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Research Article

ROLE OF ATTRACTIVE INTERACTION IN THE HIGH-T_C SUPERCONDUCTIVITY

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ABSTRACT
It is known that due to oxygen-copper virtual charge excitations, there exists an attractive term at the oxygen ion sites that can lead to changes in the on-site energies of oxygen (E_l) and copper (E_d). The resulting hybridization between copper and oxygen bands lead to attraction that is represented by t_{pd}. The role of t_{pd} in determining some of the properties of high-T_C superconductors, such as the specific heat C_V, entropy S, and the transition temperature T_C, has been studied. Finite values of t_{pd} lead to increase in T_C but the values of C_V and S decrease.

Keywords*: Virtual Charge Excitation, Hybridization, On Site Energies*

INTRODUCTION
Superconductivity can be defined as the vanishing of electrical resistance of a metallic conductor, or an alloy, or a doped semiconductor, or an insulating oxide compound at low temperatures. It was first discovered by HK Onnes in 1911. He found that the electrical resistance of pure mercury disappeared when the temperature was reduced below 4.2 K and a current of the order of 10^7 Amperes flows.
Superconductivity is now divided into two distinct parts. One is called conventional superconductivity, and other is called high temperature-superconductivity {HTSC} or unconventional superconductivity. Conventional superconductivity is understood as instability of a multielectron system due to the phonon-mediated attractive attraction interaction between the electrons resulting in the formation of Cooper pairs. The conventional superconductivity was explained on the basis of the weak coupling BCS theory [Bardeen *et al.,* 1957] based on Cooper pairs.
High- temperature superconductivity was discovered in 1986 by Bednorz and Muller. They found that LaBaCuO had a transition temperature $T_C \langle 23K$. Thus high T_C superconductors exhibit superconductivity at much higher temperatures than do the conventional superconductors. Established theories, like the BCS theories, used to explain the properties of the conventional superconductors cannot be used to explain the characteristics of the high-T_C superconductors. A new electron pairing mechanism has to be invoked to explain their properties. The high-T_C superconductors are poor conductors, with one or more CuO_2 planes, which are separated by insulating oxide layers. It is believed that CuO_2 planes form charge reservoirs, and there exists pairing interaction between the charges in the reservoir. More-over due to the oxygen-copper virtual charge excitations, there exists an attractive term at the oxygen ion sites. This can lead to changes in the on-site energies of oxygen (E_P) and copper (E_d). The hybridization between copper and oxygen bands leads to attraction and this is represented by t_{pd}. In this manuscript, the role of t_{pd} in determining some of the properties of high-T_C superconductors, such as the specific heat C_V, the entropy S, and the transition temperature T_C, has been studied. Finite values of t_{pd} lead to increase in

T_C but the values of C_V and S decrease, and these conditions are the essential requirements for obtaining the superconducting state.

Theoretical Derivations

It is clearly established that the high temperature superconductivity [HTSC] cannot be explained by using the BCS theory. A new type of pairing mechanism between the electrons has to be invoked to explain the properties of high T_C superconductors.

The structure of these HTSC compounds is explained in the introduction. It is also emphasized that there exists a pairing interaction between the charges in the charge reservoir; and there exists an attractive term at the oxygen ion sites as a result of oxygen virtual charge excitations. It seems such interactions are relevant to study the properties of high - T_C superconductors. The resulting oxygen-copper hopping due to attractive term leads to the changes in the onsite energies of oxygen (E_P) and copper (E_d). The hybridization between copper and oxygen bands is represented by t_{pd}, and the repulsion between the holes occupying the same copper orbital is u_d.

