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Signature of Anharmonicities in High Temperature Superconductors

KEYWORDS They are Anharmonicities, Phonon Line Widths, Phonon Density of States.

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ABSTRACT *Owing to the intricate mechanism of high temperature superconductivity the problem of anharmonic effects has been investigated with the help of newly developed quantum dynamics of electrons and phonons via an almost complete Hamiltonian which comprises of the effects of electrons, phonons and anharmonicities. The investigations based on the evaluation double time temperature dependent Green's function theory of electrons and phonons have been kept centralized around the anharmonic effects which is really a very complicated and unresolved problem for a very long time. The effects of anharmonicities on width, shift and phonon density of states (PDOS) have been studied. The temperature dependence of these quantities and that of pairons frequencies has also been discussed in the new framework.*

(1) INTRODUCTION

The long pending intricate predicament of anharmonic phonon-electron problem, in high temperature superconductors (HTS) gained heightened interest with time among condensed matter physicists with the fact that anharmonicity is responsible for many different properties of solids [1,2]. In several proposed mechanisms of HTSC it is always suspected that it is the phonon that helps to join the electrons into superconducting pairs. In other words, the dressing of electrons with phonons in the form of polarons, bipolarons, etc., reinvigorated the concept of attractive interaction between electrons (pairons or cooper pairs). Some of the remarkable investigations [3,4] reveal that the anharmonicity less than 1% can induce superconductivity even in the presence of coulomb repulsion which provoked us to take up this exciting issue on new grounds. Further, the effects of disorders and defects are well known which drastically change the frequency (energy) spectrum of solids may also play decisive role in understanding the problem in a wider perspective [5,6]. In the present work the problem of PDOS of HTS has been investigated the many body quantum dynamics of phonons and electrons with the help of double time thermodynamic phonon Green's functions technique. During the development of excitation spectra and PDOS, two main features are emerged; namely, (i) the temperature dependence of PDOS caused due to anharmonicities and (ii) the automated presence of pairons responsible for the phenomenon of HTSC.

(2) THE HAMILTONIAN

To investigate the many body quantum dynamics of phonons let us consider an almost complete Hamiltonian of the form (BCS type is not considered) [7,8,9]

$$H = H_e + H_p + H_{ep} + H_A + H_D \qquad (1)$$

$$H_e = \sum_q (\hbar\omega_{q\uparrow} b^*_{q\uparrow} b_{q\uparrow} + \hbar\omega_{q\downarrow} b^*_{q\downarrow} b_{q\downarrow} + \hbar\omega_{-q\uparrow} \times b^*_{-q\uparrow} b_{-q\uparrow} + \hbar\omega_{-q\downarrow} b^*_{-q\downarrow} b_{-q\downarrow}) \qquad (1a)$$

$$H_p = \sum_k \frac{\hbar\omega_k}{4}[A^*_k A_k + B^*_k B_k] \qquad (1b)$$

$$H_{ep} = \sum_{k,q} (g_k b^*_{Q\uparrow} b_{q\uparrow} + g^*_k b^*_{q\uparrow} b_{Q\uparrow} + g_k b^*_{Q\downarrow} b_{q\downarrow} + g^*_k b^*_{q\downarrow} b_{Q\downarrow}) B_k \qquad (1c)$$

$$H_A = \sum_{s\geq 3} \sum_{k_1,..,k_s} \hbar V_s(k_1,k_2,...,k_s) A_{k_1} A_{k_2} .... A_{k_s} \qquad (1d)$$

$$H_D = -\hbar \sum_{k_1,k_2} \left[C(k_1,k_2) B_{k_1} B_{k_2} \right] + \hbar \sum_{k_1,k_2} \left[D(k_1,k_2) A_{k_1} A_{k_2} \right] \qquad (1e)$$

where H_e, H_p, H_{ep}, H_A and H_D, respectively are unperturbed electron-, unperturbed phonon-, electron-phonon-, anharmonic (upto quartic terms)-, and defect contributions to the Hamiltonian H. In the above equations $b^*_q(b_q)$ and A_k, B_k are the electron creation (annihilation) and phonon field and momentum operators, respectively. Q=k+q (k and q being phonon and electron wave vectors, respectively) and g_k stand for electron-phonon coupling coefficient.The symbols $V_s(k_1,k_2,....k_s)$, $C(k_1,k_2)$ and $D(k_1,k_2)$ stand for the anharmonic coupling coefficients, mass and force constant change parameters, respectively [7,8,9].

