Role of long – range electron - phonon and coulomb interactions in high - $T_c$cuprate superconductors

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Abstract: The effect of electron – phonon and Coulomb interactions between charge carriers on the properties ofcuprate superconductors, has been studied. The expectation value of the Hamiltonian was evaluated using second quantization and many body techniques. The equation for the energy of the system at ground state was obtained from the product of the expectation value and the thermal activation factor, exp ($-E_1/kT$). Values of specific heat and entropy against absolute temperature were calculated. In these calculations, the onsite energy of oxygen (E_p) was fixed at 2.0 x 10^{-6}eV. The onsite energy of copper (E_d), hybridization energy of oxygen and copper bands (t_{pd}), the electron – phonon interaction energy, (g_{ep}) and energy due to repulsion of copper holes occupying the same orbital (u_d), were varied. From the results, it was found that increase in the values of parameters E_d, t_{pd}, g_{ep} and u_d leads to increase in the transition temperature. It was further found that entropy and specific heat decrease with increase in the values of the parameters. It is concluded that long range electron – phonon and local Coulomb interactions increase the transition temperature of superconducting cuprates. We have obtained a transition temperature of 60 K for some parameters,which correspond to the 60 K plateau ofYBaCuO oxygen content at x = 6.7

Keywords: Cuprate Superconductors, Expectation value, Coulomb interactions, Electron-Phonon interactions.

1. Introduction

Since the discovery of Superconductivity[1],attempts to explain the phenomena[2]continued, till the BCS theory[3] that could explain most of the properties of superconductors known at that time was proposed. These superconductors were metals, alloys or doped semiconductors and are referred to as BCS or conventional superconductors. However, BCS theory could not explain Meissner effect. From time to time, some short comings of BCS theory were pointed out[4].Then appeared the discovery of the so - called high temperature superconductors[5].These superconductors are copper based oxides (cuprates) which are insulators and iron – based pnictides / selenides[6].Their properties cannot be explained by the BCS theory. Various theories were proposed to explain the properties of the high - $T_c$superconductors[7], but none could explain the properties of all the high – T_c superconductors since each superconductor has properties of its own. Different properties and especially different $T_c$values seem to be related to the different electron correlation interactions in these materials. It was proposed that in some materials superconductivity emerges when the long – range anti – ferromagnetic order in their parent phase is suppressed by doping resulting in high density of charge carriers due to which the T_c values become quite large[8]. Cuprates have high – T_c=134 K and iron – based materials have low T_c=55K. The difference in T_c is related to the different electron correlation interactions in these materials. The parent phase of cuprates is a Mott insulator in which electron – electron Coulomb repulsion is very strong, whereas almost all of iron – based parent phases are poormetals, not insulators, because of weak electron correlations. Keeping in mind the reasons due to which cuprates have high T_c, and in order that iron – based superconductors have high – T_c, it would be appropriate to dope carriers into the insulating parent phase with strong electron correlation to induce an insulator – superconductor transition. Recently, even the electric field – inducedsuperconductingtransition of insulating materials have been tried successfully experimentally[9]. The crux of the problem is that to increase the value of T_c, we have to increase the density of charge carriers. This has to be done either by doping or by considering processes that will lead to the release of more mobile carriers resulting in the increase of the density of charge carriers.

The next important step is to surmise what kind of interactions can exist in a superconductor between the charge carriers. Possible interactions could be electron – lattice or what is known as electron – phonon interaction leading to Cooper pairs; exotic pairing or electron – electron interaction without the exchange of phonons[10],dipole – dipole and dipole – electron interaction[11]interactions between electrons and magnetic moments and the coexistence of electrons and holes[12]. Now, it is impossible to decide whether all the interactions could exist simultaneously in a superconductor. It would, therefore, be appropriate to consider the most probable interactions that can contribute to the physics of the problem more effectively.

It is well established that the electron – phonon interaction certainly leads to superconductivity. Next, the electron – electron and Coulomb interactions should also exist since it is the stream of electron pairs that is responsible for the superconducting current. The relative strength of the dipole – dipole, dipole – electron and electron – hole interactions is still not well established and is, therefore, not considered in our calculations. However, any interaction that can lead to the creation of a superconducting state is likely to raise the transition temperature; it may also affect the order of phase transition- the superconducting transition may be a first order phase transition (finite latent heat) or second order phase transition (no latent heat). In this manuscript, we have studied the role of long – range electron - phonon and local Coulomb interactions in studying the properties of high –$T_c$cuprate superconductors.

