

Anharmonicity and Impurity Effects on Infrared Absorption in High Temperature Superconductors

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Abstract Taking into account the effects of anharmonicities and point impurities the quantum dynamics of phonons for high temperature superconductors is developed using Green's function formalism via an almost complete Hamiltonian (without BCS Hamiltonian) which comprises the effects of (i) unperturbed electrons, (ii) unperturbed phonons, (iii) electron-phonon interactions, (iv) anharmonicities and (v) isotopic impurities. This is utilized to obtain the expressions for infrared absorption coefficient which can be resolved into diagonal and non-diagonal parts. Non-diagonal contribution arises only in impure crystals and vanishes in the case of pure crystal. The investigations are also made to study the dependence of infrared absorption coefficient on various parameters in the superconducting and normal regimes followed by numerical estimates for cuprate superconductor $YBa_2Cu_3O_{7-\delta}$. The temperature dependence of infrared absorption coefficients and automatic emergence of pairons appears as a special feature of the theory.

Keywords: high temperature superconductors, green's function, infrared absorption coefficient

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1. Introduction

Due to the direct relation between the structure of the phonon spectrum in an impure crystal and the absorption line shape the problem of the optical absorption of impurity induced crystal in the infrared and far infrared, appears as a very interesting problem [1]. We have not come across the sufficient experimental results which has offered as much information about the vibrational spectra of crystals as have been endorsed by the infrared absorption experiments. As a result of interaction of radiation (photon) the light is absorbed by the crystal without any change in the electronic state but excites or de-excites one or two phonons. The appropriate selection rule for such interactions is that only modes whose wave vector \mathbf{k} adds up to zero interact with the light incident on the crystal. The study of infrared properties of high temperature superconductors has equally attracted the theorists and experimentalists to establish the phenomenon and dynamical behavior. The far-infrared spectroscopy is used to explain the energy gap in BCS superconductors [2] as well. This interesting problem of infrared absorption with low impurity concentration using the method of Green's function of many body theory has been theoretically investigated by many authors [3-8]. The absorption coefficient of a harmonic crystal is temperature independent, while experimental evidences show that temperature plays an important role to study the absorption spectra. This arises only when nonlinear terms in the dipole moment or anharmonic terms in the potential energy are used [9]. The crystal structure is linked with

absorption bands and these bands are often observed in the infrared spectra of crystalline solids [10]. If an ionic cubic diatomic crystal absorbs the infrared light, a single band coupled with optical mode of zero propagation constant will occur. As anharmonicity alone does not give any mechanism for absorption so the intrinsic lattice absorption can be explained on the basis of second order electric moment [11]. Czerny [12] and Barnes [13] make the observations on alkali halide crystals significantly provided the existence of side band (the short wavelength side) of the chief reflection or absorption band. Some authors tried to explain these side bands using the anharmonicity approach in which the potential energy (connected with lattice vibrations) contains the higher order terms like cubic and quartic [14,15,16]. An anharmonic quantum dynamical approach is used via double time temperature dependent Green's functions to develop the theory of infrared absorption for high temperature superconductors in the following sections of the present paper:

2. The Hamiltonian

To investigate the quantum dynamics of phonons let us consider almost complete crystal Hamiltonian in the form [17,18,19,20]

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

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

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

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

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

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

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. Also, \uparrow (\downarrow) stand for spin up(down) and $\mathbf{Q} = \mathbf{k} + \mathbf{q}$ (\mathbf{k} and \mathbf{q} being phonon and electron wave vectors, respectively) and g_k stand for electron-phonon coupling coefficient. The symbols $V_s(k_1, k_2, \dots, k_s)$, $C(k_1, k_2)$ and $D(k_1, k_2)$ stand for the anharmonic coupling coefficients, mass and force constant change parameters [17, 18, 19, 20].

3. The Phonon Green's functions

To obtain the phonon line spectrum, we evaluate the double time temperature dependent retarded phonon Green's function

$$G_{k,k}^{\prime}(t-t') = -i\theta(t-t') \langle [A_k(t), A_k^*(t')] \rangle \quad (2)$$

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

$$(\omega^2 - \omega_k^2) G_{k,k}^{\prime}(\omega) = \frac{\omega_k}{\pi} \left(\eta_{k,k}^{\prime} + \langle\langle F_k(t); A_k^*(t') \rangle\rangle \right) \quad (3)$$

with

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

Which, in turns, resolves the Green's function to be obtained in terms of phonon frequency shift $\Delta_k(\omega)$ and line width $\Gamma_k(\omega)$ as

$$G_{k,k}^{\prime}(\omega) = \frac{\omega_k \eta_{k,k}^{\prime}}{\pi[\omega^2 - \tilde{\omega}_k^2 - 2\omega_k \{\Delta_k(\omega) - i\Gamma_k(\omega)\}]} \quad (5)$$

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

$$G_{k,k}^{\prime}(\omega) = \frac{\omega_k \eta_{k,k}^{\prime}}{\pi[\omega^2 - \tilde{\omega}_{kq}^2 + 2i\omega_k \Gamma_k(\omega)]} \quad (6)$$

$$\tilde{\omega}_{kq}^2 = \tilde{\omega}_{kq}^2 + 2\omega_k \Delta_k(\omega) \quad (7)$$

$\tilde{\omega}_{kq}$ and $\tilde{\omega}_{kq}$ are renormalized and perturbed mode frequencies.

