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PHONONSIN HIGH TEMPERATURE $YBa_2Cu_3O_{7-\delta}$ SUPER CONDUCTOR

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Abstract : The influence of Electron-phonon interaction, anharmonicities and point impurities phonon density of states (PDOS) of high temperature cup rate superconductors (HTS) has been investigated based on quantum dynamical many body problem using Double time thermodynamic Green's function theory via a non-BCS Hamiltonian as state of the art. The results thus obtained for phonon frequency widths and PDOS (resolved into diagonal and off diagonal contributions) are found to depend on temperature, impurity concentration etc., has been applied to numerically estimate the DOS of representative HTS $YBa_2Cu_3O_{7-\delta}$ in (i) superconducting and (ii) normal regions. The automatic appearance of pairons emerges as a special feature of the present theory.

Key words : Phonon Green's function, Lehman's representation, Phonon Density of States, Electron-

Introduction

Since the breakthrough discovery of high temperature superconductivity (HTSC) by Bednorz and Muller [1] it was heralded as one of the most interesting and fascinating area for both the theorists and experimentalists. The anharmonic electron-phonon problem in high temperature superconductors has been one of the complex and tedious problem and attracted the interest of condensed matter physicist with the fact that anharmonicity is responsible for various interesting properties of solids [2,3]. In some of the HTSC mechanisms it is proposed that phonon helps to join the two electrons to superconduct or in other words; the dressing of electron with phonons in the form of polarons, bipolarons, etc., reanimated the theory of attractive interaction between electrons. Mahan [4] and Newns [5] explained that anharmonicities less than 1 % impel the superconductivity even in the presence of coulomb repulsion. The fact that energy spectrum changed by the effects of defects and disorder provides us a platform to investigate the problem within an ample standpoint [6,7].

Every dynamical property of crystalline solids invariably needs the careful evaluation of PDOS irrespective of the method use to describe it. Hence, it is worth mentioning that the marvelous edifice of dynamical properties of solids including HTS is erected on the sound foundations of PDOS and makes it as basic building block of the problem. Using Lehman's representation PDOS is defined as [8,9]

$$N_p(\omega) = -\sum_k \mathrm{Im}G_{k,k'}(\omega) \quad (1)$$

Obviously, this form of DOS ensures that the evaluation of Green's function $G_{k,k'}(\omega)$ emerges in the heart of the problem and the sophistication involved [10, 11, 12] in state of

the art to very carefully evaluate it heralds the nature of the investigation. In the present work we have taken up Born-Mayer-Huggins potential [13-22] which is found the most suitable potential to evaluate the anharmonic interactions in HTS. This is given by

$$V_{ij} = a_{ij}\, e^{-b_{ij} r} + \frac{q_i\, q_j}{r} \qquad (2)$$

Where the symbols are well defined in reference [23]. The organization of this paper consists of the description of the Hamiltonian in section (II) with methodology and Quantum dynamics of phonons detailed in section (III). The section (IV) devoted to the PDOS, followed by the results and discussions in section (V) and conclusions drawn in section (VI).

The Hamiltonian

To investigate the many body quantum dynamics of phonons we consider an almost complete crystal Hamiltonian [24-40] of the form (without considering the BCS expressions)

$$H = H_e + H_p + H_{ep} + H_A + H_D \qquad (3)$$

$$H_e = \sum_q (\hbar\omega_{q\uparrow} b^*_{q\uparrow} b_{q\uparrow} + \hbar\omega_{q\downarrow} b^*_{q\downarrow} b_{q\downarrow} + \hbar\omega_{-q\uparrow} b^*_{-q\uparrow} b_{-q\uparrow} + \hbar\omega_{-q\downarrow} b^*_{-q\downarrow} b_{-q\downarrow}) \qquad (3a)$$

$$H_p = \sum_k \frac{\hbar\omega_k}{4} [A^*_k A_k + B^*_k B_k] \qquad (3b)$$

$$H_{ep} = \sum_{k,q} (g_k b^*_{Q\uparrow} b_{q\uparrow} + g^*_k b^*_{q\uparrow} b_{Q\uparrow} + g_k b^*_{Q\downarrow} b_{q\downarrow} + g^*_k b^*_{q\downarrow} b_{Q\downarrow}) B_k \qquad (3c)$$