2. The expectation value of the electron – phonon and coulomb interaction Hamiltonian

The electron – phonon and Coulomb interaction Hamiltonian may be written as

$$H_{epc} = g_{ep}\sum_{k,\sigma}(\alpha^{+}_{k,\sigma}\alpha_{k+X,\sigma} + \alpha^{+}_{k+X,\sigma}\alpha_{k,\sigma}) + E_p\sum_i a^{+}_{ip}a_{ip} + E_d\sum_j a^{+}_{jd}a_{jd} + t_{pd}\sum_{ij}(a^{+}_{ip}a_{jd} + a^{+}_{jd}a_{ip}) + u_d\sum_{ji}a^{+}_{jd}a^{+}_{jd}a_{ip}a_{ip} \quad (1)$$

The first term in eq. (1) represents the electron – phonon interaction energy, the second term represents the energy of oxygen ions while the third term, the energy of the copper ions, the fourth term represents the energy due to the hybridization between copper and oxygen bands, and the fifth term represents the energy due to repulsion between the holes occupying the same copper orbital.

The expectation value of H_{epc}in Eq. (1) was calculated by writing the trial wave function for such a system. The trial wave function is written as,

$$\Psi = (a_i a_i + a^{+}_j a^{+}_j)(u + v a^{+}_i a^{+}_i)\left|n,0\right\rangle \quad (2)$$

and its conjugate is

$$\Psi^{*} = \left\langle n,0\right|\left(u + v a_i a_i\right)\left(a_j a_j + a^{+}_i a^{+}_i\right) \quad (3)$$

The expectation value of the H_{epc} is written as;

$$E_n = \left\langle \Psi^{*}\left|H\right|\Psi\right\rangle \quad (4)$$

Eqs.(1), (2) and (3) were substituted in Eq. (4) to obtain

$$E_n = \left\langle n,0\right|\left(u + v a_i a_i\right)\left(a_j a_j + a^{+}_i a^{+}_i\right)\begin{bmatrix} E_p a^{+}_{ip}a_{ip} \\ +E_d a^{+}_{jd}a_{jd} \\ +t_{pd}(a^{+}_{ip}a_{jd} + a^{+}_{jd}a_{ip}) \\ +u_d a^{+}_{jd}a^{+}_{jd}a_{ip}a_{ip} \\ +g_{ep}(a^{+}_{k\sigma}a_{k+X,\sigma} + a^{+}_{k+X,\sigma}a_{k\sigma}) \end{bmatrix}(a_i a_i + a^{+}_j a^{+}_j)(u + v a^{+}_i a^{+}_i\left|n,0\right\rangle$$

(5)

After lengthy calculations using second quantization and many body techniques, and substituting for n =1, when the system is in its lowest energy state (superconducting state), andputting $u = v = \frac{1}{\sqrt{2}}$(canonical transformation formalism) in Eq. (5), one gets;

$$E_1 = 303E_p + 980E_d + 888t_{pd} + 800u_d + 720g_{ep} \quad (6)$$

3. Specific heat, entropy and transition temperature

At the temperature of interest, it is necessary to consider the difference between the states in which the hopping electron is on one site and then when it is on another site of similar symmetry or different symmetry. This difference in energy of the two sites leads to the probability amplitude Green's function which according to quantum treatment of lattice vibrations, is equivalent to the thermal activation factor,exp ($-E_1/kT$). Thus, the expectation value of the electron – phonon and Coulomb interaction Hamiltonian is multiplied by the thermal activation factor to obtain the energy,

$$E = E_1 e^{-\frac{E_1}{kT}} \tag{7}$$

The specific heat, C_v, of the system is obtained from Eq. (7) i.e.

$$C_v = \frac{\partial E}{\partial T} = E_1 \frac{\partial}{\partial T}\left(e^{-\frac{E_1}{kT}}\right) = \frac{E_1}{kT^2} e^{-\frac{E_1}{kT}} \tag{8}$$

The expression for entropy, S, is written as,

$$\int dS = \int \frac{C_v dT}{T} \tag{9}$$

such that

$$S = \int \frac{E_1}{kT^2} e^{-\frac{E_1}{kT}} \frac{dT}{T} \tag{10}$$

or

$$S = \frac{e^{-\frac{E_1}{kT}}}{T} + \frac{k}{E} e^{-\frac{E_1}{kT}} = e^{-\frac{E_1}{kT}}\left(\frac{1}{T} + \frac{k}{E}\right) \tag{11}$$

4. Results and discussions

Calculations were done using the values of different parameters that were obtained from the literature[13]forYBaCuO. Calculations using three sets of parameters whose values were changed were done to obtain the valuesC_v, S and T_c. These calculations were carried out for a constant copper on site energy E_d= 2.0 x 10^{-6}eV. The variations of $C_v$and S with absolute temperature T are as shown in Figures (1) to (6). From these figures, the transition temperature T_c is obtained.