In the second quantization formalism, the Hamiltonian H, for the assembly can be written as,

$$H = E_P \sum_i n_i^p + E_d \sum n_j^d + t_{pd} \sum_{i,j,\sigma} \left(d_{j\sigma}^+ + h.c.\right) + u_d \sum_n n_{i\uparrow}^j n_{j\downarrow}^d \quad \text{.....(1)}$$

Where p and d operators refer to the oxygen and copper ions, respectively. Each term in eq.(1) can be written in terms of the creation and annihilation operators. Here n_i^p refers to the number of electrons at the site i for oxygen, and n_j^d refers to the numbers of electrons at the site j for copper.

$$\begin{aligned} n_i^p &= a_{ip}^+ a_{ip} \\ n_d^j &= a_{jd}^+ a_{jd} \end{aligned} \quad \text{.....(2)}$$

Due to hybridization between copper and oxygen bands we have the term $\left(d_{j\sigma}^+ + h.c.\right)$ and this term can be written as $\left(a_{ip}^+ a_{jd} + a_{jd}^+ a_{ip}\right)$. We shall for the moment drop σ that represents the spin. The term $n_{i\uparrow}^d n_{j\downarrow}^d$ represents the repulsion between the holes occupying the same copper orbital. Let the creation and annihilation operators for holes be represented by 'b'. We can then write dropping spin orientation.

$$n_i^d n_j^d \rightarrow b_{jd}^+ b_{id}^+ b_{ip} b_{jp} \quad \text{.....(3)}$$

Which means the holes on repulsion in copper orbital go to oxygen from the site j in copper to the site i in oxygen, and the opposite can also happen. Now the creation of a hole results due to the disappearance of the electron, and the destruction of a hole means the appearance (creation) of an electron. To convert eq. (1) into a set of creation and annihilation operators for the electrons, this can be written as,

$$H = E_p \sum_i a_{ip}^+ a_{ip} + E_d \sum a_{jd}^+ a_{jd} + t_{pd} \sum \left(a_{ip}^+ a_{jd} + a_{jd}^+ a_{ip}\right) + u_d \sum a_{jd}^+ a_{jd}^+ a_{ip} a_{ip} \quad \text{.....(4)}$$

We have to calculate the expectation value of H by writing the trial wave function for such a system. The trial wave function ψ will be written as,

$$\psi = \left(a_i a_i + a_j^+ a_j^+\right)\left(u_i + v_i a_i^+ a_i^+\right)n,0\rangle \quad \text{.....(5)}$$

We have to calculate $\langle \psi | H | \psi \rangle$ knowing that

$$u^2 + v^2 = 1 \text{ and } u = v = \frac{1}{\sqrt{2}} \quad \text{.....(6)}$$

If E_n is the expectation value for the energy, then after lengthy calculations we get,

$$E_n = \langle \psi | H | \psi \rangle = E_p \left\{ u_i^2 \left[2n^{\frac{3}{2}} (n+1)^{\frac{3}{2}} \right] + v_i^2 \left[n^{\frac{3}{2}} (n+1)^{\frac{3}{2}} \right] \right\} +$$

$$E_d \left\{ u_i^2 \left[2n^{\frac{3}{2}} (n+1)^{\frac{3}{2}} \right] + v_i^2 \left[n^{\frac{3}{2}} (n+1)^{\frac{3}{2}} \right] \right\} + t_{pd} \left\{ n_i^2 \left[4n^{\frac{3}{2}} (n+1)^{\frac{3}{2}} \right] + v_i^2 \left[2n^{\frac{3}{2}} (n+1)^{\frac{3}{2}} \right] \right\} \quad \text{.....(7)}$$

$$+ u_d \left\{ u_j^2 \left[2n^2 (n+1)^2 \right] + v_i^2 \left[n^3 (n+1)^3 \right] \right\}$$

For $n = 1$

$$E_1 = 5.66E_p + 5.66E_d + 11.31t_{pd} + 8u_d \quad \text{.....(8)}$$

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 gives the probability amplitude Green's function which according to quantum treatment of lattice vibrations. Is equivalent to the thermal activation factor $e^{-\frac{E_n}{kT}}$.

