuring a finite

quasi-particle weight z_k at zero temperature. This may account for the cross over in resistivity from T to T^2 seen in some of the high T_c compounds [10].

In order to calculate the Raman scattering amplitude, it is necessary to evaluate the phonon response in the system which will depend on the coupling of phonons to the charge carriers. The Hamiltonian for usual electron-phonon coupled system is given as

$$H_p = \sum_q \omega_q a_q{}^\dagger a_q \tag{2}$$

$$H_{e-p} = g \sum_{k,q,\sigma} c^\dagger_{k+q,\sigma} c_{k,\sigma} (a_q + a_{-q}{}^\dagger) \tag{3}$$

$a_{-q}{}^\dagger(a_q)$ are the qth creation (annihilation) operators for phonon with the frequencies ω_q, g being its coupling to the charge carrier density.

Usually, in normal metals the scattering of light [11] proceeds as follows: The incident photon excites an electron-hole pair, which either emits or absorbs a phonon due to the electron-phonon interaction in the system. Finally, the electron and hole recombine giving rise to the scattered photons. In such a process the scattered intensity of the photon will be proportional to the sum of the imaginary part of the particle-hole polarisability and the phonon spectral density function, both evaluated at $q = 0$ (Fig.1(a)). But in a nested Fermi liquid, besides the $q = 0$ optic phonon there exists an another one for $q = Q$ which is Raman active. The coupling of the later phonons to the charge carriers is same as that of the former, but the self-energies in the two cases differ remarkably. This is obvious due to the fact that the momenta in eqn.(2-3) take an extra value Q

because of the Fermi surface nesting. Hence the Hamiltonian for the coupled electron-phonon system in a nested Fermi liquid is same as that of eqn.(2-3) when q is replaced by Q. Thus, in the present case, Raman intensity will acquire an additional contribution coming from the sum of the imaginary part of the particle-hole polarisability for $q = Q$ and the spectral density function for $q = Q$ phonons (Fig.1(b)).

For the evaluation of the phonon response of the system, one must therefore consider both types of phonons and calculate the self-energies they acquire due to the interaction with the charge carriers present in the system. The phonon propagator is given as

$$D_q(\omega) = (\omega_q/\pi)[\omega^2 - \omega_q^2 - \Pi(q,\omega)]^{-1} \tag{4}$$

where $\Pi(q,\omega)$ is the phonon self energy arises due to the electron-phonon interactions. The phonon self-energy is evaluated with the help of the diagonal part of the electronic Hamiltonian which yields

$$\Pi(q,\omega) = 4\pi g^2 \omega_q \sum_{k,\sigma} \frac{< n_{k+q} > - < n_k >}{\omega + \epsilon_{k+q} - \epsilon_k} \tag{5}$$

where $< n_k >$ is the Fermi-Dirac distribution. This expression vanishes for $q = 0$ which implies that the particle-hole polarisability $\chi^{p-h}(q,\omega)$ for $q = 0$ also vanishes. On the other hand, for $q = Q$ phonons, the self-energy exists. The imaginary part of the phonon self-energy in the later case is obtained by carrying out the summation which yields

$$Im\Pi(Q,\omega) = -(\frac{4\pi g^2 N(0)}{\omega_Q})\omega_Q^2 \tanh(\frac{\omega}{4T}) \tag{6}$$

where N(0) is the density of states at the Fermi level which is assumed to be constant and ω_Q being the frequency of the $q = Q$ phonons. This shows that the particle-hole polarisability for $q = Q$ case is similar to that of the marginal Fermi liquid which is given as

$$Im\chi^{p-h}(Q,\omega) = -(\frac{\pi N(0)}{2}) \tanh(\frac{\omega}{4T}) \tag{7}$$

The real part of the phonon self-energy is calculated with the help of Kramers-Kronig analysis.

Once the phonon self energies are known, the Green's functions and hence the spectral density functions are calculated. The spectral density function which is the imaginary part of the Green's function is given as

$$S(0(Q),\omega) = -2ImD_{q=0(Q)}(\omega + i\eta_{0(Q)}) \tag{8}$$

$$= -\frac{2\omega_{0(Q)}(2\omega\eta_{0(Q)} + Im\Pi(0(Q),\omega))}{\pi([\omega^2 - \omega_{0(Q)}^2 - \eta_{0(Q)}^2 - Re\,\Pi(0(Q),\omega)]^2 + [2\omega\eta_{0(Q)} + Im\Pi(0(Q),\omega)]^2)} \tag{9}$$

where $\eta_{0(Q)}$ are the intrinsic widths of the phonons with frequencies ω_0 and ω_Q. Thus with the knowledge of the polarisabilities and the phonon spectral density functions the Raman intensity in a nested Fermi liquid is calculated. The expression for the Raman intensity $I(\omega)$ is given by

$$I(\omega) \sim (1 + n(\omega))[-Im\chi^{p-h}(0,\omega) - Im\chi^{p-h}(Q,\omega) + S(0,\omega) + S(Q,\omega)] \tag{10}$$

where $n(\omega)$ is the Bose factor, $\chi^{p-h}(0(Q),\omega)$ being the polarisabilities in the particle-hole channel for $q = 0$ and $q = Q$ respectively and $S(0(Q),\omega)$ are the corresponding spectral density functions for both the phonons.