4. The Phonon Frequency Width

The phonon line width enables one to investigate many dynamical properties of crystalline solids, e.g., life times, the phonon frequency (energy) spectrum and density of states which can be obtained in the following form [17,21]:

$$\Gamma_k(\omega) = \Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \quad (8)$$

$$\Gamma_k^D(\omega) = \sum_{k_1} [\pi \mathcal{E}(\omega) R^D(k, k_1) \omega_{k_1} \delta(\omega^2 - \tilde{\omega}_{k_1}^2) + 4\pi \omega_k^{-1} N R^{Dep}(k, k_1) |\tilde{\omega}| \delta(\omega^2 - \tilde{\omega}_k^2)] \quad (8a)$$

$$\Gamma_k^{3A}(\omega) = 18\pi \mathcal{E}(\omega) \sum_{k_1, k_2} |V_3(k_1, k_2, -k)|^2 \eta_1 A_\alpha \quad (8b)$$

$$\Gamma_k^{3D}(\omega) = 144\pi \mathcal{E}(\omega) \sum_{k_1, k_2} |V_3(k_1, k_2, -k)|^2 \times R^c(k, k_1) \omega_k^{-1} \eta_1 A_\alpha \quad (8c)$$

$$\Gamma_k^{ep}(\omega) = \pi \omega_k^{-2} |g_k|^2 \sum_q \left[\bar{N}_{qQ\uparrow} \Omega_\uparrow \omega_{1q}^c \times \delta(\omega - 4\tilde{\omega}_{qQ\uparrow}) + \bar{N}_{qQ\uparrow} \Omega_\uparrow \omega_{2q}^c \times \delta(\omega - \tilde{\Omega}_\uparrow) + 3\bar{N}_{qQ\downarrow} \Omega_\downarrow \omega_{3q}^c \times \delta(\omega - \tilde{\Omega}_\downarrow) + \bar{N}_{qQ\downarrow} \gamma_1 \omega_{4Q\downarrow}^c \times \delta(\omega - \tilde{\Omega}_\downarrow) \right] + 128\pi \sum_{k,q} \omega_k^{-2} |g_k|^4 \times \left[\tilde{n}_k N(Q_\uparrow) \delta(\omega - \Omega_1) + \tilde{n}_k N(q_\uparrow) \times \delta(\omega - \Omega_2) + \tilde{n}_k N(Q_\downarrow) \delta(\omega - 2\Omega_3) - 2\omega_k^{-1} \tilde{\omega}_k^2 \hat{N}^2 \mathcal{E}(\omega) \delta(\omega^2 - \tilde{\omega}_k^2) \right] \quad (8d)$$

various symbols are well defined in the references elsewhere [17,21].

5. The Infrared Absorption Coefficients

The optical absorption coefficient which is related to Green's function can be given by [5],

$$\alpha(\omega) = \frac{4\pi\omega}{\eta c} \text{Im} \left[\sum_{\alpha, \beta} \sum_{l, l'} e_i(l) e_j(l') t_\alpha t_\beta (2\pi / \hbar) \langle\langle U_{i\alpha}(l, t); U_{j\beta}(l', O) \rangle\rangle_\omega \right] \quad (9)$$

In the above equation $\langle\langle \dots \rangle\rangle_\omega$ is the Fourier transform of phonon Green's function, t_α is the

polarization vector of incident radiation, c is the speed of electromagnetic radiation, η is the refractive index and $e_i(l)$ is the charge on the i -th atom in the l -th unit cell. For diatomic crystal and $\mu_{\alpha}^{-1} = M_1 M_2 (M_1 + M_2)^{-1}$ is the reduced mass. Eq. (9) can be written in the form [22]

$$\alpha(\omega) = \left(\frac{4\pi N e^2}{\eta c} \right) \left(\frac{\pi \mu \omega}{\omega_0} \right) \text{Im } G_{k,k'}(\omega) \quad (10)$$

Using Eq. (6) in (10) the absorption coefficient can be obtained in the following form

$$\alpha(\omega) = \left(\frac{8\pi N e^2 \mu}{\eta c} \right) \frac{\omega_k \eta_{kk'} \Gamma_k(\omega)}{[(\omega^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 \Gamma_k^2(\omega)]} \quad (11)$$

The Absorption coefficient given in Eq. (11) can be separated into diagonal and non-diagonal contributions, namely;

$$[\alpha(\omega) = \alpha_d(\omega) + \alpha_{nd}(\omega)]$$

$$\alpha_d(\omega) = \frac{P_c \omega_k \Gamma_k(\omega)}{[(\omega^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 \Gamma_k^2(\omega)]} \quad (12)$$

$$\alpha_{nd}(\omega) = \frac{P_c C(-k, k') \Gamma_k(\omega)}{[(\omega^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 \Gamma_k^2(\omega)]} \quad (13)$$

where $P_c = 8\pi N e^2 \mu / \eta c$. For $k \neq k'$ the non-diagonal contribution arises and it chiefly depends on the mass change parameter $C(-k, k')$. This contribution is momentous only for impurity induced crystal and vanishes for a pure crystal. Now making use of Eq. (8) in Eq. (12) and after some algebra we can derived the expression for diagonal contribution in the following form

$$\begin{aligned} \alpha_d^D(\omega) &= P_c \omega_k A_D(\omega) \left[1 - 4\omega_k^2 A(\omega) \right. \\ &\quad \times \left(\Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \right)^2 \\ &\quad + 2\Gamma_k^D(\omega) \left(\Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \right) \\ &\quad \left. \times \left\{ 1 - 4\omega_k^2 A(\omega) [\Gamma_k^D(\omega)]^2 \right\} \right] \quad (14) \end{aligned}$$