Thus the values of energy are to be multiplied by the thermal activation factor, *i.e.*,

$$E = E_n e^{-\frac{E_n}{kT}} \quad \text{.....(9)}$$

Now the specific heat, C_V ,of the system is written as,

$$C_V = \frac{\partial E}{\partial T} = E_n \frac{\partial}{\partial T} \left(e^{-\frac{E_n}{kT}} \right) = \frac{E_n}{kT^2} e^{-\frac{E_n}{kT}} \quad \text{.....(10)}$$

The entropy, S , of the system is given by

$$S = C_V \log T$$

.....(11)

The transition temperature T_C will be given by

$$\left(\frac{\partial C_V}{\partial T} \right)_{T=T_C} = 0 \quad \text{.....(12)}$$

The calculation gives T_C as

$$T_C = \frac{E_n}{2k} \quad \text{.....(13)}$$

Numerical Calculations

Numerical values of C_V are obtained from eq. (10), that of S are obtained from eq. (11), and T_C is obtained from eq. (13).

The parameters used in the calculation are obtained from the Literature and we have done three sets of calculations using three sets of parameters. The parameter regime relevant to HTSC systems has been chosen. In the conventional superconductors, the condensation energy per electron is surprisingly very small [Khanna 2008], being of the order of 10^{-7}ev, which is equivalent to a thermal energy of about a millidegree Kelvin. In high-T_C superconductors since the transition to the superconducting state takes place at temperatures of the order of 100K, the condensation energy per electron could be much higher than 10^{-7}ev. We assume that it could be of the order of 10^{-4}ev.

RESULTS

Calculations using three sets of increasing parameters for u_d and E_p in eq. (10) and (11) have been carried out and the influence of t_{pd} on T_C, C_V and S investigated. These calculations have been carried out for a constant copper on site energy E_d of 2.0 x 10^{-4}ev. The variations of C_V and S with temperature T are as shown in Figure s. 1(a) to (3b).

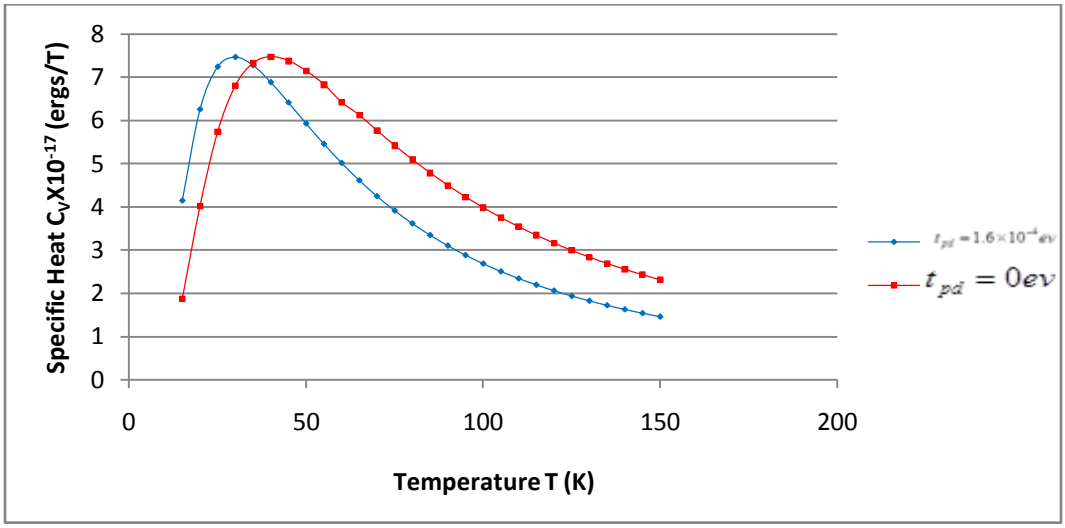

Figure 1(a): Variation of Specific Heat with temperature when $E_p = 0.00035$ ev, $E_d = 0.0002$ ev and $u_d = 0.00025$ ev.

