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TO STUDY FREE ENERGY DIFFERENCE OF PALARON EFFECTS IN HIGH-Tc SUPERCONDUCTORS:

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ABSTRACT

Considering that a number of normal state experiments on HTSC are consistent with conduction by small polarons, several workers have developed specific model based on polaron effects, but they are all phenomenological. The strong electron phonon interaction renormalizes the carrier mass and shifts the atomic level. In narrow band crystals it leads to the well-defined polaron band ("small" polaron). If the lattice is soft enough to allow sufficient local deformation to overcome the near neighbour Sits occurs. Superconductivity can result from the Bose Einstein condensation of mobile charged bosons, i.e., bipolarons.We start with the model Hamiltonian consisting of the following parts.

$$H = \sum_{K,\sigma} \in_K C^{+}_{K\sigma} C_{K\sigma} + \sum_{K,q,\sigma} \left[U(q) C^{+}_{K+q,\sigma} C_{K,\sigma} dq + U^{*}(q) C^{+}_{Kq} C_{K+q,\sigma} d^{+}_{q} \right]$$

$$+ \sum_{K,K',q,\sigma,\sigma'} V(q) C^{+}_{K+q,\sigma} C^{+}_{K'-q,\sigma'} C_{K',\sigma'} C_{K\sigma} + \sum_{q} \omega_q d^{+}_{q} dq$$

Here, $\in_K$ denotes the bare initial electron dispersion in a rigid latice, $C_{K,\sigma}$ and d_q are the electron and phonon operators, , respectively, ω_q represents the phonon dispersion, $\vec{K}, \vec{K}', \vec{q}$ the first wave vectors, and phonon the spin of the electrons, First and fourth terms of the Hamiltonian denote the free electron and phonon subsystems respectively. Second and third terms are Frohilch electron phonon U and coulomb V interactions in the ordinary one band Hamiltonian respectively. In strong Coupling narrow band superconductors the second term in the Hamiltonian is dominating.

Keywords: *Free Energy Difference*

INTRODUCTION

In the 214 and 123 systems superconductivity is obtained mostly in the orthorehmbic phase with metal oxygen bonds being different in the X and Y axes. Popescu et al.have shown that T_C in $YBa_2Cu_3O_7$ increases with the orthorhombic distraction (b-a)/a of the unit cell. This does not mean that superconductivity is connected with the structural transition. Never the less, this point towards the conclusion that some parameters of the mechanisms (electronic or phononic) responsible for superconductivity become favourable in the distorted phase. Also, the orthorhombic distortion particularly of the copper oxygen square may be connected with the ordering of some chemical species.

The above mentioned classes of high - T_C copper oxide superconductors are now well established. These systems are p-type superconductors, i.e., the materials have been doped such that majority carriers are holes. Recently, electron doped superconductors $Ln_{1.85}$ $Ce_{0.15}Cu$ O_{4-y}(LnPr, Nd and Sm) , $Ln_{1.85}$ $Th_{0.15}$ CuO_{4-y} (Ln = Pr and Nd) , $Eu_{1.85}Ce_{o.15}CuO_{4-y}$, Nd_2 CuO_{4-x-y} and $Sm_{1.85}$ $Th_{o.15}$ Cu O_{4-y} have also been discovered. These layered coppered oxides are of considerable interest because half effect measurements and charge balance indicate that electrons are the charge carriers rather than holes as in the case of p- type cuprate superconductors. The superconducting transition - temperature (T) onsets for these systems vary between ~ 12 K for $Eu_{1.85}Ce_{0.15}CuO_{4-y}$ and ~ 24 K for $Nd_{1.85}$ $Ce_{0.15}$ CuO_{4-y} .

The family of $(Nd_{1-x}Ce_x)_2$ CuO_4 compounds where Ce Can be replaced by Th and Nd by La, Sm or Pr have a formula unit similar to '214 system except that they are doped by replacing the trivelant rare earth by a tetravalent, instead of divalent atom. These materials have, like the cuprates, a tetragonal structure where the perovskites is further distorted by removal of the apical oxygens of the octahedra and bringing them to the face centres to form O_4 squares (similar to those in CuO_2 planes).

In addition to the above mentioned high-T_C systems, the following notable discoveries have also been reported:

(i) Series of cuprates of the type $T1Ca_1$-x $Ln_xSr_2Cu_2O_{7+6}$ showing electron or hole superconductivity depending on X .