The change in Raman intensity due to the variation in phonon frequency at different temperatures is depicted in Figs.2(a,b). The basic feature observed here is the appearance of a constant background intensity which can be attributed to the scattering of charge carriers in the system since it is an outcome of the particle-hole polarisability due to nesting of the Fermi surface. It should also be noted that both the phonons ride over the background intensity. As it can be seen from Figs.2(a,b) that there are changes in the frequency as well as in the line width of the $q = Q$ phonon on varying the temperature where as there is no change for the case of the $q = 0$ phonon. This is due to the fact that the particle-hole polarisability and hence the phonon self-energy vanishes for $q = 0$ but for $q = Q$ it is finite. Of course, an intrinsic width ($\eta_{0(Q)}$) has been provided to both the phonons besides the natural one which comes out from the imaginary part of the self- energies otherwise the $q = 0$ phonon would have been observed as a δ-function peak in the Raman spectra. On reducing the temperature, the intensity of the $q = Q$ phonon decreases and its frequency hardens with broadening in the line width for ($\omega_Q = 2\omega_0$) (Fig.2(a)) but in the case where ($\omega_0 = 2\omega_Q$)(Fig.2(b)) it softens with again broadening in the line width. The frequency softening of the $q = Q$ phonon is in accordance with the experimentally observed spectrum [4] which could be associated with the nesting of the Fermi surface in the high T_c materials.

In this letter, an attempt has been made to explain the frequency softening of the $500cm^{-1}$ phonon in the deoxygenated sample of YBCO, observed in the normal state Raman spectra [4]. It seems that the nested Fermi liquid theory successfully accounts for this observation. This is due to the fact that a broad electronic continuum can be derived in the frame work of the model. Also, many of the rare earth and transition metals such as Dy, Er and Y which have nested Fermi surface also show constant background intensity in the Raman spectra experimentally [12].

The nested Fermi liquid proposed by Ruvalds et al [8], is valid at a temperature which is higher than twice of the SDW/CDW gap. Therefore, since the validity criteria for the theory as a function of temperature and electron coupling suggest that the higher order corrections may be particularly important at low temperature near the phase transition instability, it requires further study in view of the SDW/CDW phases where one has considerable Fermi surface nesting. It is worth while to extend this analysis to more sophisticated cases such as the spin bag calculations [13]. However, the electron-phonon coupling in this case for $q = Q$ will be different from the usual one since it will be directly proportional to the SDW/CDW gap [14]. Such calculations in a correlated metallic state have already been carried out in an earlier paper [15].

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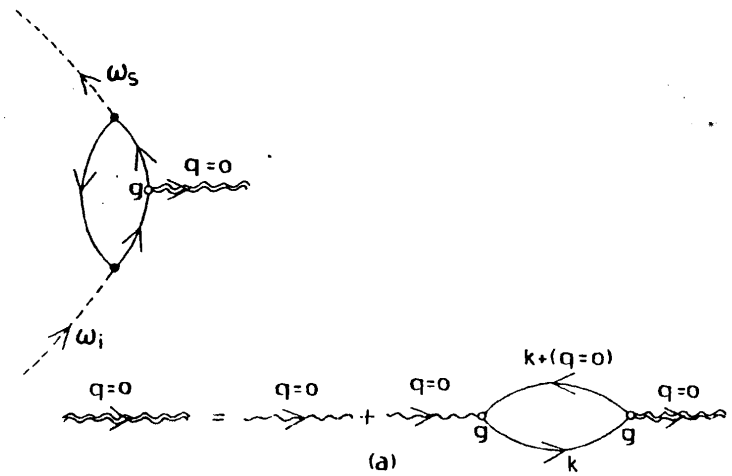
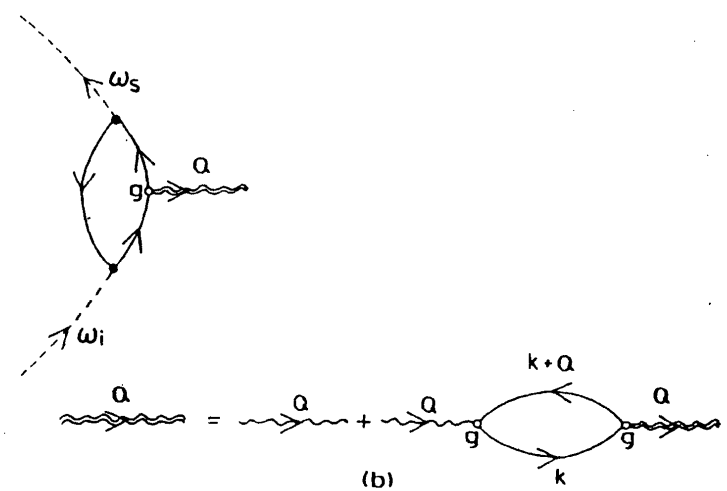
FIGURE CAPTIONS

Figure 1: Feynman diagram for phonon-Raman scattering in a nested Fermi liquid. Lowest order processes: (a) for $q = 0$ and (b) for $q = Q$.