Figure 1 (a) shows that the role of t_{pd} on the specific heat C_V is to increase the transition Temperature T_C from $30K$ to $40K$. The values of C_V at the transition temperature T_C are almost identical.

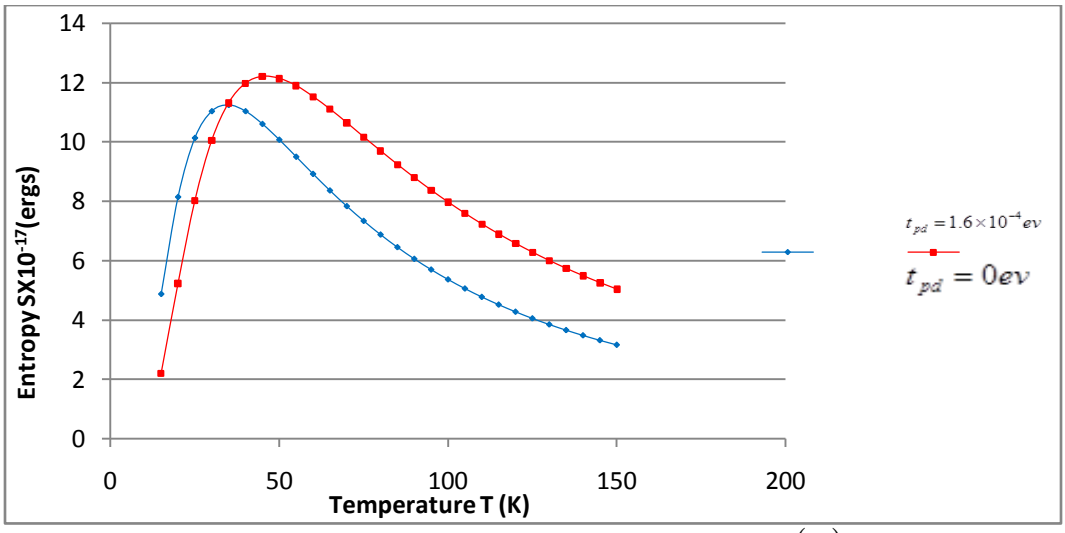

Figure 1(b): Variation of Entropy S (ergs) with temperature $T(K)$ where $E_p = 0.00035$ ev, $E_d = 0.0002$ ev and $u_d = 0.00025$ ev.

Figure 1(b) shows the increase of entropy from 11.26 erg/K to 12.5 erg/K when the hybridization interaction t_{pd} is reduced to zero. The effect of this reduction is also to increase the transition temperature T_C from 35K to 45K.