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

$$H_D = -\hbar \sum_{k_1,k_2} \left[C(k_1,k_2) B_{k_1} B_{k_2} \right] + \hbar \sum_{k_1,k_2} \left[D(k_1,k_2) A_{k_1} A_{k_2} \right] \qquad (3e)$$

where H_e, H_p, H_{ep}, H_A and H_D, respectively are unperturbed electron Hamiltonian [32,36,41] unperturbed phonon Hamiltonian [36], electron-phonon Hamiltonian [32], anharmonic (upto quartic terms) Hamiltonian [28,38], and defect Hamiltonian [37,38,40] H. Here **Q=k+q,** where **q** is the electron wave vector, g_k is the electron-phonon coupling coefficient.The terms $b^*_q (b_q)$ and A_k, B_k are the electron creation (annihilation) and phonon field and momentum operators, respectively. 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 [28,37,38], mass and force constant change parameters, respectively[24,29,37,38].

Quantum Dynamics Of Phonons

The evaluation of double time temperature dependent retarded Green's function [42]

$$G_{k,k'}(t-t') = -i\theta(t-t') < [A_k(t), A^*_{k'}(t')] > \qquad (4)$$

can be carried out by the quantum dynamical approach via Hamiltonian [3] and Dyson equation method in the form

$$G_{k,k'}(\omega) = \frac{\omega_k \eta_{k,k'}}{\pi[\omega^2 - \tilde{\omega}^2_k - 2\omega_k \tilde{P}(k,k',\omega)]} \qquad (5)$$

Where the response function $\tilde{P}(k,k^{'},\omega)=\Delta_k(\omega)-i\Gamma_k(\omega)$, with $\Delta_k(\omega)$ and $\Gamma_k(\omega)$ are phonon frequency widths and phonon frequency shifts, respectively. After some tedious analytic algebraic simplification yields the phonon line widths in the following form as

$$\Gamma_k(\omega)=\Gamma_k^D(\omega)+\Gamma_k^{3A}(\omega)+\Gamma_k^{3D}(\omega)+\Gamma_k^{ep}(\omega) \quad (6)$$

$$\Gamma_k^D(\omega)=\sum_{k_1}[\pi\varepsilon(\omega)R^D(k,k_1)\omega_{k_1}\delta(\omega^2-\tilde{\omega}_{k_1}^2)+4\pi\omega_k^{-1}NR^{Dep}(k,k_1)|\tilde{\omega}|\delta(\omega^2-\tilde{\omega}_k^2)] \quad (6a)$$

$$\Gamma_k^{3A}(\omega)=18\pi\varepsilon(\omega)\sum_{k_1,k_2}|V_3(k_1,k_2,-k)|^2\eta_1 A_\alpha \quad (6b)$$

$$\Gamma_k^{3D}(\omega)=144\pi\varepsilon(\omega)\sum_{k_1,k_2}|V_3(k_1,k_2,-k)|^2R^c(k,k_1)\omega_k^{-1}\eta_1 A_\alpha \quad (6c)$$

$$\Gamma_k^{ep}(\omega)=\pi\omega_k^{-2}|g_k|^2\sum_q\Big[\bar{N}_{qQ\uparrow}\Omega_\uparrow\omega_{1q\uparrow}^c\delta(\omega-4\tilde{\omega}_{qQ\uparrow})+\bar{N}_{qQ\uparrow}\Omega_\uparrow\omega_{2q\uparrow}^c$$
$$\delta(\omega-\tilde{\Omega}_\uparrow)+3\bar{N}_{qQ\downarrow}\Omega_\downarrow\omega_{3q\downarrow}^c\delta(\omega-\tilde{\Omega}_\downarrow)+\bar{N}_{qQ\downarrow}\gamma_1\omega_{4Q\downarrow}^c$$
$$\delta(\omega-\tilde{\Omega}_\downarrow)\Big]+128\pi\sum_{k,q}\omega_k^{-2}|g_k|^4\Big[\tilde{n}_kN(Q_\uparrow)\delta(\omega-\Omega_1)+\tilde{n}_kN(q_\uparrow)$$
$$\delta(\omega-\Omega_2)+\tilde{n}_kN(Q_\downarrow)\delta(\omega-2\Omega_3)-2\omega_k^{-1}\tilde{\omega}_k^2\hat{N}^2\varepsilon(\omega)\,\delta(\omega^2-\tilde{\omega}_k^2)\Big] \quad (6d)$$

The various symbols appears in the above equations are well defined in the references elsewhere [11,12,23,42].