$$\begin{aligned} \alpha_d^{3A}(\omega) &= P_c \omega_k A_{3A}(\omega) \left[1 - 4\omega_k^2 A(\omega) \right. \\ &\quad \times \left(\Gamma_k^D(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \right)^2 \\ &\quad + 2\Gamma_k^{3A}(\omega) \left(\Gamma_k^D(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \right) \\ &\quad \left. \times \left\{ 1 - 4\omega_k^2 A(\omega) [\Gamma_k^{3A}(\omega)]^2 \right\} \right] \quad (15) \end{aligned}$$

$$\begin{aligned} \alpha_d^{3D}(\omega) &= P_c \omega_k A_{3D}(\omega) \left[1 - 4\omega_k^2 A(\omega) \right. \\ &\quad \times \left(\Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{ep}(\omega) \right)^2 \\ &\quad + 2\Gamma_k^{3D}(\omega) \left(\Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{ep}(\omega) \right) \\ &\quad \left. \times \left\{ 1 - 4\omega_k^2 A(\omega) [\Gamma_k^{3D}(\omega)]^2 \right\} \right] \quad (16) \end{aligned}$$

$$\begin{aligned} \alpha_d^{ep}(\omega) &= P_c \omega_k A_{ep}(\omega) \left[1 - 4\omega_k^2 A(\omega) \right. \\ &\quad \times \left(\Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) \right)^2 \\ &\quad + 2\Gamma_k^{ep}(\omega) \left(\Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) \right) \\ &\quad \left. \times \left\{ 1 - 4\omega_k^2 A(\omega) [\Gamma_k^{ep}(\omega)]^2 \right\} \right] \quad (17) \end{aligned}$$

Where

$$A_D(\omega) = \frac{\Gamma_k^D(\omega)}{[(\omega^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^D(\omega)]^2]} ;$$

$$A_{3A}(\omega) = \frac{\Gamma_k^{3A}(\omega)}{[(\omega^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^{3A}(\omega)]^2]} ;$$

$$A(\omega) = \frac{1}{[(\omega^2 - \bar{\omega}_k^2)^2]} ;$$

$$A_{3D}(\omega) = \frac{\Gamma_k^{3D}(\omega)}{[(\omega^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^{3D}(\omega)]^2]} ;$$

$$A_{ep}(\omega) = \frac{\Gamma_k^{ep}(\omega)}{[(\omega^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]}$$

The terms in the square brackets of Eqs. (14) to (17) can be further simplified to give

$$\begin{aligned} \alpha_d^D(\omega) &= P_c \omega_k A_D(\omega) \left[1 - 8\omega_k^2 A(\omega) \Gamma_k^D(\omega) \right. \\ &\quad \times \left\{ \left(\Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \right)^2 \right\} \\ &\quad \left. \times \left\{ 1 - 4\omega_k^2 A(\omega) [\Gamma_k^D(\omega)]^2 \right\} \right] \quad (18) \end{aligned}$$

$$\begin{aligned} \alpha_d^{3A}(\omega) &= P_c \omega_k A_{3A}(\omega) \left[1 - 8\omega_k^2 A(\omega) \Gamma_k^D(\omega) \right. \\ &\quad \times \left\{ \left(\Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \right)^2 \right\} \\ &\quad \left. \times \left\{ 1 - 4\omega_k^2 A(\omega) [\Gamma_k^{3A}(\omega)]^2 \right\} \right] \quad (19) \end{aligned}$$

$$\begin{aligned} \alpha_d^{3D}(\omega) &= P_c \omega_k A_{3D}(\omega) \left[1 - 8\omega_k^2 A(\omega) \Gamma_k^{3D}(\omega) \right. \\ &\quad \times \left\{ \left(\Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{ep}(\omega) \right)^2 \right\} \\ &\quad \left. \times \left\{ 1 - 4\omega_k^2 A(\omega) [\Gamma_k^{3D}(\omega)]^2 \right\} \right] \quad (20) \end{aligned}$$

$$\begin{aligned} \alpha_d^{ep}(\omega) &= P_c \omega_k A_{ep}(\omega) \left[1 - 8\omega_k^2 A(\omega) \Gamma_k^{ep}(\omega) \right. \\ &\quad \times \left\{ \left(\Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) \right)^2 \right\} \\ &\quad \left. \times \left\{ 1 - 4\omega_k^2 A(\omega) [\Gamma_k^{ep}(\omega)]^2 \right\} \right] \quad (21) \end{aligned}$$

Which after further simplification yield,

$$\begin{aligned} \alpha_d^D(\omega) = P_c \omega_k A_D(\omega) & \left[1 - \left\{ 4\omega_k^2 A(\omega) [\Gamma_k^D(\omega)]^2 \right\} \right. \\ & - 8\omega_k^2 A(\omega) \Gamma_k^D(\omega) \\ & \times \left\{ \left(\Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \right) \right\} \\ & + 32\omega_k^4 A(\omega) [\Gamma_k^D(\omega)]^3 \\ & \left. \times \left\{ \left(\Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \right) \right\} \right] \end{aligned} \quad (22)$$

$$\begin{aligned} \alpha_d^{3A}(\omega) = P_c \omega_k A_{3A}(\omega) & \left[1 - \left\{ 4\omega_k^2 A(\omega) [\Gamma_k^{3A}(\omega)]^2 \right\} \right. \\ & - 8\omega_k^2 A(\omega) \Gamma_k^{3A}(\omega) \\ & \times \left\{ \left(\Gamma_k^D(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \right) \right\} \\ & + 32\omega_k^4 A(\omega) [\Gamma_k^{3A}(\omega)]^3 \\ & \left. \times \left\{ \left(\Gamma_k^D(\omega) + \Gamma_k^{3D}(\omega) + \Gamma_k^{ep}(\omega) \right) \right\} \right] \end{aligned} \quad (23)$$