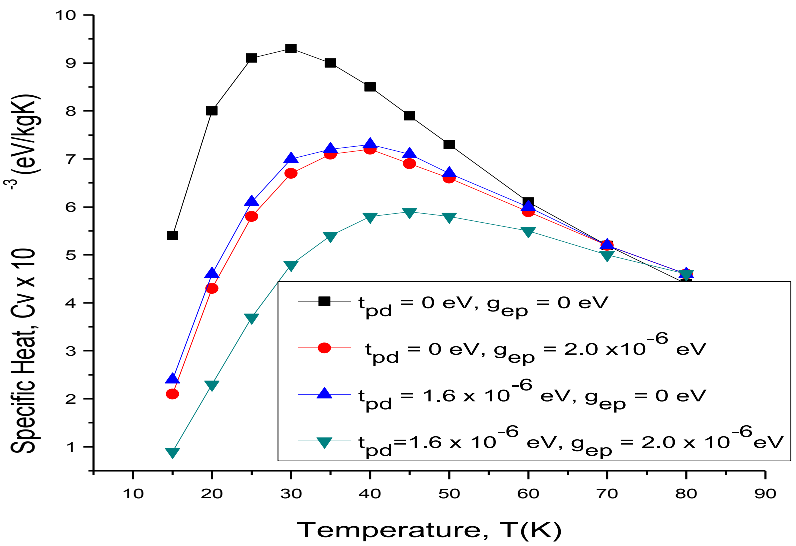

Fig.1: Variation of Specific Heat with temperature (E_p = 3.5 x 10^{-6}eV and u_d = 2.5 x 10^{-6}eV) forYBaCuO

The graph depicting the variation of C_v against T shows that $C_v$increases with $T$and attains a peak value and thereafter, decreases with further increase in T.

The peak values of C_{vs} are 9.3 x 10^{-3}eV/kgK, 7.2 X 10^{-3}eV/kgK, 7.3 x 10^{-3}eV/kgK and 7.2 X 10^{-3}eV/kgK for the parameterst_{pd} and g_{ep}which occur at 30 K, 40 K, 40 K and 45 K, respectively, and these temperatures are the transition temperatures.

These results show that as t_{pd} and g_{ep} are increased, the peak value of C_v reduce but T_c increases.

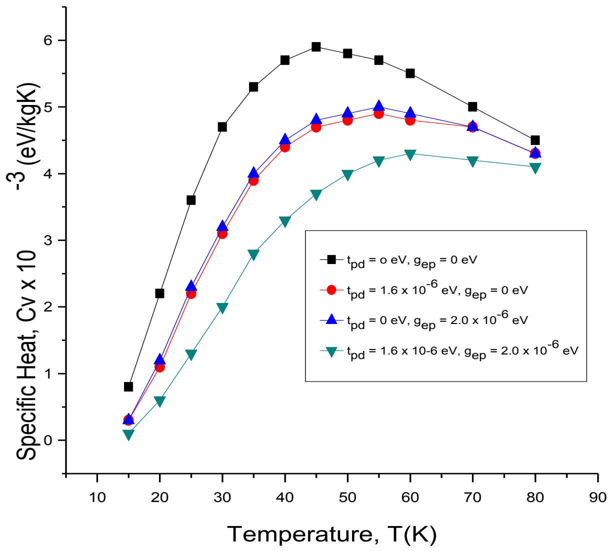

Figure 2: Variation of Specific heat with absolute temperature(E_p = 5.5 x 10^{-6}eV and u_d = 5.5 x 10^{-6}eV) for YBaCuO

From Figure (2) , C_V increases with absolute temperature and attains a peak value and thereafter, decreases with further increase in absolute temperature. The peak values of $C_V$are 5.9 x 10^{-3}eV/kgK, 4.9 x 10^{-3}eV/kgK, 5.0 x 10^{-3}eV/kgK and 4.3 x 10^{-3}eV/kgK which occur at the transition temperatures T_c, i.e., 45 K, 55 K, 55 K and 60 K, respectively. These transition temperatures are higher than the values obtained in Figure (1). These results show that as $t_{pd}$and g_{ep} are increased, the peak value of $C_v$decreases but T_c increases.