Phonon Density Of States Of High Temperature Superconductors

Using Eqs. (6) in (5) and then in (1) the expression for PDOS can be written in the form

$$N_p(\omega)=-\sum_k \mathrm{Im}G_{k,k'}(\omega) \quad (7)$$

The PDOS represented by Eq.(7) can be separated into diagonal and non-diagonal contributions

$$N_p(\omega)=N_p(\omega)_d+N_p(\omega)_{nd} \quad (8)$$

After some algebra, the diagonal part of PDOS can be obtained in a more explicit form as [11,12,42]

$$N_p(\omega)_d=N_p^{3A}(\omega)_d+N_p^D(\omega)_d+N_p^{3D}(\omega)_d+N_p^{ep}(\omega)_d \quad (9)$$

$$N_p^D(\omega)_d=\xi_v\pi\omega_k^2\sum_{k_1}\Big[\varepsilon(\tilde{\omega}_{k_1})R^D(k,k_1)\omega_{k_1}+16\omega_k^{-1}NR^{Dep}(k,k_1)\Big]\tilde{\Omega}(k_1,k) \quad (9a)$$

$$N_p^{3A}(\omega)_d=18\pi\xi_v\sum_{k_1,k_2}|V_3(k_1,k_2,-k)|^2\eta_1\omega_k^2A_\alpha^{(1)} \quad (9b)$$

$$N_p^{3D}(\omega)_d = 144\pi\xi_v \sum_{k_1,k_2} |V_3(k_1,k_2,-k)|^2 R^c(k,k_1)\omega_k^{-1}\eta_1\omega_k^2 A_\alpha^{(1)} \quad (9c)$$

$$\begin{aligned} N_p^{ep}(\omega)_d = {} & \xi_v\pi\left\{\omega_k^{-2}|g_k|^2 \sum_q \left[\bar{N}_{qQ\uparrow}\Omega_\uparrow\omega_{1q\uparrow}^c\Omega_1(qQ\uparrow,k) + \bar{N}_{qQ\uparrow}\Omega_\uparrow\omega_{2Q\uparrow}^c\right.\right. \\ & \times\Omega_2(qQ\uparrow,k) + 3\bar{N}_{qQ\downarrow}\Omega_\downarrow\omega_{3q\downarrow}^c\Omega_3(qQ\downarrow,k) + \bar{N}_{qQ\downarrow}\gamma_1\omega_{4Q\downarrow}^c \\ & \left.\times\Omega_3(qQ\downarrow,k)\right]\omega_k^2 + 128\sum_{k,q}\omega_k^{-2}|g_k|^4\left[\tilde{n}_k N(Q_\uparrow)\Omega_4(Q\uparrow,k) + \tilde{n}_k N(q_\uparrow)\right. \\ & \times\Omega_5(q\uparrow,k) + \tilde{n}_k N(Q\downarrow)\Omega_6(Q\downarrow,k) + \tilde{n}_k N(q\downarrow)\Omega_7(q\downarrow,k) - 2\omega_k^{-1}\tilde{\omega}_k^2 \\ & \left.\left.\times\hat{N}^2\varepsilon(\tilde{\omega}_k)\tilde{\Omega}(k)\right]\right\} \end{aligned} \quad (9d)$$