(ii) A series of high- T_C lead cuprate superconductors with formula $Pb_2Sr_2ACu_3O_{8+\delta}$ (A = a mixture of lanthanide and alkaline earth elements containing Cu^{+1} in high proportion [37, 38 J.

(iii) Non - Copper oxide high - T_C superconductor Ba_{1-x} K_x Bi O_{3-y} (x ˜ 0.4) exhibiting superconductivity at about 30 K. This system displays a simple cubic perovskite crystal structure below T_C. Thus it appears to be a high - T_C system without the 2-dimensional metal - oxygen arrays so critical to superconductivity in cuprate superconductors.

(iv) (iv) Fullerene - alkali metal compounds such as $C_{60}K_3$ and $C_{60}Rb_3$ also exhibit high temperature superconductivity. In these new compounds C_{60} is made only of carbon atoms, and is similar to graphite. The transition temperature (T_C 20 K) for these fullerence compounds are much higher than for similar graphite intercalation compounds such as C_8K and C_8Rb (T_C~ 0.1 K). More than one crystal structure has been observed, but the basic packing scheme of nearly spherical C_{60} molecules is close to afcc structure. First measurements of the upper and lower critical field indicate that A_3C_{60} is a type II superconductor with a coherence length of 20-40 A° and a magnetic penetration length of several thousand A°. Preliminary H_{c1} and H_{c2} measurements indicate a quite high density of states and Summerfield parameter ϒ about 50-100 m J/k per mole K_3C_{60}. This new class of materials has a particular structure.

Several group of observations which researchers have indicate that reported superconductivity could occur at substantially higher temperatures, perhaps even at room temperature. However, the highest T_C obtained so far is 125 K, that of the compound $T1_2Ba_2Ca_2Cu_3O_{10}$.

The question of electronic structure of high- T_C superconductors is still open. According to the band structure calculations in the self consistent field approximation these compounds must have half filled band formed mainly due to the hybridization of $3d_{x^2-y^2}$ Cu and $2p_\sigma$, O orbitals in the CuO_2 plane. On the other hand, estimates of the coulomb interaction of electrons show that the self consistent field approximation is not applicable and these compounds are close to Mott insulators. Photon, electron and position spectroscopies provide important information about the electronic states and a comparison with electronic structure calculations indicate that, while many features can be interpreted in terms of existing calculations, self energy corrections or 'correlations' are important for a more detailed understanding.

OBJECTIVES

To study free energy difference

RESEARCH METHODOLOGY

Free energy Difference = $\langle F_S - F_N \rangle$ **:**

The free energy difference between the superconducting and normal state can be obtained by means of the formula.

$$\frac{[F_S - F_N]}{V} = \left[\int_0^\Delta d\Delta \left[\Delta^2 \frac{d}{d\Delta}\left(\frac{1}{|U|}\right)\right]\right] \quad \text{... (1a)}$$

Here,

$$U = g\left(\frac{\omega_q}{2V}\right)^{\frac{1}{2}} \quad \text{and} \quad \omega_q = \hbar q v_0 = \frac{\hbar^2 q^2}{2m} \quad \text{... (1b)}$$

From equation (1) we can rewrite it in the following way

$$\langle\langle C^+_{-K''} \downarrow; \ C^+_{K'} \uparrow\rangle\rangle = \frac{(\omega + \Delta)}{\omega^2 - F^2_{K''} - (Z + \Delta)^2} \quad \text{... (2)}$$

So superconducting gap parameter Δ will become

$$\Delta = \sum_K \frac{(Z + \Delta)}{\omega^2 - F^2_{K''} - (Z + \Delta)^2} \quad \text{... (3)}$$

We have changed summnation over K into an integration

using the formula : $\sum_{K''} \simeq N(0) \int_{-\hbar\omega_D}^{+\hbar\omega_D} d \in_{K''}$

or $$\sum_{K} \simeq N(0) \int_{-\hbar\omega_D}^{+\hbar\omega_D} d \in_{K''} \qquad \text{... (4)}$$

$$\therefore \qquad \Delta = \int_{-\hbar\omega_D}^{+\hbar\omega_D} N(0)\ dF_{K''} \frac{(Z+\Delta)}{\left[\omega^2 - F_{K''}^2 - (Z+\Delta)^2\right]} \qquad \text{... (5)}$$

On simplification equation (5), we obtain as follows:

$$\therefore \qquad \Delta = \int_{-\hbar\omega_D}^{+\hbar\omega_D} \frac{(Z+\Delta)\tanh \frac{\beta}{2}\sqrt{F_{K''}^2 + (Z+\Delta)^2}}{2\sqrt{\left[F_{K''}^2 + (Z+\Delta)^2\right]}} \qquad \text{... (6)}$$