(3) THE PHONON GREEN'S FUNCTIONS

In order to obtain the phonon line spectrum,

let us consider the evaluation of double time temperature dependent retarded Green's function

$$G_{q,q'}(t-t') = -i\theta(t-t') < [A_k(t), A^*_{k'}(t')] >$$

where $\theta(t-t')$ is the Heaviside unit step function.

Double differentiation of equation (2) with respect to t followed by the Fourier transformation yields

$$(\omega^2 - \omega_k^2) G_{k,k'}(\omega) = \frac{\omega_k}{\pi} \left(\eta_{k,k'} + \ll F_k(t); A^*_{k'}(t') \gg \right) \qquad (3)$$

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with

$$\eta_{k,k'} = \delta_{k,k'} + 4\omega_k^{-1}\sum_{k_1} C(k_1,-k)\delta_{k_1,k'} \qquad (4)$$

The second term in equation (3) contains the

hierarchy of higher order of Green's functions $\ll F_k(t); A^*_{k'}(t') \gg$. For further simplification we adopt the equation motion technique to evaluate the Green's function $\ll F_k(t); A^*_{k'}(t') \gg$

with respect to t' which enables us to formulate the Green's function $G_{k,k'}(\omega)$ in terms of Dyson's equation as

$$G_{k,k'}(\omega) = G_k^0(\omega)\delta_{k,k'} + G_k^0(\omega)\tilde{P}(k,k',\omega)G^0_{k'}(\omega)$$
$$= G_k^0(\omega)\delta_{k,k'} + G_k^0(\omega)\pi(k,k',\omega)G_{k'}(\omega) \qquad (5)$$

where symbols, $\tilde{P}(k,k',\omega)$ $G_k^0(\omega) = \omega_k / \pi(\omega^2 - \omega_k^2)$ and $\pi(k,k',\omega)$ stand for

the zeroth order (unperturbed) Green's function, response function and phonon self energy function respectively and are readily obtainable in the form [10]

where $\Delta_k(\omega)$ and $\Gamma_k(\omega)$ describe phonon frequency (energy)

$$G_{k,k'}(\omega) = \frac{\omega_k \eta_{k,k'}}{\pi[\omega^2 - \tilde{\omega}_k^2 - 2\omega_k\{\Delta_k(\omega) - i\Gamma_k(\omega)\}]} \qquad (6)$$

shift and line width $\tilde{P}(k,k',\omega) = \Delta_k(\omega) - i\Gamma_k(\omega)$. During the calcula-

tion of response function 268 higher order Green's functions are encountered. The higher order Green's functions are decoupled using the appropriate decoupling scheme [8]. After simplification only 39 Green's functions contribute significantly and the rest either vanish identically or have negligibly small contribution. The remaining Green's functions are quantum dynamically evaluated via a renormalized electron and phonon Hamiltonians as

$$H^e_{\text{Ren}} = \sum_q (\hbar\tilde{\omega}_{q\uparrow} b^*_{q\uparrow} b_{q\uparrow} + \hbar\tilde{\omega}_{q\downarrow} b^*_{q\downarrow} b_{q\downarrow} + \hbar\omega_{-q\uparrow}$$
$$\times b^*_{-q\uparrow} b_{-q\uparrow} + \hbar\omega_{-q\downarrow} b^*_{-q\downarrow} b_{-q\downarrow}) \qquad (7)$$

$$H^p_{\text{Ren}} = \frac{\hbar}{4}\sum_k \left[\frac{\tilde{\omega}_k^2}{\omega_k} A_k^* A_k + \omega_k B_k^* B_k\right] \qquad (8)$$