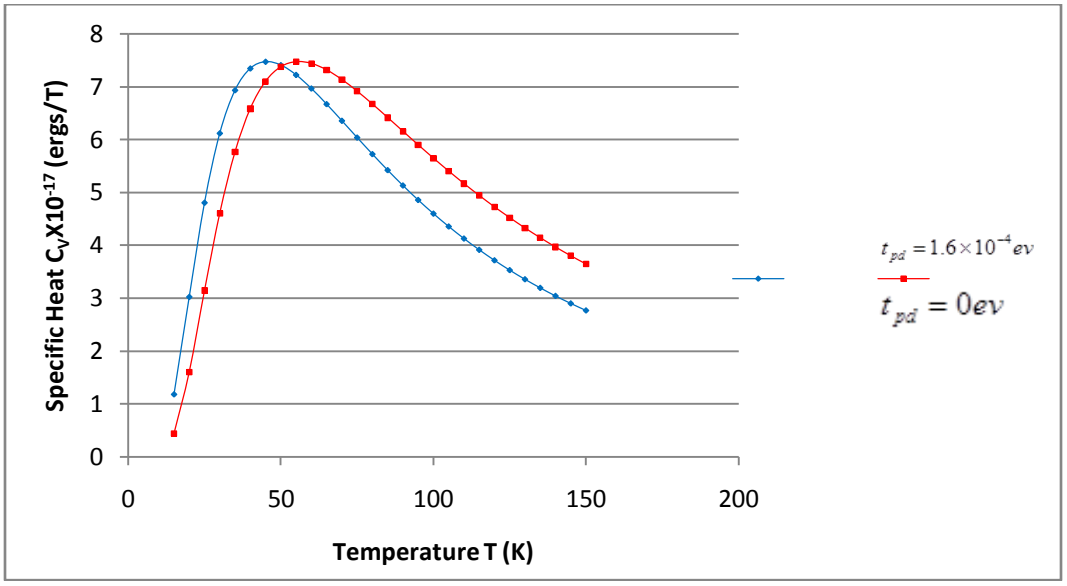

Figure 2(a): Variation of Specific Heat C_V (ergs/T) with temperature T (K) when $E_p = 0.00055$ ev, $E_d = 0.0002$ ev and $u_d = 0.00055$ ev.

In Figure 2(a) th values of C_V at the transition temperature are not affected by t_{pd} but the transition temperature T_C is increased from 45K to 55K.

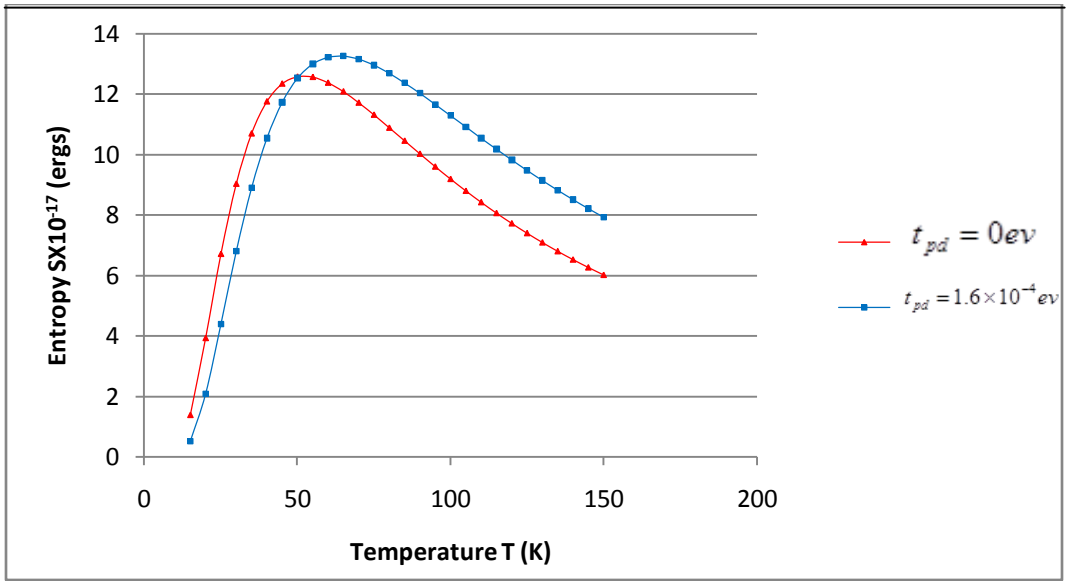

Figure 2(b): Variation of Entropy S (ergs) with temperature T (K) when $E_p = 0.00055$ ev, $E_d = 0.0002$ ev and $u_d = 0.00045$ ev.