Rearrangement yields

$$\frac{1}{|U|N(0)} = \sum_{K} \frac{\left(\frac{Z+\Delta}{\Delta}\right)\tan h\left(\frac{\beta}{2}\sqrt{F_{K''}^2 + (Z+\Delta)^2}\right)}{2\sqrt{F_{K''}^2 + (Z+\Delta)^2}} \qquad \text{... (7)}$$

Where Z, $F_{K''}$ are same as in equation (1).

The zero temperature gap Δ (T = 0) $\equiv\Delta_0$ can also be obtained from (7) as

$$\frac{\Delta_0}{|U|N(0)} = \sum_{K} \frac{(Z+\Delta_0)}{\sqrt{F_{K''}^2 + (Z+\Delta_0)^2}}, \quad \text{at} \quad T=0 \qquad \text{... (8)}$$

Thus from equations (1) and (8), one obtains on integrating by parts:

$$\frac{[F_S - F_N]}{V} = \left[\frac{\Delta^2}{|U|} - 2N(0)\int_0^{\hbar\omega_D} dF_{K''}\left[\int_0^{\Delta} d\Delta \frac{(Z+\Delta)\tan h\left(\frac{\beta E}{2}\right)}{E}\right]\right] \qquad \text{... (9)}$$

We have made the substitution

$$E = \left[F_{K''}^2 + (Z+\Delta)^2\right]^{\frac{1}{2}} \qquad \text{... (10)}$$

Equation (9) can be further reduced to the following equation on evaluating Δ integral

$$\frac{[F_S - F_N]}{V} = \left[\frac{\Delta^2}{|U|} - \frac{4N(0)}{\beta}\int_0^{\hbar\omega_D} dF_{K''}\log\left[\frac{\cosh\left(\frac{\beta E}{2}\right)}{\cosh\left(\frac{\beta E'}{2}\right)}\right]\right] \qquad \text{... (11)}$$

$$\frac{[F_S - F_N]}{V} = \left[\frac{\Delta^2}{|U|} - \frac{4N(0)}{\beta}\int_0^{\hbar\omega_D} dF_{K''}\left[\log\left(1+e^{-\beta E} + \frac{1}{2}\beta(E-E')\right)\right]\right.$$

$$\left. + \frac{4N(0)}{\beta}\int_0^{\hbar\omega_D} dF_{K''}\left[\log\left(1+e^{-\beta E'}\right)\right]\right] \qquad \text{... (12)}$$

Making use of equation (1) and

$$E' = \left[F_{K''}^2 + Z^2\right]^{\frac{1}{2}} \qquad \text{... (13)}$$

It can be put into following form as :

$$\frac{[F_S - F_N]}{V} = \left[\frac{\Delta^2}{|U|} - N(0)\left[\frac{1}{2}\Delta(2Z-\Delta) + (Z-\Delta)^2\log\frac{(2\hbar\omega_D)}{(Z-\Delta)}\right.\right.$$

$$\left. - Z^2\log\left(\frac{2\hbar\omega_D}{2}\right)\right] + \frac{1}{3}\pi^2 N(0)(k_B T)^2$$

$$\left. - 4N(0)k_B T\int_0^{\hbar\omega_D} dF_{K''}\log\left(1+e^{-\beta E}\right)\right] \qquad \text{... (14)}$$

Since $\hbar\omega_D \rangle\rangle k_B T$ the last integral in equation (14) have been evaluated by extending in to infinity.

DATA ANALYSIS

Free Energy Difference (F_S – F_N)

Taking equation (11) for unit volume and changing the variable of integration, we rewrite equation (11) as follows:

$$[F_S - F_N] = \left[\frac{\Delta^2}{|U|} - 4N(0)k_B T \int_0^{\hbar\omega_D} dF_{K''} \ln\left[\frac{\cosh\left(\frac{\beta E}{2}\right)}{\cosh\left(\frac{\beta E'}{2}\right)}\right]\right] \quad \text{... (15)}$$