After appropriate algebraic simplification the Green's function takes the form

$$G_{k,k'}(\omega + i\varepsilon) = \frac{\omega_k \eta_{k,k'}}{\pi[\omega^2 - \overline{\omega}_{kq}^2 + 2i\omega_k\Gamma_k(\omega)]} \qquad (9)$$

$$\overline{\omega}_{kq}^2 = \tilde{\omega}_{kq}^2 + 2\omega_k\Delta_k(\omega) \qquad (10)$$

where $\tilde{\omega}_{kq}$ and $\overline{\omega}_{kq}$ are the renormalized and perturbed mode

frequency mode frequencies can be readily obtainable in the form

$$\tilde{\omega}_{kq}^2 = \tilde{\omega}_k^2 + \tilde{\omega}_q^2 \; ; \;\; \tilde{\omega}_q^2 = \omega_k\omega_q \qquad (11)$$

$$\tilde{\omega}_k^2 = \omega_k^2 - \omega_k[\omega_k^D + \omega_k^A + \omega_k^{AD}] \qquad (12)$$

$$\omega_q = -8\omega_k^{-1}|g_k|^2[N(Q_\uparrow) + N(q_\uparrow) + N(Q_\downarrow)$$
$$+ N(q_\downarrow)] + 32\omega_k^{-2}\sum_q |g_k|^2[(8\omega_q^c + 8\omega_Q^c)$$
$$\times n_c(Q) + (5\omega_q^c + 2\omega_Q^c)n_c(q) + 3\omega_{Q\uparrow}$$
$$\times N(Q_\uparrow) + 3\omega_{Q\downarrow}N(Q_\downarrow) + 3\omega_{Q\uparrow}N(q_\uparrow)$$
$$+ (4\omega_{q\downarrow} + 2\omega_{Q\downarrow})N(q_\downarrow)] \qquad (13)$$

$$\omega_k^A = 48\sum_{k_1,k_2} \omega_{k_1}/\tilde{\omega}_{k_1} V_4(k_1,k_2,k_1,-k)$$
$$\times \coth\left(\frac{\beta\hbar\omega_{k_1}}{2}\right) \qquad (14)$$

$$\omega_k^D = 8D(k_1,-k) + 8C(k_1,-k) + 32\omega_k^{-1}$$
$$\times \sum_{k_1} C(k_1,-k)D(k_1,-k_1) + 32\omega_k^{-1}$$
$$\times \sum_{k_1} C(k_1,-k_1)D(k_1,-k) + 32\omega_k^{-1}$$
$$\times \sum_{k_1} C(k_1,-k_1)C(k_1,-k) \qquad (15)$$

$$\omega_k^{AD} = 192\omega_k^{-1}\sum_{k_1,k_2} \omega_{k_1}/\tilde{\omega}_{k_1} V_4(k_1,k_2,k_1,-k_1)$$
$$\times C(k_1,-k_1)\coth\left(\frac{\beta\hbar\omega_{k_1}}{2}\right) + 64\omega_k^{-1}$$
$$\times \sum_{k_1,k_2} C(k_1,-k_1)V_4(k_1,k_2,k_1,-k_1)$$
$$+ 256\omega_k^{-2}\sum_{k_1,k_2} C(k_1,-k_1)C(k_1,-k)$$
$$\times V_4(k_1,k_2,-k_1,-k_1) \qquad (16)$$

During this process of evaluation of Green's function the auto emergence of pairons (cooper pairs, bipolarons) is encountered with renormalized pairon frequency given by

$$\tilde{\omega}_q^c = 32\hbar^{-2}\omega_k^{-1}\sum_q |g_k|^2[(8\omega_q^c + \omega_Q^c)n_c(Q)$$
$$+ (5\omega_q^c + \omega_Q^c)n_c(q)] \qquad (17)$$

The pairon occupancy $n_c(\gamma)$ appearing in above equations

can be obtained in the form

$$n_c(\gamma) = [\exp(\beta\hbar\tilde{\omega}_\gamma^c) - 1]^{-1}; \gamma = (q,Q) \qquad (18a)$$

$$N(\gamma_\sigma) = [\exp(\beta\hbar\tilde{\omega}_{\gamma\sigma}^c) + 1]^{-1}; \sigma = (\uparrow,\downarrow) \qquad (18b)$$

This reveals that the renormalized pairon frequency is not a simple quantity but depends on temperature and electron phonon coupling coefficient and wave vector combinations.