After the same process the non-diagonal contribution to PDOS can be resolved in the form

$$N_p(\omega)_{nd} = N_p^D(\omega)_{nd} + N_p^{3D}(\omega)_{nd} + N_p^{Dep}(\omega)_{nd} \quad (10)$$

$$N_p^D(\omega)_{nd} = 4\xi_v\pi\omega_k\sum_{k_1}\left[\varepsilon(\tilde{\omega}_{k_1})R^D(k,k_1)\omega_{k_1} + 16\omega_k^{-1}NR^{Dep}(k,k_1)C(k',-k)\tilde{\Omega}(k_1,k)\right. \quad (10a)$$

$$N_p^{3D}(\omega)_{nd} = 72\xi_v\eta_1\omega_k A_\alpha^{(1)}C(k',-k)\left[1+8R^c(k,k_1)\omega_k^{-1}\right] \quad (10b)$$

$$\begin{aligned} N_p^{Dep}(\omega)_{nd} = {} & 4\xi_v\pi\left\{\omega_k^{-2}|g_k|^2\sum_q C(k',-k)\left[\bar{N}_{qQ\uparrow}\Omega_\uparrow\omega_{1q\uparrow}^c\Omega_1(qQ\uparrow,k) + \bar{N}_{qQ\uparrow}\Omega_\uparrow\right.\right. \\ & \times\omega_{2Q\uparrow}^c\Omega_2(qQ\uparrow,k) + 3\bar{N}_{qQ\downarrow}\Omega_\downarrow\omega_{3q\downarrow}^c\Omega_3(qQ\downarrow,k) + \bar{N}_{qQ\downarrow}\gamma_1\omega_{4Q\downarrow}^c \\ & \times\Omega_3(qQ\downarrow,k)\left]\omega_k + 512\sum_{k,q}\omega_k^{-2}|g_k|^4 C(k',-k)\left[\tilde{n}_k N(Q_\uparrow)\right.\right. \\ & \times\Omega_4(Q\uparrow,k) + \tilde{n}_k N(q_\uparrow)\Omega_5(q\uparrow,k) + \tilde{n}_k N(Q\downarrow)\Omega_6(Q\downarrow,k) \\ & \left.\left.+\tilde{n}_k N(q\downarrow)\Omega_7(q\downarrow,k) - 2\omega_k^{-1}\tilde{\omega}_k^2\hat{N}^2\varepsilon(\tilde{\omega}_k)\tilde{\Omega}(k)\right]\omega_k\right\} \end{aligned} \quad (10c)$$

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

$$\Omega_{\binom{2}{3}}\left(\begin{pmatrix} qQ\uparrow \\ qQ\downarrow \end{pmatrix},k\right)=\left[3\tilde{\omega}_{\binom{qQ\uparrow}{qQ\downarrow}}+\tilde{\omega}^{c}_{qQ}\right]\left[\left(3\tilde{\omega}_{\binom{qQ\uparrow}{qQ\downarrow}}+\tilde{\omega}^{c}_{qQ}\right)^{2}-\bar{\omega}_{k}^{-2}\right]^{-2}$$

$$\Omega_{\binom{4}{5}}\left(\begin{pmatrix} Q\uparrow \\ q\downarrow \end{pmatrix},k\right)=\left[7\tilde{\omega}_{\binom{Q\uparrow}{q\downarrow}}+\tilde{\omega}^{c}_{\binom{Q}{q}}\right]^{2}\left[\left(7\tilde{\omega}_{\binom{Q\uparrow}{q\downarrow}}+\tilde{\omega}^{c}_{\binom{Q}{q}}\right)^{2}-\bar{\omega}_{k}^{-2}\right]^{-2}$$

$$\Omega_{\binom{6}{7}}\left(\begin{pmatrix} Q\uparrow \\ q\downarrow \end{pmatrix},k\right)=\left[6\tilde{\omega}_{\binom{Q\downarrow}{q\downarrow}}+\tilde{\omega}^{c}_{\binom{Q}{q}}\right]^{2}\left[\left(6\tilde{\omega}_{\binom{Q\downarrow}{q\downarrow}}+\tilde{\omega}^{c}_{\binom{Q}{q}}\right)^{2}-\bar{\omega}_{k}^{-2}\right]^{-2};\ \xi_{v}=\frac{V}{\pi^{3}v_{p}^{3}}$$