Figure 2(b) shows that the role of non application of t_{pd} is to increase the transition temperature T_C from 50K to 65K and to increase entropy S from 12.54erg to 13.49erg at the transition temperature T_C

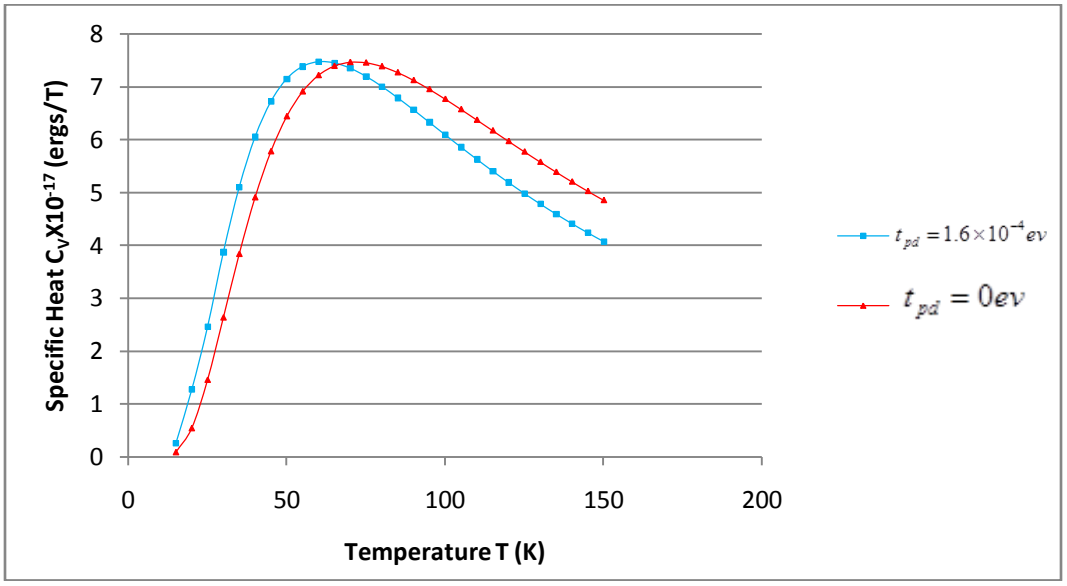

Figure 3(a): Variation of Specific Heat C_V (ergs/T) with temperature T (K) when $E_p = 0.00075$ ev, $E_d = 0.0002$ ev and $u_d = 0.00065$ ev.

Figure 3(a) shows that the transition temperature T_C is increased from 60K to 70K with a small reduction in C_V at the transition temperature when t_{pd} is switched on.

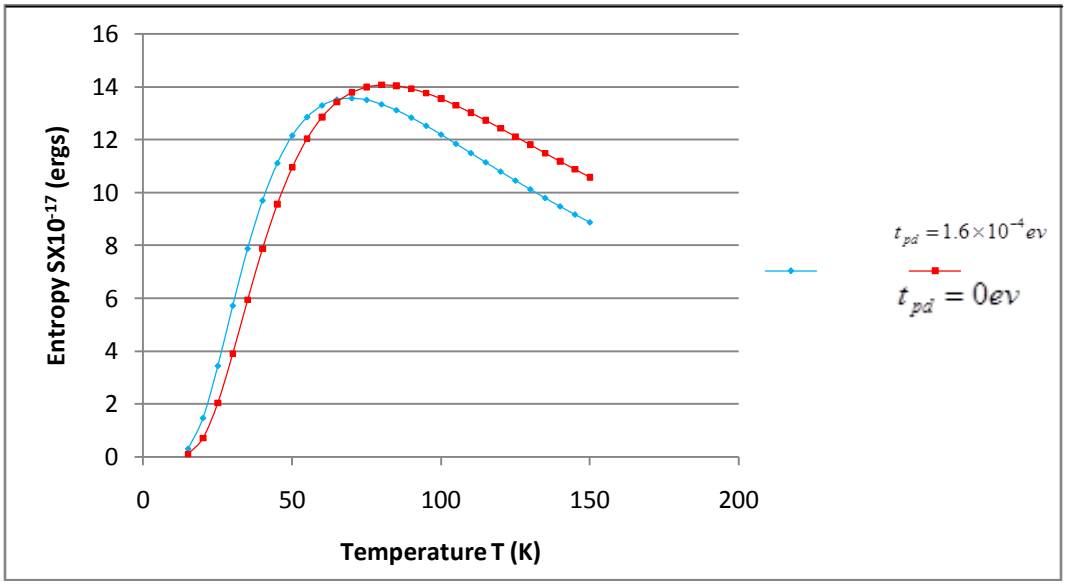

Figure 3(b): Variation of entropy S (ergs) with Temperature T (K) when $E_p = 0.00075$ ev, $E_d = 0.0002$ ev and $u_d = 0.00065$ ev.