$$\begin{aligned} \alpha_d^{3D}(\omega) = P_c \omega_k A_{3D}(\omega) & \left[1 - \left\{ 4\omega_k^2 A(\omega) [\Gamma_k^{3D}(\omega)]^2 \right\} \right. \\ & - 8\omega_k^2 A(\omega) \Gamma_k^{3D}(\omega) \\ & \times \left\{ \left(\Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{ep}(\omega) \right) \right\} \\ & + 32\omega_k^4 A(\omega) [\Gamma_k^{3D}(\omega)]^3 \\ & \left. \times \left\{ \left(\Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{ep}(\omega) \right) \right\} \right] \end{aligned} \quad (24)$$

$$\begin{aligned} \alpha_d^{ep}(\omega) = P_c \omega_k A_{ep}(\omega) & \left[1 - \left\{ 4\omega_k^2 A(\omega) [\Gamma_k^{ep}(\omega)]^2 \right\} \right. \\ & - 8\omega_k^2 A(\omega) \Gamma_k^{ep}(\omega) \\ & \times \left\{ \left(\Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) \right) \right\} \\ & + 32\omega_k^4 A(\omega) [\Gamma_k^{ep}(\omega)]^3 \\ & \left. \times \left\{ \left(\Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{3D}(\omega) \right) \right\} \right] \end{aligned} \quad (25)$$

The higher order terms with cubic and higher powers add negligibly small contribution [7,19,20] and can be dropped from above Eqs. (22) to (25). Thus making use of substantial contributions only the Eqs. (22) to (25) can be further simplified to give

$$\begin{aligned} \alpha_d^D(\omega) = P_c \omega_k A_D(\omega) & \left[1 - 4\omega_k^2 A(\omega) \Gamma_k^D(\omega) \right. \\ & \left. \times \left\{ \Gamma_k^D(\omega) + 2\Gamma_k^{3A}(\omega) + 2\Gamma_k^{ep}(\omega) \right\} \right] \end{aligned} \quad (26)$$

$$\begin{aligned} \alpha_d^{3A}(\omega) = P_c \omega_k A_{3A}(\omega) & \left[1 - 4\omega_k^2 A(\omega) \Gamma_k^{3A}(\omega) \right. \\ & \left. \times \left\{ \Gamma_k^{3A}(\omega) + 2\Gamma_k^D(\omega) + 2\Gamma_k^{ep}(\omega) \right\} \right] \end{aligned} \quad (27)$$

$$\begin{aligned} \alpha_d^{3D}(\omega) = P_c \omega_k A_{3D}(\omega) & \left[1 - 4\omega_k^2 A(\omega) \Gamma_k^{3D}(\omega) \right. \\ & \left. \times \left\{ \Gamma_k^{3D}(\omega) + 2\Gamma_k^D(\omega) + 2\Gamma_k^{ep}(\omega) \right\} \right] \end{aligned} \quad (28)$$

$$\begin{aligned} \alpha_d^{ep}(\omega) = P_c \omega_k A_{ep}(\omega) & \left[1 - 4\omega_k^2 A(\omega) \Gamma_k^{ep}(\omega) \right. \\ & \left. \times \left\{ \Gamma_k^{ep}(\omega) + 2\Gamma_k^D(\omega) + 2\Gamma_k^{3A}(\omega) \right\} \right]. \end{aligned} \quad (29)$$

Thus the final form of absorption coefficients can be obtained as

$$\begin{aligned} \alpha_d^D(\omega) = P_c \omega_k \sum_{k_1} & \left[\pi R^D(k, k_1) \omega_{k_1} (2\tilde{\omega}_{k_1})^{-1} \right. \\ & \left. + 8\pi \omega_k^{-1} N R^{Dep}(k, k_1) \right] A_D^{k_1}(\omega) \end{aligned} \quad (30)$$

$$\begin{aligned} \alpha_d^{3A}(\omega) = 18\pi P_c \omega_k \sum_{k_1, k_2} & |V_3(k_1, k_2, -k)|^2 \eta_1 \\ & \times \left[S_{+\alpha} \omega_{+\alpha} A_{3A}^{+\alpha}(\omega) + S_{-\alpha} \omega_{-\alpha} A_{3A}^{-\alpha}(\omega) \right] \end{aligned} \quad (31)$$

$$\begin{aligned} \alpha_d^{3D}(\omega) = 144\pi P_c \omega_k \sum_{k_1, k_2} & |V_3(k_1, k_2, -k)|^2 \\ & \times R^c(k, k_1) \omega_k^{-1} \eta_1 \times \left[\begin{aligned} & S_{+\alpha} \omega_{+\alpha} A_{3D}^{+\alpha}(\omega) \\ & + S_{-\alpha} \omega_{-\alpha} A_{3D}^{-\alpha}(\omega) \end{aligned} \right] \end{aligned} \quad (32)$$