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

Results And Discussions

Taking Y(1) ion at the centre of the system a mesh of 38 atoms/lattice sites (Ba(2), Cu(16) and O(20) ions) is observed for the model calculations in which Cu-O layer has Cu(8) and O(4), Cu-O_2 layer has Cu(8) and O(8) and Ba-O layer has Ba(2) and O(8) atoms. The digits appearing in brackets with elements stand for their number taken up for numerical estimation. Above investigations reveal that the PDOS can be resolved into diagonal and non-diagonal contributions. Further, with special references to the high temperature superconductivity and present form of PDOS, being temperature dependent can be studied into (i) superconducting and (ii) normal regimes.In order to verify above obtained results we apply to a model crystal $YBa_2Cu_3O_{7-\delta}$ with following physical constantsas given below

Symbol	Value	Symbol	Value
a	$3.8\times10^{-8}\ cm$	$\hbar$	$1.05\times10^{-27}\ cm^2\ gm\sec^{-1}$
b	$3.9\times10^{-8}\ cm$	v_p	$4\times10^{5}\ cm/\sec$
c	$11.60\times10^{-8}\ cm$	V	$171.912\times10^{-24}\ cm^3$
g_k	0.5	k_B	$1.3807\times10^{-16}\ cm^2\ gm\sec^{-2}\ K$
T	50 K	ω_Q^c	$1.1783\times10^{14}\ \sec^{-1}$
f	.05263	ω_Q	$3.0343\times10^{13}\ \sec^{-1}$
Mass (Y)	$147.58\times10^{-24}\ gm$	$\phi^{II}(r)$	$1.13\times10^{6}\ erg\sec^{-2}$
Mass (Ba)	$66.95\times10^{-24}\ gm$	$\phi^{III}(r)$	$-1.14\times10^{14}\ erg\sec^{-3}$
$\phi^{IV}(r)$	$2.14\times10^{21}\ erg\sec^{-4}$		

Fig. (1) and Fig. (2) show the diagonal contribution and non-diagonal contribution of PDOS for

$YBa_2Cu_3O_{7-\delta}$ superconductor. It is evident from Fig. (3) and Fig. (4) that as temperature is increased to 50K to 300K (above critical temperature) the nature of PDOS curves changes, showing temperature dependent nature of PDOS which is the main feature of the present theory. Hence, PDOS not only dependents upon energy but also on impurity concentration and temperature.

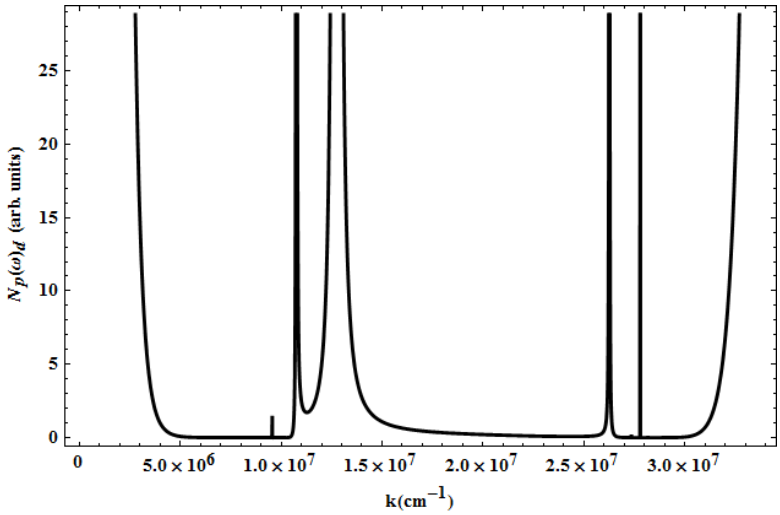

Figure 1. Nature of $N_p(\omega)_d$ for $YBa_2Cu_3O_{7-\delta}$ in Superconducting region.