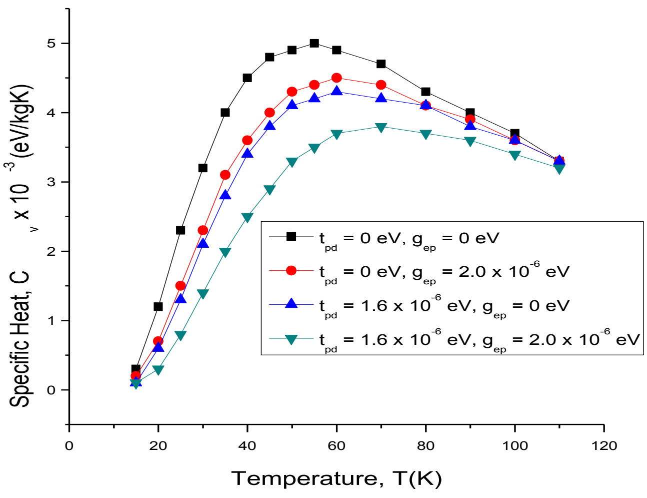

Figure 3: Variation of Specific Heat with absolute Temperature (E_p = 7.5 x 10^{-6}eV and u_d = 6.5 x 10^{-6}eV) for YBaCuO.

From Figure (3), one notices that $C_v$increases with absolute temperature and attains a peak value and thereafter, decreases with further increase in absolute temperature. The maximum values of C_v are 5.0 x 10^{-3}eV/kgK, 4.5 x 10^{-3}eV/kgK and 3.8 x 10^{-3}eV/kgK , and these occur at the transition temperatures 55 K, 60 K, 60 K and 70 K, respectively.

The values of C_v are lower as compared to the values obtained in Fig. (1) and (2). However, the values of T_c obtained are higher. These results show that as t_{pd} and g_{ep} are increased, the peak values of C_v decrease, but the values of T_c increase.

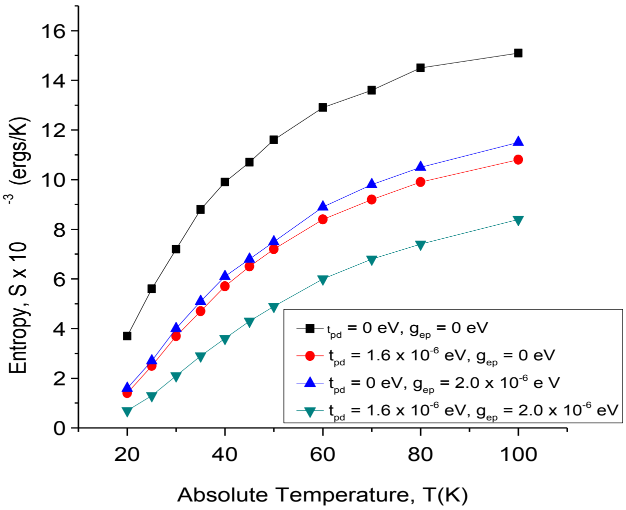

Figure 4: Variation of Entropy with absolute Temperature (E_p = 3.5 x 10^{-6}eV and u_d = 2.5 x 10^{-6}eV) forYBaCuO

From Figure (4), *S* increases with absolute temperature. The increase is large for lower values of absolute temperature as compared to higher values of absolute temperature. The graphs above change from non - linear to linear shape at around $T_c \approx$ 60 K for all the curves. Entropy values for different parameters are 9.0 x 10^{-3} ergs/K, 5.0 X 10^{-3} ergs / K, 4.3 X 10^{-3} ergs/ K and 4.0 x 10^{-3} ergs/K ,respectively.

The results show that as t_{pd} and $g_{ep}$are increased, the values of S reduce. However, the transition temperature increases with increase in values oft_{pd} and g_{ep}.

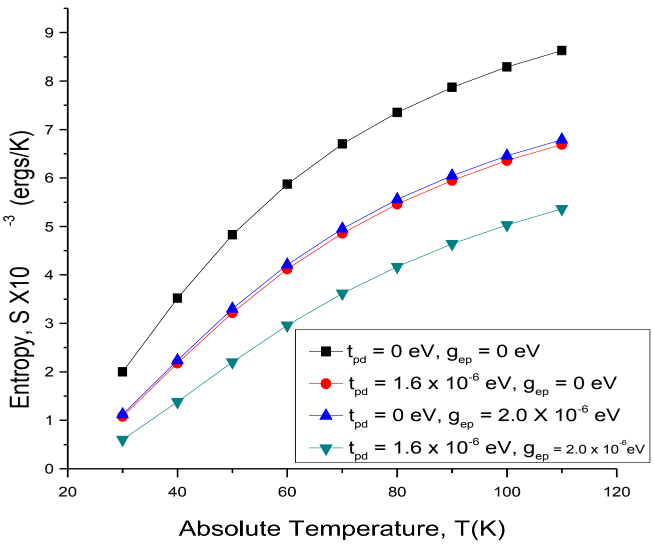

Figure 5: Variation of entropy with absolute temperature (E_p = 5.5 x 10^{-6}eV and u_d = 5.5 x 10^{-6}eV) for YBaCuO