Figure 3(b) shows the small change in S at the transition temperature and the increase in transition temperature T_C from 60K to 70K as t_{pd} is increased.

DISCUSSION

The objective of the study was to understand as to what role the attractive interaction between the charge carriers plays in determining the properties of high-T_C superconductors. The essential properties that have been studied are the specific heat C_V, entropy S and the transition temperature, T_C, of a superconductor.

The phonon mediated attractive interaction between the electrons resulting in the formation of Cooper pairs was able to explain the essential properties of the conventional superconductors via what is called the BCS theory. The expression for the transition temperature T_C is given by (Khanna, 2008).

$$kT_C = 1.14\hbar\omega_D e^{\frac{-1}{VD(E_P)}} \quad \text{.....(14)}$$

Hence T_C is determined by the interaction energy V. It is not exactly known whether V should be pure attractive, pure repulsive, or a combination of attraction and repulsion.

Another relation of importance according to BCS theory [Bardeen, Cooper, Schrieffer 1957] is the equation relating $\Delta(T)$- the energy gap, and T_C, i.e.,

$$\frac{2\Delta(T_C)}{kT_C} = 3.5 \quad \text{.....(15)}$$

For high-T_C superconductors, experimental measurement for T_C give

$$\frac{2\Delta(T)}{kT_C} = 5 \to 8 \quad \text{.....(16)}$$

Eq.(14) shows that for T_C to be large, the electron phonon coupling constant or interaction V should be large. Self consistent band structure calculations have also shown that the values of V should be large.

Now we have a variety of high-T_C - superconducting materials, but what is common in all of them is the existence of the Cu-O layers or planes. It is believed that these Cu-O planes (CuO_2) planes form a charge reservoir, planes being separated by oxide layers, and there exists pairing interactions between charges in the reservoir. It is now believed that in addition to such interactions, there may exist attractive term at the oxygen on sites as a result of oxygen-copper virtual exchange and charge excitations. The strong oxygen on-site attraction is quite relevant to high-temperature superconductors. Large variations on the effective spin correlations have also been observed and this changes sign with increasing oxygen-copper hopping. This leads to changes in the on-site energies of oxygen (E_p) and copper (E_d). The hybridization between copper and oxygen bands is represented by t_{pd}, and this is the term that contributes attractive interaction to the system, its effect on the specific heat C_V, the entropy S, and the transition temperature T_C has been studied in this manuscript. For different values of u_d, E_p, E_d and t_{pd} eqs.(10) and (11) have been used to obtain numerical values of C_V, S and T_C. Using these values graphs have been drawn for S and C_V and these graphs are shown in Figure s.1 to 3.

The graphs clearly show that as C_V changes with T, at some definite value of T, the slope of the graph changes sign. The temperature at which this happens is called the transition temperature T_C, and this

marks the transition to the superconducting state. The shape of the $C_V - T$ indicates that it is a second order phase transition.

When the attractive term t_{pd} is finite, values of C_V and S decrease: whereas when $t_{pd} = 0$ the values of C_V and S are higher. Hence when there is a finite term, the values of C_V and S decrease, and these conditions are necessary for obtaining a superconducting state.

On the other hand, the graphs clearly show that T_C is higher for finite values of t_{pd}. Thus for a superconductor for which t_{pd} is finite (not) zero the magnitude of T_C will be large. Hence if superconductors with large t_{pd} can be manufactured, it may be possible to have room temperature superconductors. It is therefore concluded the hybridization between copper and oxygen bands can lead to increase in the value of T_C.

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