Using equations (2), (10) and (12) we rewrite equation (15) taking $\in_{K''} = y\hbar\omega_D$ and $\Delta = x \times 10^{-14}$ erg

$$[F_S - F_N] = \left[\frac{\Delta^2}{|U|} - 4N(0)k_B T(\hbar\omega_D)\times\right.$$

$$\left.\times \int_0^1 dy \ln\left[\frac{\cosh\left[\frac{\hbar\omega_D}{2k_B T}\left\{(y+0.578)^2 + \left(\frac{2\Delta}{\hbar\omega_D}\right)^2\right\}\right]^{1/2}}{\cosh\left[\frac{\hbar\omega_D}{2k_B T}\left\{(y+0.578)^2\right\}\right]^{1/2}}\right]\right]$$

$$[F_S - F_N] = \left[221.63\times 10^{-18} \times x^2 - 36.21\times 10^{-18} \times T \times\right.$$

$$\left.\times \int_0^1 dy \ln\left[\frac{\cosh\left[\frac{57.97}{T}\left\{(y+0.578)^2 + (1.25x)^2\right\}\right]^{1/2}}{\cosh\left[\frac{57.97}{T}\left\{(y+0.578)^2\right\}\right]^{1/2}}\right]\right] \quad \text{... (16)}$$

The value of free energy difference at various temperature are given in Table 1.

Table 1

S. No.	Temperature	$[F_S - F_N]$	$\lvert H_C \rvert \times 10^{-9}$

	T (K)	10^{-18} (erg/mole)	(K Gauss)
1.	5	-1750.335	209.7396
2.	10	-1974.879	222.7871
3.	15	-2146.16	232.2474
4.	20	-2289.812	239.8942
5.	25	-2303.884	245.7970
6.	30	-2501.386	250.7323
7.	35	-2568.729	254.0850
8.	40	-2616.11	256.4176
9.	45	-2615.556	256.3905
10.	50	-2586.141	254.9447
11.	55	-2508.79	251.1031
12.	60	-2384.212	244.7892
13.	65	-2194.734	234.8609
14.	70	-1944.605	221.0729
15.	75	-1605.387	200.8675
16.	80	-1197.401	173.4761
17.	85	-675.7065	130.3163
18.	90	-5.092192	11.31285

Variation of Critical Field with Temperature

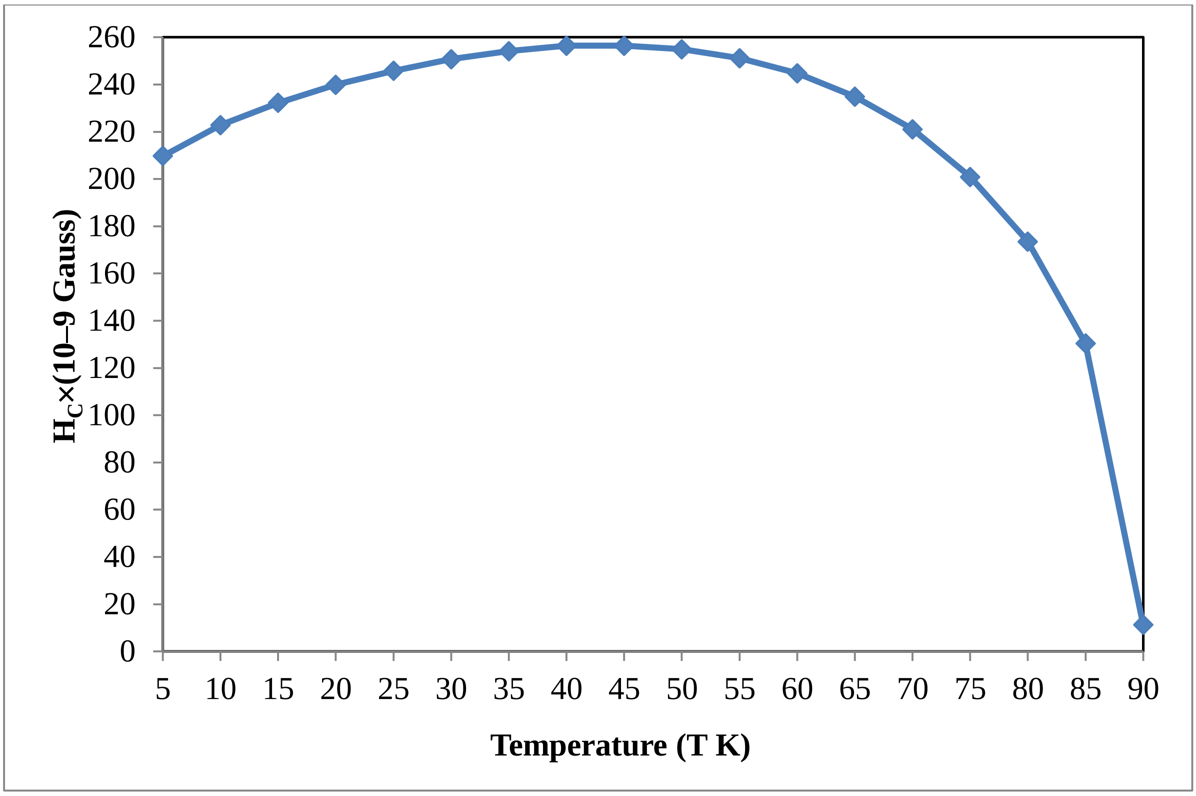
H_C×(10–9 Gauss)
260
240
220
200
180
160
140
120
100
80
60
40
20
0
5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90
Temperature (T K)