Figure 2: Raman intensity in a nested Fermi liquid as a function of reduced frequency: (a) for $\omega_Q = 2\omega_0$ and for $\omega_0 = 2\omega_Q$.





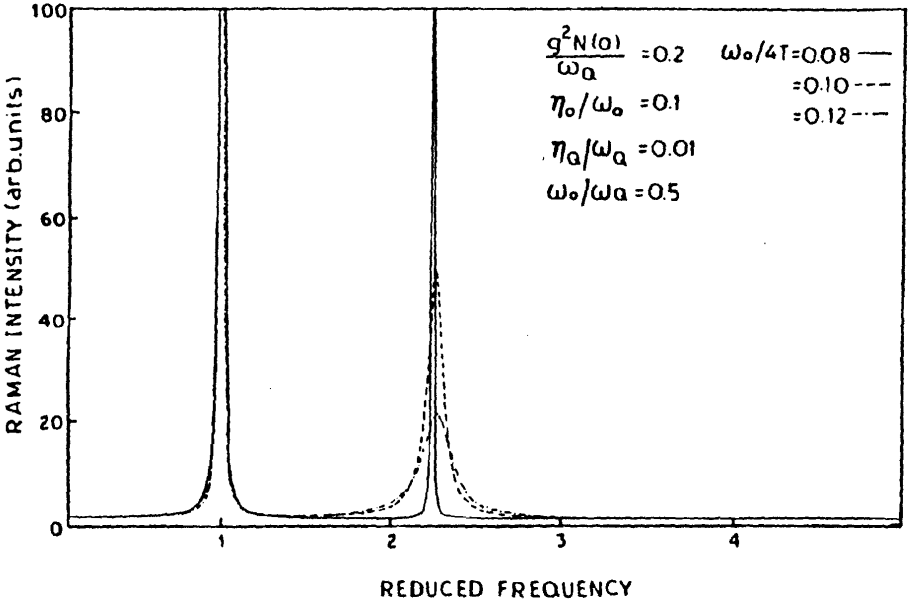

$\frac{g^2N(0)}{\omega_Q}$ =0.2
$\omega_0/4T$=0.08
=0.10
=0.12
η_0/ω_0 =0.1
η_Q/ω_Q =0.01
ω_0/ω_Q =0.5
RAMAN INTENSITY (arb.units)
REDUCED FREQUENCY

Fig.2 (a)

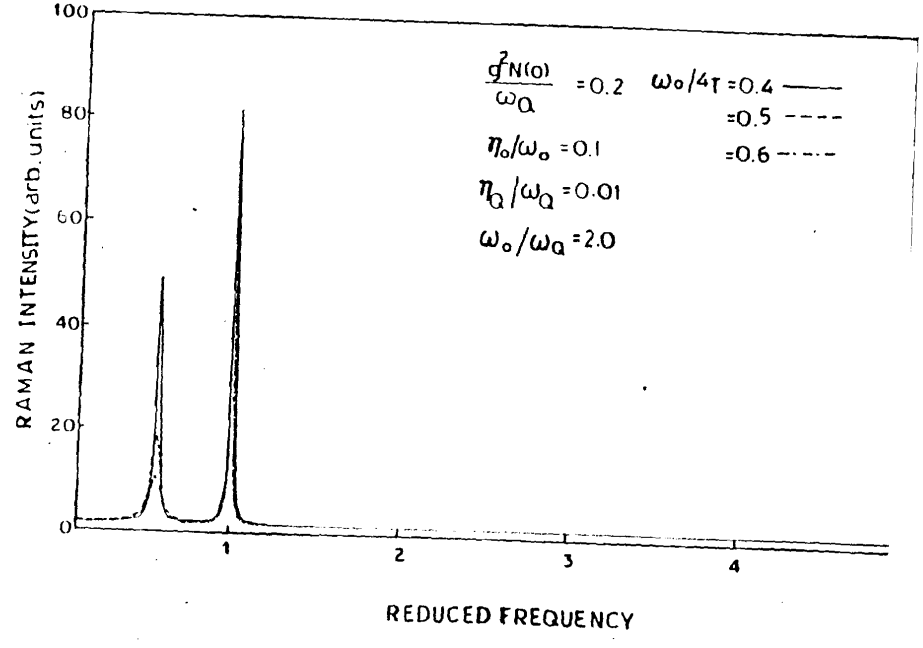

$\frac{g^2N(0)}{\omega_Q}$ =0.2
$\omega_0/4T$ =0.4
=0.5
=0.6
η_0/ω_0 =0.1
η_Q/ω_Q =0.01
ω_0/ω_Q =2.0
RAMAN INTENSITY(arb. units)
REDUCED FREQUENCY

Fig.2 (b)