$$\begin{aligned} \alpha_d^{ep}(\omega) = P_c \pi \omega_k^{-1} |g_k|^2 & \sum_q \left[\frac{\bar{N}_{qQ\uparrow} (3\omega_{qQ\uparrow} + \omega_{qQ}^c) \omega_{1q\uparrow}^c}{[(16\tilde{\omega}_{qQ\uparrow}^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]} \right. \\ & + \frac{\bar{N}_{qQ\uparrow} (3\omega_{qQ\uparrow} + \omega_{qQ}^c) \omega_{2q\uparrow}^c}{[\{(3\tilde{\omega}_{qQ\uparrow} + \tilde{\omega}_{qQ}^c) - \bar{\omega}_k^2\}^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]} \\ & + \frac{3\bar{N}_{qQ\downarrow} (3\omega_{qQ\downarrow} + \omega_{qQ}^c) \omega_{3q\downarrow}^c}{[\{(3\tilde{\omega}_{qQ\downarrow} + \tilde{\omega}_{qQ}^c) - \bar{\omega}_k^2\}^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]} \\ & \left. + \frac{\bar{N}_{qQ\downarrow} (4\omega_{q\downarrow} + 2\omega_{Q\downarrow} + \omega_{qQ\downarrow}^c) \omega_{4Q\downarrow}^c}{[\{(3\tilde{\omega}_{qQ\downarrow} + \tilde{\omega}_{qQ}^c) - \bar{\omega}_k^2\}^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]} \right] \\ & + 128 P_c \pi \omega_k \sum_{k,q} |g_k|^4 \omega_k^{-2} \\ & \times \left[\frac{\tilde{n}_k N(Q\uparrow)}{[\{(7\tilde{\omega}_{Q\uparrow} + \tilde{\omega}_Q^c) - \bar{\omega}_k^2\}^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]} \right. \\ & + \frac{\tilde{n}_k N(q\uparrow)}{[\{(7\tilde{\omega}_{q\uparrow} + \tilde{\omega}_q^c) - \bar{\omega}_k^2\}^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]} \\ & + \frac{\tilde{n}_k N(Q\downarrow)}{[\{(6\tilde{\omega}_{Q\downarrow} + 2\tilde{\omega}_Q^c) - \bar{\omega}_k^2\}^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]} \\ & + \frac{\tilde{n}_k N(q\downarrow)}{[\{(6\tilde{\omega}_{q\downarrow} + 2\tilde{\omega}_q^c) - \bar{\omega}_k^2\}^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]} \\ & \left. - \frac{2\omega_k^{-1} \tilde{\omega}_k^2 \hat{N}^2 (2\tilde{\omega}_k)^{-1}}{[\{(6\tilde{\omega}_{Q\downarrow} + 2\tilde{\omega}_Q^c) - \bar{\omega}_k^2\}^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]} \right] \end{aligned} \quad (33)$$

And similarly the non-diagonal contribution can be obtained as

$$\alpha_{nd}^D(\omega) = P_c \omega_k C(-k, k') \sum_{k_1} \left[\pi R^D(k, k_1) \omega_{k_1} (2\tilde{\omega}_{k_1})^{-1} + 8\pi \omega_k^{-1} N R^{Dep}(k, k_1) \right] A_D^{k_1}(\omega) \quad (34)$$

$$\alpha_{nd}^{3A}(\omega) = 18\pi P_c \omega_k C(-k, k') \sum_{k_1, k_2} |V_3(k_1, k_2, -k)|^2 \eta_1 \times \left[S_{+\alpha} \omega_{+\alpha} A_{3A}^{+\alpha}(\omega) + S_{-\alpha} \omega_{-\alpha} A_{3A}^{-\alpha}(\omega) \right] \quad (35)$$

$$\alpha_{nd}^{3D}(\omega) = 144\pi P_c \omega_k C(-k, k') \sum_{k_1, k_2} |V_3(k_1, k_2, -k)|^2 \times R^c(k, k_1) \omega_k^{-1} \eta_1 \times \left[S_{+\alpha} \omega_{+\alpha} A_{3D}^{+\alpha}(\omega) + S_{-\alpha} \omega_{-\alpha} A_{3D}^{-\alpha}(\omega) \right] \quad (36)$$

$$\begin{aligned} \alpha_{nd}^{ep}(\omega) = & P_c \pi \omega_k^{-1} |g_k|^2 C(-k, k') \\ & \sum_q \left[\frac{\bar{N}_{qQ\uparrow} (3\omega_{qQ\uparrow} + \omega_{qQ}^c) \omega_{1q\uparrow}^c}{[(16\tilde{\omega}_{qQ\uparrow}^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2]} \right. \\ & + \frac{\bar{N}_{qQ\uparrow} (3\omega_{qQ\uparrow} + \omega_{qQ}^c) \omega_{2q\uparrow}^c}{\{[(3\tilde{\omega}_{qQ\uparrow} + \tilde{\omega}_{qQ}^c)^2 - \bar{\omega}_k^2]^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2\}} \\ & + \frac{3\bar{N}_{qQ\downarrow} (3\omega_{qQ\downarrow} + \omega_{qQ}^c) \omega_{3q\downarrow}^c}{\{[(3\tilde{\omega}_{qQ\downarrow} + \tilde{\omega}_{qQ}^c)^2 - \bar{\omega}_k^2]^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2\}} \\ & \left. + \frac{\bar{N}_{qQ\downarrow} (4\omega_{q\downarrow} + 2\omega_{Q\downarrow} + \omega_{qQ\downarrow}^c) \omega_{4Q\downarrow}^c}{\{[(3\tilde{\omega}_{qQ\downarrow} + \tilde{\omega}_{qQ}^c)^2 - \bar{\omega}_k^2]^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2\}} \right] \\ & + 128P_c \pi \omega_k C(-k, k') \sum_{k, q} |g_k|^4 \omega_k^{-2} \\ & \times \left[\frac{\tilde{n}_k N(Q\uparrow)}{\{[(7\tilde{\omega}_{Q\uparrow} + \tilde{\omega}_Q^c)^2 - \bar{\omega}_k^2]^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2\}} \right. \\ & + \frac{\tilde{n}_k N(q\uparrow)}{\{[(7\tilde{\omega}_{q\uparrow} + \tilde{\omega}_q^c)^2 - \bar{\omega}_k^2]^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2\}} \\ & + \frac{\tilde{n}_k N(Q\downarrow)}{\{[(6\tilde{\omega}_{Q\downarrow} + 2\tilde{\omega}_Q^c)^2 - \bar{\omega}_k^2]^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2\}} \\ & + \frac{\tilde{n}_k N(q\downarrow)}{\{[(6\tilde{\omega}_{q\downarrow} + 2\tilde{\omega}_q^c)^2 - \bar{\omega}_k^2]^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2\}} \\ & \left. - \frac{2\omega_k^{-1} \tilde{\omega}_k^2 \hat{N}^2 (2\tilde{\omega}_k)^{-1}}{\{[(6\tilde{\omega}_{Q\downarrow} + 2\tilde{\omega}_Q^c)^2 - \bar{\omega}_k^2]^2 + 4\omega_k^2 [\Gamma_k^{ep}(\omega)]^2\}} \right] \quad (37) \end{aligned}$$