(4) PHONON FREQUENCY WIDTH

The phonon line width is responsible for many different dynamical properties of crystalline solids, e.g., the phonon frequency (energy) spectrum, life times and DOS and this can be obtained from response function in the following form [9]:

$$\Gamma_k(\omega) = \Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \qquad (19)$$

$$\Gamma_k^D(\omega) = \sum_{k_1}[\pi\varepsilon(\omega)R^D(k,k_1)\omega_{k_1}\delta(\omega^2 - \tilde{\omega}_{k_1}^2)$$
$$+ 4\pi\omega_k^{-1}NR^{Dep}(k,k_1)|\tilde{\omega}|\delta(\omega^2 - \tilde{\omega}_k^2)] \qquad (19a)$$

$$\Gamma_k^{3A}(\omega) = 18\pi\varepsilon(\omega)\sum_{k_1,k_2}|V_3(k_1,k_2,-k)|^2\eta_1 A_\alpha \qquad (19b)$$

$$\Gamma_k^{ep}(\omega) = \pi\omega_k^{-2}|g_k|^2\sum_q\Big[\bar{N}_{qQ\uparrow}\Omega_\uparrow\omega^c_{1q\uparrow}$$
$$\times\delta(\omega - 4\tilde{\omega}_{qQ_\uparrow}) + \bar{N}_{qQ\uparrow}\Omega_\uparrow\omega^c_{2q\uparrow}$$
$$\times\delta(\omega - \tilde{\Omega}_\uparrow) + 3\bar{N}_{qQ\downarrow}\Omega_\downarrow\omega^c_{3q\downarrow}$$
$$\times\delta(\omega - \tilde{\Omega}_\downarrow) + \bar{N}_{qQ\downarrow}\gamma_1\omega^c_{4Q\downarrow}$$
$$\times\delta(\omega - \tilde{\Omega}_\downarrow)\Big] + 128\pi\sum_{k,q}\omega_k^{-2}|g_k|^4$$
$$\times\Big[\tilde{n}_k N(Q_\uparrow)\delta(\omega - \Omega_1) + \tilde{n}_k N(q_\uparrow)$$
$$\times\delta(\omega - \Omega_2) + \tilde{n}_k N(Q_\downarrow)\delta(\omega - 2\Omega_3)$$
$$- 2\omega_k^{-1}\tilde{\omega}_k^2\hat{N}^2\varepsilon(\omega)\,\delta(\omega^2 - \tilde{\omega}_k^2)\Big] \qquad (19c)$$

$$\Gamma_k^{3D}(\omega) = 144\pi\varepsilon(\omega)\sum_{k_1,k_2}|V_3(k_1,k_2,-k)|^2$$
$$\times R^c(k,k_1)\omega_k^{-1}\eta_1 A_\alpha \qquad (19d)$$

$$\tilde{\Omega}_{\uparrow\downarrow} = 3\tilde{\omega}_{qQ\uparrow\downarrow} + \tilde{\omega}^c_{qQ};\; \Omega_{\uparrow\downarrow} = 3\omega_{qQ\uparrow\downarrow} + \omega^c_{qQ} \qquad (20a)$$

$$\gamma_1 = (4\omega_{q\downarrow} + 2\omega_{Q\downarrow} + \omega^c_{qQ});\; \Omega_1 = 7\omega_{Q\uparrow} + \tilde{\omega}^c_Q \qquad (20b)$$

$$\Omega_2 = 7\omega_{q\uparrow} + \tilde{\omega}^c_Q;\; \Omega_3 = 3\tilde{\omega}_{Q\downarrow} + \tilde{\omega}^c_Q \qquad (20c)$$

Volume : 3 | Issue : 4 | April 2013 | ISSN - 2249-555X

The superscript 'c' on various terms stands for the pairons (cooper pairs or bipolarons). Various symbols appearing in above equations are defined as follows:

$$A_\alpha = [S_{+\alpha}\omega_{+\alpha}\delta(\omega^2-\tilde{\omega}_{+\alpha}^2)+S_{-\alpha}\omega_{-\alpha} \times \delta(\omega^2-\tilde{\omega}_{-\alpha}^2)] \quad (21)$$

$$R^D(k,k_1) = |D(k_1,-k)|^2 + 8|C(k_1,-k)|^2 \left[1+16\omega_k^{-2}|D(k_1,-k)|^2+8\omega_k^{-1} \times |D(k_1,-k)|^2\right] + 16C(k_1,-k) \times\left[D(k_1,-k)+4\omega_k^{-1}|D(k_1,-k)|^2\right] \quad (22a)$$