The diagonal contribution for PDOS for YBCO superconductor has been portrayed in fig. (1) with in superconducting region. From Fig (1) we have seen that there are 8 peaks at 5.56 meV, 18.98 meV, 21.36 meV, 25.11 meV, 52.01 meV, 54.18 meV,54.18 meV and 64.66 meV for diagonal contribution of PDOS for $YBa_2Cu_3O_{7-\delta}$ superconductor. The 11 peaks of 1.305 meV, 18.98 meV, 20.37 meV, 21.35 meV, 25.31 meV, 38.36 meV, 52.01 meV, 53.98 meV, 54.97 meV, 55.96 meV and 62.29 meV has been critically analysed for non-diagonal contribution of PDOS for $YBa_2Cu_3O_{7-\delta}$ in superconducting region.

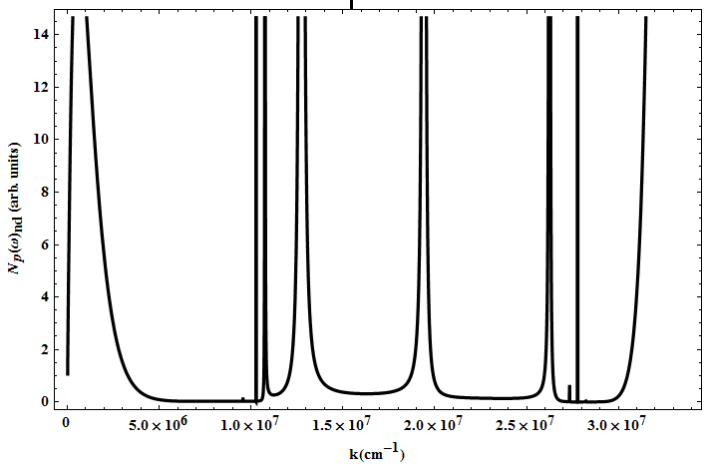

Figure 2. Variation of $N_p(\omega)_{nd}$ for $YBa_2Cu_3O_{7-\delta}$ in Superconducting region.

Here Fig (3) and Fig (4) confirmed that the number of peaks decreases as there is a transition

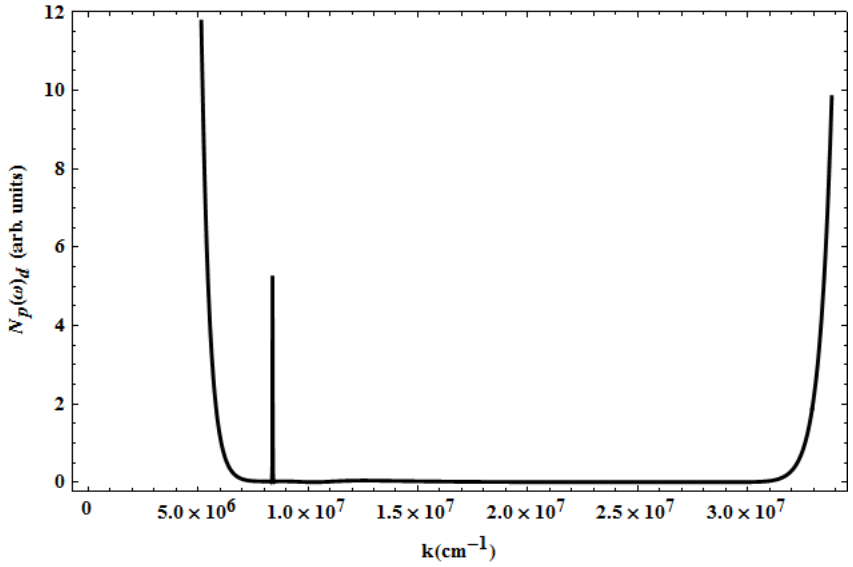

Figure 3. Behaviour of $N_p(\omega)_d$ for $YBa_2Cu_3O_{7-\delta}$ in normal region.

From Fig (3) we observed that as temperature increased there exists only 3 peaks at 10.24 meV, 16.59 meV and 67.03 meV for diagonal contribution of PDOS in normal region.