Where

$$A_D^{k_1}(\omega) = \frac{1}{\left[(\tilde{\omega}_{k_1}^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^D(\omega)]^2 \right]} ;$$

$$A_{3A}^{+\alpha}(\omega) = \frac{(|2\tilde{\omega}_{+\alpha}|)^{-1}}{\left[(\tilde{\omega}_{+\alpha}^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^{3A}(\omega)]^2 \right]} ;$$

$$A_{3A}^{-\alpha}(\omega) = \frac{(|2\tilde{\omega}_{-\alpha}|)^{-1}}{\left[(\tilde{\omega}_{-\alpha}^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^{3A}(\omega)]^2 \right]} ;$$

$$A_{3D}^{+\alpha}(\omega) = \frac{(|2\tilde{\omega}_{+\alpha}|)^{-1}}{\left[(\tilde{\omega}_{+\alpha}^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^{3D}(\omega)]^2 \right]} ;$$

$$A_{3D}^{-\alpha}(\omega) = \frac{(|2\tilde{\omega}_{-\alpha}|)^{-1}}{\left[(\tilde{\omega}_{-\alpha}^2 - \bar{\omega}_k^2)^2 + 4\omega_k^2 [\Gamma_k^{3D}(\omega)]^2 \right]}$$

6. Results and Discussions

The results thus obtained can be analyzed for a model cuprate crystal $YBa_2Cu_3O_{7-\delta}$. For the purpose of numerical estimation following physical constants have been used:

$$\begin{aligned} a &= 3.8 \times 10^{-8} \text{ cm}, \quad b = 3.9 \times 10^{-8} \text{ cm}, \quad c = 11.60 \times 10^{-8} \text{ cm}, \\ g_k &= 0.5, \quad \eta = 1, \quad f = 0.05263, \quad \text{Mass of } Y = 147.58 \times 10^{-24} \text{ gm}, \\ \hbar &= 1.05 \times 10^{-27} \text{ cm}^2 \text{ gm sec}^{-1}, \quad \mu = 3.57 \times 10^{-23} \text{ gm}, \\ k_B &= 1.3807 \times 10^{-16} \text{ cm}^2 \text{ gm sec}^{-2} \text{ K}, \\ \phi^{II}(r) &= 1.13 \times 10^6 \text{ erg sec}^{-2}, \\ \phi^{III}(r) &= -1.14 \times 10^{14} \text{ erg sec}^{-3}. \end{aligned}$$

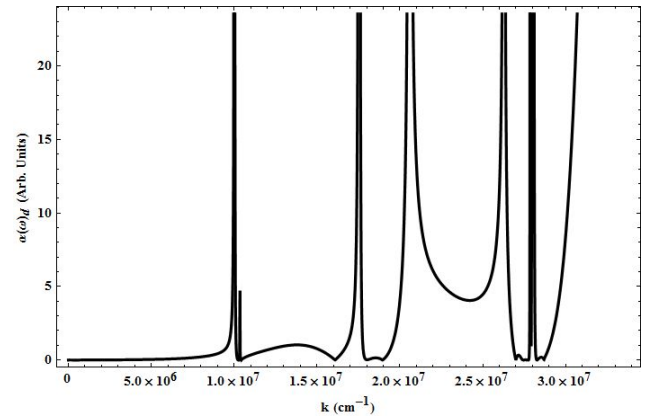


Figure 1. Nature of $\alpha(\omega)_d$ for $YBa_2Cu_3O_{7-\delta}$ in superconducting region

A careful investigation reveals that the diagonal contribution to infrared absorption coefficient exhibits 11 peaks corresponding to the energies 19.85 meV, 20.51 meV, 27.37 meV, 34.80 meV, 40.79 meV, 52.01 meV, 53.78 meV, 55.17 meV, 55.56 meV, 56.36 meV and 60.75 meV in the superconducting region which is depicted in Figure 1.

Correspondingly, the contribution due to various individual processes is shown in Figure 2, which confirms that the contribution due to anharmonic processes and impurities is extremely sensitive as compared to others. The emergence of several peaks at various k-values with different magnitudes due to individual processes is self-explanatory. The three dimensional behaviour of

absorption coefficient with varying temperature and phonon wave vector is depicted in Figure 3.