$$R^{Dep}(k,k_1) = |g_k|^2\left[D(k_1,-k)+C(k_1,-k) \times\left(1+4\omega_k^{-1}D(k_1,-k)\right)\right]+16\omega_k^{-1} \times |C(k_1,-k)|^2\left[1+4\omega_k^{-1}D(k_1,-k)\right] \quad (22b)$$

$$R^c(k,k_1) = C(k_1,k)+2\omega_k^{-1}|C(k_1,-k)|^2 \quad (22c)$$

$$R^c(k,k_1) = C(k_1,k)+2\omega_k^{-1}|C(k_1,-k)|^2 \quad (22d)$$

$$S_{\pm\alpha} = n_{k_2} \pm n_{k_1};\ \eta_{i-1} = \frac{\omega_{k_1}\omega_{k_2}....\omega_{k_i}}{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}....\tilde{\omega}_{k_i}} \quad (23)$$

$$n_{k_i} = \coth\left(\frac{\beta\hbar\omega_{k_i}}{2}\right);\ \tilde{n}_{k_i} = \frac{\tilde{\omega}_{k_i}}{\omega_{k_i}}\coth\left(\frac{\beta\hbar\omega_{k_i}}{2}\right) \quad (24)$$

$$\omega_{\pm\alpha} = \tilde{\omega}_{k_1} \pm \tilde{\omega}_{k_2} \quad (25a)$$

$$\omega_{qQ\left(\uparrow\atop\downarrow\right)} = \omega_{q\left(\uparrow\atop\downarrow\right)} + \omega_{Q\left(\uparrow\atop\downarrow\right)} \quad (25b)$$

$$\tilde{\omega}_{qQ\left(\uparrow\atop\downarrow\right)} = \tilde{\omega}_{q\left(\uparrow\atop\downarrow\right)} + \tilde{\omega}_{Q\left(\uparrow\atop\downarrow\right)} \quad (25c)$$

$$\omega_{qQ}^c = \omega_q^c + \omega_Q^c \quad (25d)$$

$$\omega^c_{\left(1q\uparrow\atop 2Q\uparrow\right)} = 13\omega_{\left(q\uparrow\atop Q\uparrow\right)} + 11\omega_{\left(Q\uparrow\atop q\uparrow\right)} + 4\omega_{qQ}^c \quad (25e)$$

$$\omega^c_{\left(3q\downarrow\atop 4Q\downarrow\right)} = 7\omega_{\left(q\downarrow\atop Q\downarrow\right)} + 5\omega_{\left(Q\downarrow\atop q\downarrow\right)} + 4\omega_{qQ}^c \quad (25f)$$

$$N = N(Q_\uparrow)+N(q_\uparrow)+N(Q_\downarrow)+N(q_\downarrow) \quad (26a)$$

$$\bar{N}_{qQ\left(\uparrow\atop\downarrow\right)} = N_{q\left(\uparrow\atop\downarrow\right)} + N_{Q\left(\uparrow\atop\downarrow\right)} \quad (26b)$$

(5) PHONON FREQUENCY SHIFTS

The phonon frequency shift which is the real part of phonon Green's function is given by

$$\Delta_k(\omega) = \Delta_k^D(\omega)+\Delta_k^{3A}(\omega)+\Delta_k^{3D}(\omega)+\Delta_k^{ep}(\omega) \quad (27)$$

$$\Delta_k^D(\omega) = \sum_{k_1} R^D(k,k_1)D(\omega,\tilde{\omega}_{k_1})^{-1}+16\omega_k^{-1}N \times\left[D_1(\omega,\tilde{\omega}_{k_1})-\tilde{\omega}_{k_1}D(\omega,\tilde{\omega}_{k_1})\right] \times R^{Dep}(k,k_1) \quad (27a)$$

$$\Delta_k^{3A}(\omega) = 18\sum_{k_1,k_2}|V_3(k_1,k_2,-k)|^2\eta_1 D_s(\omega,\omega_{\pm\alpha}) \quad (27b)$$

$$\Delta_k^{3D}(\omega) = 144\sum_{k_1,k_2}|V_3(k_1,k_2,-k)|^2 R^c(k,k_1)\omega_k^{-1} \times\eta_1 D_s(\omega,\omega_{\pm\alpha}) \quad (27c)$$