From Figure (5) , S increases with absolute temperature. The graphs change from non - linear to linear shape at temperatures of about 60 K. The entropy values for different parameters are 4.8 x 10^{-3} ergs/K, 4.3 x 10^{-3} ergs/K, 4.2 X 10^{-3} ergs/ K and 3.5 x 10^{-3} ergs/K, respectively. These results show that as t_{pd} and g_{ep} are increased, the values of S reduce.

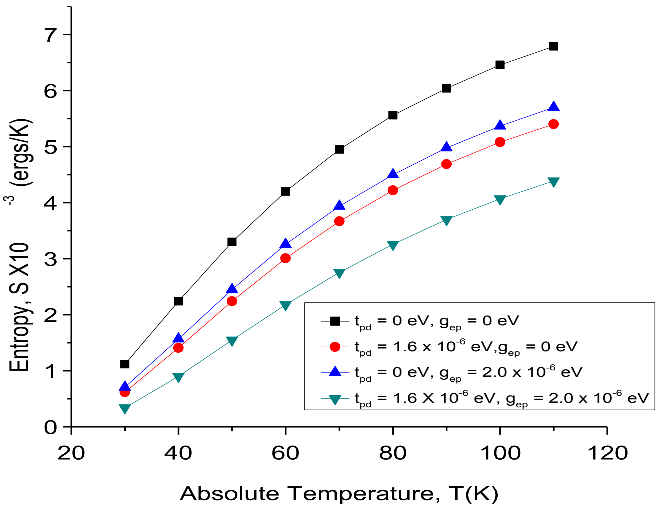

Figure 6: Variation of Entropy with absolute Temperature (E_p = 7.5 x 10^{-6}eV and u_d = 6.5 x 10^{-6}eV) for YBaCuO

From Figure (6), S increases with absolute temperature. The graphs change from non - linear to linear shape at temperatures of about 60 Kwith corresponding values of entropy of 4.2 x 10^{-3} ergs/K, 3.8 X 10^{-3} ergs/K, 3.5 X 10^{-3} ergs/K and 3.0 x 10^{-3} ergs/K, respectively.

These values of S are lower compared with values obtained from Fig. (4)and(5), but the values of T_c are higher. These results show that as t_{pd} and g_{ep} are increased, the values of Sreduce.

The highest transition temperature obtained by us is, $T_c \approx 70\,K$, but the highest experimental value for the T_c of $YBa_2Cu_3O_x$ is of the order of 93 K. One transition temperature that is common for different values of parameters is $T_c = 60\,K$. The phase diagram[13] of $YBa_2Cu_3O_x$ at x = 6.7 shows that there is a plateau at $T_c = 60\,K$. This is the so called 60 K plateau. In our calculations, $S - T$ graphs change from non – linear to linear shape at 60 K, and $C_v - T$ graphs show a transition around 60 K. Hence, our calculations are applicable to the superconducting compound $YBa_2Cu_3O_x$ for x = 6.7, and this emphasizes the correctness of our calculations.

Conclusion

The combined effects of electron – phonon and Coulomb interactions on the transition temperature of high - $T_c$cuprate superconductors were investigated by using the electron – phonon and Coulomb interaction Hamiltonian. The expectation value of the electron – phonon and Coulomb interaction Hamiltonian was calculated using second quantization and many body techniques.

The effects of E_p, E_d, t_{pd}, u_d and g_{ep} on T_c were determined from the graphs of specific heat and entropy against absolute temperature. From the study, it was found that increase in the values of the parametersE_p, E_d,t_{pd}, u_d and g_{ep}lead to increase in T_c, reduction in the entropy and variation of specific heat showing a transition from normal to superconducting state.

However, Coulomb interaction is a local interaction, whereas the electron – phonon interaction is a long – range, non – local interaction, we have to explore the conditions under which both the interactions make significant contributions to the superconducting state, or both compete with each other such that one process alone makes a significant contribution to the superconducting state. Our next attempt will be to study the effect of the competition between the electron – phonon interaction and Coulomb interaction on the properties of high – T_c superconductors.

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