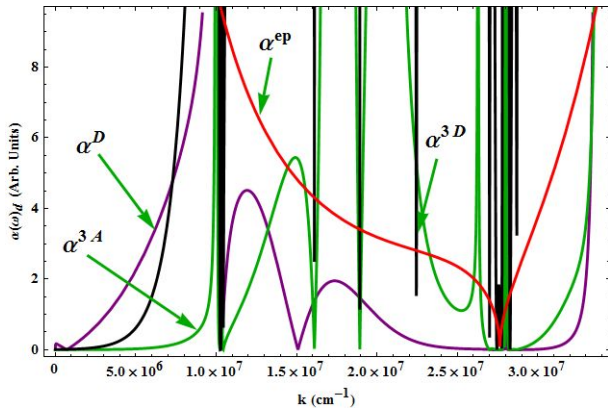


Figure 2. Various contributions to $\alpha(\omega)_d$ for $YBa_2Cu_3O_{7-\delta}$ in superconducting region

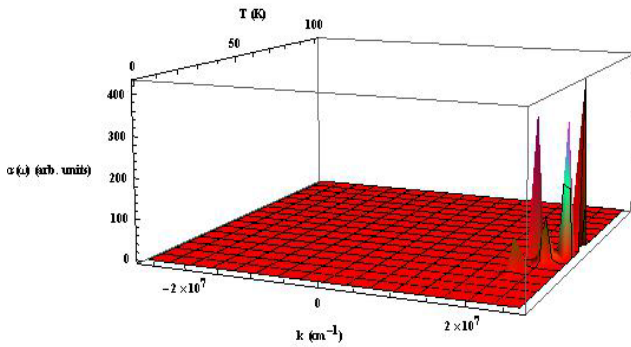


Figure 3. 3D depiction of $\alpha(\omega)$ for $YBa_2Cu_3O_{7-\delta}$ with k and T in superconducting region

Below transition temperature this graphics clearly exhibits sharp five absorption peaks of variable heights at different temperatures appearing at higher side of the phonon wave vector. Similarly, Figure 4 portrays the typical 3-D behaviour of $\alpha(\omega)$ with ω_q and phonon wave vector at the higher end of k .

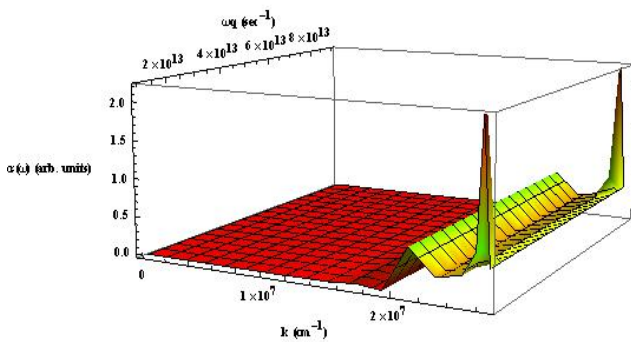


Figure 4. 3D depiction of $\alpha(\omega)$ for $YBa_2Cu_3O_{7-\delta}$ with ω_q and k in superconducting region

Further, the three dimensional variation of $\alpha(\omega)$ has been depicted with ω_q and temperature in Figure 5 where one can see large number of peaks with different heights and nature. The appearance of large number of peaks, however have not been observed through any experiment but one may observe and confirm them with the help of high resolution experiments in future.

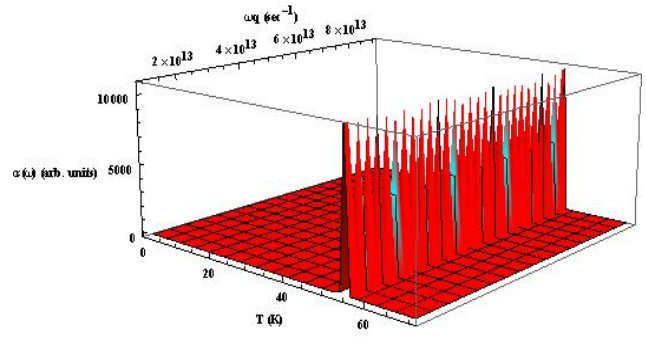


Figure 5. 3D Nature of $\alpha(\omega)$ for $YBa_2Cu_3O_{7-\delta}$ with ω_q and T in superconducting region

After a careful inspection of diagonal contribution it can be plotted to observe its significance which is portrayed as Figure 6. The infrared absorption coefficient shows 8 various peaks at 18.69 meV, 21.28 meV, 27.88 meV, 40.7 meV, 52.01 meV, 55.73 meV, 56.55 meV and 62.09 meV normal region.

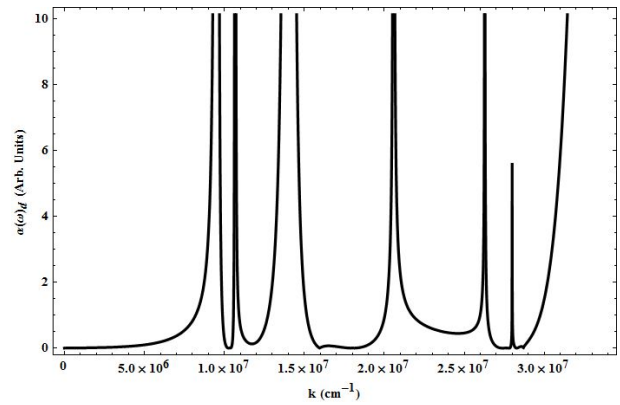


Figure 6. Behaviour of $\alpha(\omega)_d$ for $YBa_2Cu_3O_{7-\delta}$ in normal region

Comparatively this contribution is of lower magnitude as compared to the diagonal part, but the sensitivity is of similar intensity.