$$\Delta_k^{ep}(\omega) = \omega_k^{-2}|g_k|^2\sum_q\Big[\bar{N}_{qQ\uparrow}\Omega_\uparrow\big\{\omega^c_{1q\uparrow} \times(\omega-4\omega_{qQ\uparrow})^{-1}+\omega^c_{2Q\uparrow}(\omega-\tilde{\Omega}_\uparrow)^{-1}\big\} + \bar{N}_{qQ\downarrow}3\Omega_\downarrow\omega^c_{3q\downarrow}(\omega-\tilde{\Omega}_\downarrow)^{-1}+\gamma_1\omega^c_{4Q\downarrow} \times(\omega-\tilde{\Omega}_\downarrow)^{-1}\Big]+128\sum_{k,q}\omega_k^{-2}\tilde{n}_k \times N(q_\uparrow)(\omega-\tilde{\Omega}_2)^{-1}+\tilde{n}_k N(Q_\downarrow) \times(\omega-2\tilde{\Omega}_3)^{-1}+\tilde{n}_k N(q_\downarrow)(\omega-2\tilde{\Omega}_3) -2\tilde{\omega}_k^2\hat{N}^2\omega_k(\omega^2-\tilde{\omega}_k^2)\Big] \quad (27d)$$

$$D_s[\omega,\omega_{\left(+\alpha\atop+\beta\right)}] = S_{\left(+\alpha\atop+\beta\right)}\omega_{\left(+\alpha\atop+\beta\right)}(\omega^2-\tilde{\omega}_{-\alpha}^2)^{-1} + S_{\left(-\alpha\atop-\beta\right)}\omega_{\left(-\alpha\atop-\beta\right)}(\omega^2-\tilde{\omega}_{-\beta}^2)^{-1} \quad (28a)$$

$$D(\omega,\tilde{\omega}_i) = (\omega^2-\tilde{\omega}_i^2)^{-1} \quad (28b)$$

$$D_1(\omega,\tilde{\omega}_i) = D(\omega,\tilde{\omega}_i)^{-1} \quad (28c)$$

(6) PHONON DENSITY OF STATES

Using Lehman's representation the PDOS is defined as

$$N_p(\omega) = -\sum_k \mathrm{Im}G_{k,k'}(\omega) = \sum_k \eta_{k,k'}J(k,\omega) \quad (29)$$

where

$$J(k,\omega) = \frac{2\omega_k^2\Gamma_k(\omega)}{\pi[\omega^2-\tilde{\omega}_k^2-2\omega_k\Delta_k(\omega)]^2} \quad (30)$$

The PDOS represented by equation (32) can be separated into diagonal and non-diagonal contribution in the form

$$N_p(\omega) = N_p(\omega)_d + N_p(\omega)_{nd} \quad (31)$$

where

$$N_p(\omega)_d = \sum_k J(k,\omega) \quad (31a)$$

$$N_p(\omega)_{nd} = 4\sum_{k,k' \atop k\neq k'}\frac{C(-k,k')}{\omega_k}J(k,\omega) \quad (31b)$$

Making the use of equation (33) and replacing the summation sign by integral, $N_p(\omega)_d$ and $N_p(\omega)_{nd}$ can be written as

After some algebra, the diagonal part of PDOS can be obtained in a more explicit form as

$$N_p(\omega)_d = \xi_v\int\frac{\omega^2\omega_k^2\Gamma_k(\omega)d\omega}{(\omega^2-\bar{\omega}_k^2)^2} \quad (32a)$$

$$N_p(\omega)_{nd} = 4\xi_v\int\frac{\omega^2\omega_k\Gamma_k(\omega)C(k,-k')d\omega}{(\omega^2-\bar{\omega}_k^2)^2} \quad (32b)$$

with

$$N_p(\omega)_d = N_p^{3A}(\omega)_d + N_p^D(\omega)_d + N_p^{3D}(\omega)_d + N_p^{ep}(\omega)_d \quad (33)$$

$$N_p^D(\omega)_d = \xi_v\pi\omega_k^2\sum_{k_1}\left[\varepsilon(\tilde{\omega}_{k_1})R^D(k,k_1)\omega_{k_1}+16 \times\omega_k^{-1}NR^{Dep}(k,k_1)\right]\tilde{\Omega}(k_1,k) \quad (33a)$$

$$N_p^{3A}(\omega)_d = 18\pi\xi_v\sum_{k_1,k_2}|V_3(k_1,k_2,-k)|^2\eta_1\omega_k^2A_\alpha^{(1)} \quad (33b)$$