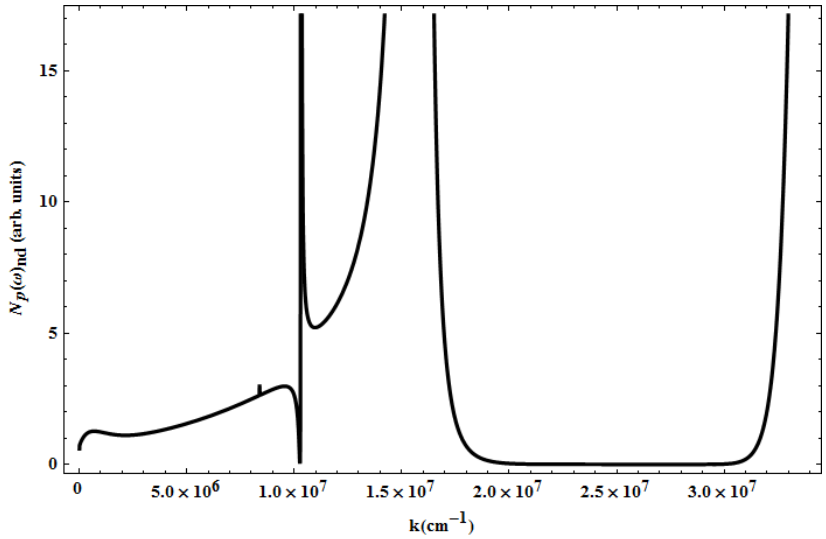

Figure 4. Nature of $N_p(\omega)_{nd}$ for $YBa_2Cu_3O_{7-\delta}$ in normal region.

We understand from Fig (4) that there are 5 peaks arising at 1.076 meV, 16.61 meV, 21.36 meV, 30.45 meV and 65.25 meV, for non-diagonal PDOS in normal region.

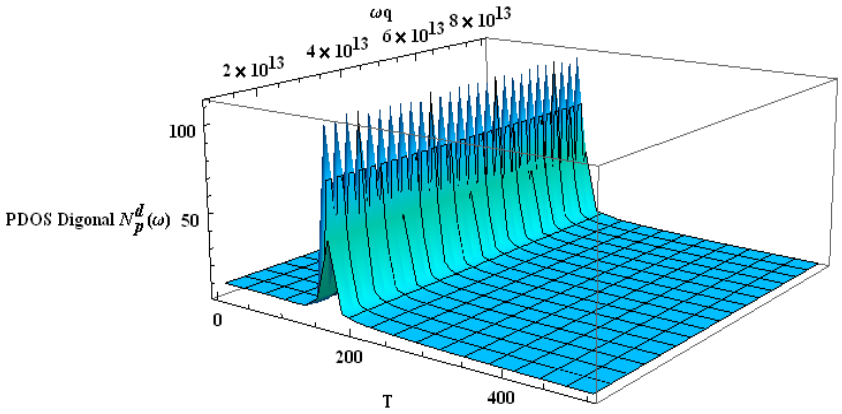

Figure 5. 3D depiction of $N_p(\omega)_{nd}$ for $YBa_2Cu_3O_{7-\delta}$ in superconducting region.

The three dimensional graphic has been portrayed for diagonal contribution of PDOS with the variation of T and ω_q. We can observe there arises large number of peaks near 150 K temperature with different height which are very sensitive in nature.

Conclusions

The PDOS shows significant dependence on temperature, impurity concentration and electron-phonon coupling and appears as a salient feature of the theory.There is the auto emergence of pairon without taking the BCS Hamiltonian.It also infers from the present theory that taking the effects of anharmonicity, defect and electron-phonon contributions, the system $YBa_2Cu_3O_{7-\delta}$ is numerically analysedand found in goodagreement with experimental results.A large number of peaks are arising for the various contributions of PDOS within two regions, discussed with a special framework. The highly sensitive nature of electron-phonon coupling is also observed to contribute significantly for the rapid variation in PDOS.The highly sensitive nature of PDOS can certainly be useful in deriving and undertaking the various dynamical properties of cuprate superconductors in the superconducting and normal regimes, e.g., various electronic and thermal transport properties, electronic and lattice heat capacities, infrared and far infrared absorption, microwave attenuation and Raman scattering. As a final comment the theory developed on the new foundations is equally applicable for various high T_c superconductors.

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