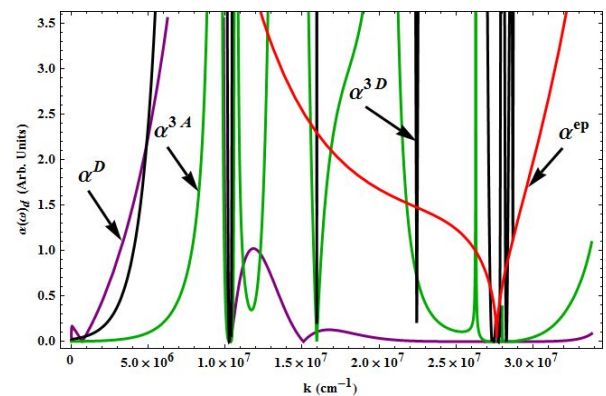


Figure 7. Various contributions to $\alpha(\omega)_d$ for $YBa_2Cu_3O_{7-\delta}$ in normal region

Figure 7 also shows the various contributions for diagonal infrared absorption coefficient in normal region with various peaks.

7. Conclusions

Taking into account the anharmonicities, impurity and electron-phonon effects, the infrared absorption coefficient

has been derived in terms of diagonal and non-diagonal contributions. The various components of infrared absorption coefficient depend upon electron-phonon coupling, temperature and concentration. As we go from superconducting to normal region the nature of curves change sharply with substantial modifications in the phonon spectra. It has been confirmed that infrared absorption coefficient not only depends upon defect concentration but also on temperature, renormalized mode and pairons frequencies which emerges as a new feature of present theory. This theory which is very unique and complex, gives a very good treatment of high temperature superconductors and is applicable for other systems also. The peculiar feature of the theory is the auto-emergence of pairons during the quantum dynamical developments where no use of BCS Hamiltonian has been made. It emerges from the present study that the optical absorption (infrared absorption) for high temperature superconductors can be made successfully with the help of present theory in both superconducting and normal regions.

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References

- [1] K. Patnaik and J. Mahanty, Infrared Absorption due to Substitutional Impurity in Cubic Crystals, *Phys. Rev.*, 155, 987, 1967.
- [2] T. Timusk, D. A. Bonn, J. E. Greedan, C. V. Satger, J. D. Garrett, A. H. O'Reilly, M. Reedyk, K. Kamaras, C. D. Porter, S. L. Herr and D. B. Tanner, Infrared properties of $YBa_2Cu_3O_{7-\delta}$, *Phys. C*, 153, 1744, 1988.
- [3] Maradudin, A. A. In astrophysics and the many-body problem. Benjamin, New York, 1963.
- [4] G. Benedek and G. F. Nardelli, Lattice response functions of imperfect crystals: Effects due to a local change of mass and short-range interaction, *Phys. Rev.*, 155, 1004, 1967.
- [5] R. J. Elliott and D. W. Taylor, Vibrations of random dilute alloys. *Proc. R. Soc. London A*, 296, 161, 1967.
- [6] Martin, T. P, Impurity-induced infrared absorption in a monatomic fcc lattice, *Phys. Rev.*, 160, 686, 1967.
- [7] Maradudin, A. A, Advances in research and applications, solid state physics. vols. 18 and 19. edited by F. Seitz and D. Turnbull (Academic Press, New York) 1966.
- [8] Genzel, L, Optical properties of solids. edited by S Nudelman and S S Mitra, 1969.
- [9] Semwal, B. S. and Sharma, P. K, Dielectric susceptibility and infrared absorption in an anharmonic crystals, *Prog. Theo. Phy.*, 51, 639, 1974.
- [10] Florence H. Forziati and Rowen. John W, Effect of changes in crystalline structure on the infrared absorption spectrum of cellulose, *J. Res. Nat. Bur. Stand.*, 46, 38, 1951.
- [11] Lax, M. and Burstein, E, Infrared lattice absorption in ionic and homopolar crystals, *Phys. Rev.*, 97, 39, 1955.
- [12] Czerny, M, Measurement on the rock salt in ultra red for testing the theory of dispersion. *Z. Physik*, 65, 600, 1930.
- [13] Barnes, R. B. and Czerny, M, Messungen am NaCl und KCl im Sprktrabereich inder ultraroten Eigenschwingungen. *Z. Physik*, 72, 447, 1931.
- [14] Born, M. and Blackman, M, Uber die feinstruktur der reststrahlen. *Z. Physik*, 82, 551, 1933.
- [15] Blackman, M, Die feinstruktur der reststrahlen. *Z. Physik*, 86, 421, 1933.
- [16] Robert Brattain, R., Barnes, R. B. and Seitz, F, On the structure and interpretation of the infrared absorption spectra of crystals. *Phys. Rev.*, 48, 582, 1935.
- [17] Ashokan, Vinod, Indu, B. D. and Dimri, A. Kr, Signature of electron-phonon interactions in high temperature superconductors, *AIP Advances*, 1, Article ID:032101, 2011.
- [18] K. N. Pathak, Theory of anharmonic crystals., *Phys. Rev.*, 139, 1569, 1965.
- [19] Indu, B. D, Theory of lattice specific heat of an isotopically disordered anharmonic crystal, *Int. J. Mod. Phys. B*, 4, 1379, 1990.
- [20] Indu, B. D, Enhanced phonon density of states in impure anharmonic crystals, *Mod. Phys. Lett. B*, 6, 1665, 1992.
- [21] Singh, Hempal, Singh, Anu, Ashokan, Vinod and Indu, B. D, Signature of anharmonicities in high temperature superconductors, *Ind. J. Appl. Res.*, 3, 35, 2013.
- [22] Painuli, C. P, Jagdish Chandra, and Indu, B. D, Infrared absorption in defect induced anharmonic solids, *Pramana. J. Phys.*, 40, 345, 1993.