$$N_p^{3D}(\omega)_d = 144\pi\xi_v\sum_{k_1,k_2}|V_3(k_1,k_2,-k)|^2R^c(k,k_1) \times\omega_k^{-1}\eta_1\omega_k^2A_\alpha^{(1)} \quad (33c)$$

$$N_p^{ep}(\omega)_d = \xi_v\pi\Big\{\omega_k^{-2}|g_k|^2\sum_q\Big[\bar{N}_{qQ\uparrow}\Omega_\uparrow\omega^c_{1q\uparrow} \times\Omega_1(qQ\uparrow,k)+\bar{N}_{qQ\uparrow}\Omega_\uparrow\omega^c_{2Q\uparrow} \times\Omega_2(qQ\uparrow,k)+3\bar{N}_{qQ\downarrow}\Omega_\downarrow\omega^c_{3q\downarrow} \times\Omega_3(qQ\downarrow,k)+\bar{N}_{qQ\downarrow}\gamma_1\omega^c_{4Q\downarrow} \times\Omega_3(qQ\downarrow,k)\Big]\omega_k^2+128\sum_{k,q}\omega_k^{-2}|g_k|^4 \times\Big[\tilde{n}_kN(Q_\uparrow)\Omega_4(Q\uparrow,k)+\tilde{n}_kN(q_\uparrow) \times\Omega_5(q\uparrow,k)+\tilde{n}_kN(Q\downarrow)\Omega_6(Q\downarrow,k) +\tilde{n}_kN(q\downarrow)\Omega_7(q\downarrow,k)-2\omega_k^{-1}\tilde{\omega}_k^2 \times\hat{N}^2\varepsilon(\tilde{\omega}_k)\tilde{\Omega}(k)\Big]\Big\} \quad (33d)$$

Volume : 3 | Issue : 4 | April 2013 | ISSN - 2249-555X

with

$$A_{\alpha}^{(1)} = \left[\varepsilon(\omega_{+\alpha})S_{+\alpha}\omega_{+\alpha}\Omega(+\alpha,k) + \varepsilon(\omega_{-\alpha}) \times S_{-\alpha}\omega_{-\alpha}\Omega(-\alpha,k)\right] \quad (34)$$

Similarly, the non-diagonal contribution to PDOS can be expressed in the form

$$N_p(\omega)_{nd} = N_p^D(\omega)_{nd} + N_p^{3D}(\omega)_{nd} + N_p^{Dep}(\omega)_{nd} \quad (35)$$

$$N_p^D(\omega)_{nd} = 4\xi_v \pi \omega_k \sum_{k_1}\left[\varepsilon(\tilde{\omega}_{k_1})R^D(k,k_1)\omega_{k_1} + 16\omega_k^{-1} N R^{Dep}(k,k_1)C(k',-k)\tilde{\Omega}(k_1,k)\right. \quad (35a)$$

$$N_p^{3D}(\omega)_{nd} = 72\xi_v\eta_1\omega_k A_\alpha^{(1)}C(k',-k) \times\left[1+8R^c(k,k_1)\omega_k^{-1}\right] \quad (35b)$$

$$\begin{aligned} N_p^{Dep}(\omega)_{nd} = 4\xi_v\pi\Big\{&\omega_k^{-2}|g_k|^2\sum_q C(k',-k)\Big[\bar{N}_{qQ\uparrow} \times\Omega_\uparrow\omega^c_{1q\uparrow}\Omega_1(qQ\uparrow,k) + \bar{N}_{qQ\uparrow}\Omega_\uparrow \\ &\times\omega^c_{2Q\uparrow}\Omega_2(qQ\uparrow,k) + 3\bar{N}_{qQ\downarrow}\Omega_\downarrow\omega^c_{3q\downarrow} \times\Omega_3(qQ\downarrow,k) + \bar{N}_{qQ\downarrow}\gamma_1\,\omega^c_{4Q\downarrow} \\ &\times\Omega_3(qQ\downarrow,k)\Big]\omega_k + 512\sum_{k,q}\omega_k^{-2} \times|g_k|^4 C(k',-k)\Big[\tilde{n}_k N(Q_\uparrow) \\ &\times\Omega_4(Q\uparrow,k) + \tilde{n}_k N(q_\uparrow)\Omega_5(q\uparrow,k) + \tilde{n}_k N(Q\downarrow)\Omega_6(Q\downarrow,k) + \tilde{n}_k N(q\downarrow)\Omega_7(q\downarrow,k) \\ &- 2\omega_k^{-1}\tilde{\omega}_k^2\,\hat{N}^2\varepsilon(\tilde{\omega}_k)\tilde{\Omega}(k)\Big]\omega_k\Big\} \end{aligned} \quad (35c)$$