Fig. 1 (a)

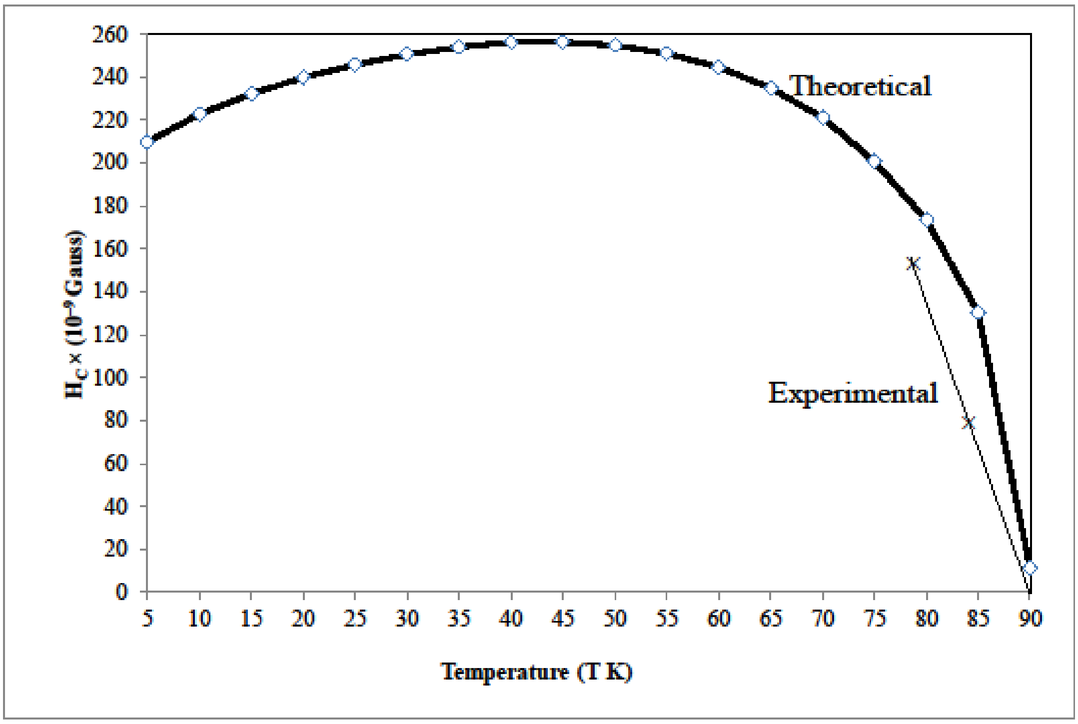

Fig 1(b) . Variation of Critical Field with Temperature

CONCLUSION

Photo induced conductivity and photo - modulation optical conductivity EXAFS measurements on the radial distribution function of particular clusters of atoms ion channeling and resonant neutron absorption measurements clearly demonstrate that charge carriers in cuprate superconductors have characterstics of small polarons. It is generally accepted that electronically the copper based superconductors belong to the class of charge transfer insulators which are close to the ionic limit and with strong onsite correlations on the Cu sites in the CuO_2 layers. Based upon these ideas, we have developed a microscopic theory of high $-T_C$ superconductivity considering Frohlich's Hamiltonian and electron - electron interaction. We have seen that our theory satisfactorily explains several features of new high $T_C$cuprates superconductors, $YBa_2Cu_3O_{7-\delta}$. We have shown that BCS theory is applicable to these systems, only with the difference that usual electron - phonon interaction is replaced by the interactions of pairs of electrons with opposite momenta and spin - in the strong coupling limit. We derived the mean - field normal and anomalous Green's functions.

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