with

$$\Omega_1(qQ\uparrow,k) = (4\tilde{\omega}_{qQ\uparrow})^2(16\tilde{\omega}^2_{qQ\uparrow} - \bar{\omega}_k^2)^{-2} \quad (36a)$$

$$\Omega_{\binom{2}{3}}\left(\binom{qQ\uparrow}{qQ\downarrow},k\right) = \left[3\tilde{\omega}_{\binom{qQ\uparrow}{qQ\downarrow}} + \tilde{\omega}^c_{qQ}\right] \times\left[\left(3\tilde{\omega}_{\binom{qQ\uparrow}{qQ\downarrow}} + \tilde{\omega}^c_{qQ}\right)^2 - \bar{\omega}_k^{-2}\right]^{-2} \quad (36b)$$

$$\Omega_{\binom{4}{5}}\left(\binom{Q\uparrow}{q\downarrow},k\right) = \left[7\tilde{\omega}_{\binom{Q\uparrow}{q\downarrow}} + \tilde{\omega}^c_{\binom{Q}{q}}\right]^2 \times\left[\left(7\tilde{\omega}_{\binom{Q\uparrow}{q\downarrow}} + \tilde{\omega}^c_{\binom{Q}{q}}\right)^2 - \bar{\omega}_k^{-2}\right]^{-2} \quad (36c)$$

$$\Omega_{\binom{6}{7}}\left(\binom{Q\uparrow}{q\downarrow},k\right) = \left[6\tilde{\omega}_{\binom{Q\downarrow}{q\downarrow}} + \tilde{\omega}^c_{\binom{Q}{q}}\right]^2 \times\left[\left(6\tilde{\omega}_{\binom{Q\downarrow}{q\downarrow}} + \tilde{\omega}^c_{\binom{Q}{q}}\right)^2 - \bar{\omega}_k^{-2}\right]^{-2} \quad (36d)$$

$$\xi_v = \frac{V}{\pi^3 v_p^3} \quad (37)$$

V is the volume of the unit cell and v_p is the velocity of phonon.

(7) RESULTS AND DISCUSSION

Let us carefully inspect the general trends of this formulation. The PDOS has been resolved into diagonal and non-diagonal components. The non-diagonal part $N_p(\omega)_{nd}$ chiefly emerges due to the presence of impurities and vanishes in case of pure crystals. The anisotropic dispersion can be well described with the help of disorder and anharmonicity in HTS.

Here the BCS type Hamiltonian has not been taken but this theory presents the evaluation of pairons and appears as a salient feature of theory. Every term of PDOS in the present theory is found to be temperature dependent via a large number of phonon, electron and pairon distribution functions like $S_{\binom{\pm\alpha}{\pm\beta}}, \bar{N}(\varepsilon_{kc}), \bar{n}(\tilde{\varepsilon}_{qc})$. Due to the presence of the terms like $D_s[\omega,\omega_{\binom{\alpha}{\beta}}]$ $D(\omega,\tilde{\omega}_i)$, $D_1(\omega,\tilde{\omega}_i)$, $\Omega_1(qQ\uparrow,k)$, etc, a large number of peaks in the PDOS curves can be predicted which would be confirmed in high resolution experiments.

(8) CONCLUSIONS

These investigations presents the general theory and show that the localized anharmonic phonon-electron interaction is a novel problem in high temperature superconductivity studies. Further, this formulation successfully describes the evaluation of pairons without considering the BCS type Hamiltonian. The pairon frequency, renormalized mode frequency and PDOS are found to be heavily influenced by impurity concentration, electron-phonon coupling and temperature. The temperature dependence of these quantities via various distribution functions (occupation numbers) emerges as a new feature of the theory and obviously is the consequence of the anharmonicities.

(8) AKNOWLEDGEMENT

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