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TO STUDY DENSITY OF STATES OF POLARON EFFECTS IN HIGH-Tc SUPERCONDUCTORS:

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ABSTRACT

High-T_C Copper oxides discovered so far are characterized by the two dimensional Cu-O planes. The superconductivity can be controlled by doping an appropriate carriers to these CuO₂ sheets. From structural points of view the intervening components between the points of CuO₂ sheets play an important role in structure stabilization adjusting the carrier density in the CuO₂ sheets. The layered cuprate superconductors are now well established. The majority carriers in these systems are holes. Recently, electron doped high temperature superconductors Ln_{1.85} Ce_{0.15}CuO_{4-y} (Ln = Pr, Nd and Sm) have also been discovered. Hall effect measurements and charge balance indicate that in electron doped superconductors, electron are the charge carriers rather than holes. A series of cuprates of the type T1 Ca_{1-x}Ln_x Sr₂Cu₂O₇₊₈ have also been reported which shows electron or hole superconductivity depending on x. In addition to the above mentioned high-T_C superconductors several other notable discoveries have also been made (i) series of lead cuprates of the type Pb₂Ca_{1-x} Ln_xSn₂ Cu₃O₈ containing Cu¹⁺ in high proportions, (ii) non copper oxide high - T_C superconductors Ba_{1-x}KxBiO_{3-y} (x~0.4) exhibiting superconductivity at about 30K (iii) 2222 compounds Bi₂Sr₂ (Ln_{1-x}Ce_{x)₂} Cu₂O_{10+y} dL₁ = Sm, Eu or Gd), having double CuO₂paramidal sheets between double layered units with an onset transition temperature around 25K.

Keywords: density of states

INTRODUCTION

Since Anderson's proposal that strongly correlated one - band Hubbard model near half filling in the square lattice includes essential physics of high - T_C cuprate superconductors, extensive study has been made along this line. The simplest is t - J model. For applying the t - J model to the cuprate oxides it is assumed that electron - or - hole doping causes the spin defects with electric charge on copper sites so that the defects can be looked upon as holes on Cu sites.

In addition to above mechanisms, several other mechanisms, e.g. chemical mechanism, copper d - d excitation model, Magnon exchange pairing mechanism. Real space pairing, correlated charge fluctuation mechanism have also been proposed.

So far we have discussed some possible novel mechanisms of electron pairing that have been suggested for high - T_C superconductivity.

These cuprate superconductors start as an insulator and become metallic on doping by metal impurities or oxygen excess and go to a superconducting phase below T_c . Even the normal state properties of these systems

are puzzling and they are referred to as strange metals. These systems are much more complicated compared to ordering metals and alloys.

The experimental observations made on these systems now put serious restrictions on some models discussed above. It appears that superconductivity is of BCS type. i.e. s-wave pairing, the main difference are in having a very short coherence length. Anisotropy and very minor role of phonon induces pairing mechanism. The usual features such as energy gap, discontinuity in the heat capacity singlet s-wave pairing, type-II behaviour are all seen.

Experiments also indicate that the pairing interactions in these systems are not driven by magnetic origin rather they compete with the process.

The strong electron correlations, which without any doubt are present in these materials 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 - all these experiments provide strong evidence that charge carriers in the high-T_C superconducting materials have characterstics of small polarons. An excess electron (hole) in a crystal produces a polarization of the lattice which surrounds it due to an interaction between the electron and the ions. Zubarevelectron have shown that direct electron interaction can lead to superconductivity. Cooper pairs are formed of electrons with opposite momenta and spins starting with the ordinary one - band Hamiltonian, including the Frohlich electron - phonon U and Coulomb V interactions, together with usual BCS interaction we propose to develop the theory of high temperature superconductivity in cuprate oxides - following Green's function technique and equation of motion method. Using this model we propose to serive expression for superconducting order parameter (Δ), critical temperature (T_c), specific heat. density of states N(w), Free energy and critical Field. We shall apply our results to the system Y Ba₂ Cu₃ O_{6+δ}.

OBJECTIVES

To study density of states

RESEARCH METHODOLOGY

One of the important functions to be determined and the one which is most susceptible to experimental verification is the density of states as a function the excitation energy \in_{K} .

The density of states per atom per spin, N (ω) is given by

$$N(\omega) = \lim_{\epsilon \to 0} \frac{i}{2\pi N} \sum_{K} \left\{ G_{\uparrow\uparrow} \left(K, \omega + i \epsilon \right) - G_{\uparrow\uparrow} \left(K, \omega - i \epsilon \right) \right\} \qquad \dots (1)$$

Here, $G\uparrow\uparrow(k,\omega)$ is the one particle Green's function.

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Using equation
$$\sum_{K} \cong N(0) \int d \in_{K}$$
 we rewrite equation as:

$$G_{K''}(\omega) = \left\langle \left\langle C_{K''\uparrow}; C_{K'\uparrow}^{+} \right\rangle \right\rangle = \frac{1}{2\pi} \frac{(\omega + F_{K''})}{(\omega^{2} - \alpha \omega - \gamma)}$$
$$= \frac{(\omega + F_{K''})}{\omega^{2} - F_{K''}^{2} - (Z + \Delta)^{2}} \qquad \dots (2)$$

Here, $F_{K''} = \in_{K''} + M_{K''}(-\omega) - S_{K''} \approx \in_{K''} + M_{K''}(-\omega)$

$$Z = N_{K''\sigma'}(\omega) - T_{K''\sigma''}(\omega) + \Delta$$

$$\approx N_{K''\sigma''}(-\omega) - T_{K''\sigma''}(-\omega) + \Delta$$

$$\Delta \approx \Delta^{+}, N_{K''\sigma''}(\omega) = N_{K''\sigma''}(-\omega)$$

$$T_{K''\sigma''}(\omega) = T_{K''\sigma''}(-\omega) \qquad \dots (3)$$

Thus

$$G_{\uparrow\uparrow}(\omega) = \frac{1}{2} \left[\frac{\left(\frac{F_{K^{*}}}{y} + 1\right)}{(\omega - y)} - \frac{\left(\frac{F_{K^{*}}}{y} - 1\right)}{(\omega + y)} \right] \qquad \dots (4)$$

Where,

$$y^{2} = \left[F_{K^{n}}^{2} + (Z + \Delta)^{2}\right] \qquad ... (5)$$

Using the following properties of δ -function

$$\delta(\mathbf{x}) = \frac{1}{2\pi i} \left\{ \frac{1}{\mathbf{x} - \mathbf{i} \in} -\frac{1}{\mathbf{x} + \mathbf{i} \in} \right\} \qquad \dots (6)$$

$$\delta\{g(t_n)\} = \sum_{n} \frac{1}{|g't_n|} \delta(t - t_n) \qquad \dots (7)$$

Where, $g(t_n) = 0$; $g'(t_n) \neq 0$

and using equation,

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$$\sum_{K'} = \int \frac{d^3 \vec{K'}}{(2\pi)^3} = N(E_F) \int_{-\hbar\omega_D}^{-\hbar\omega_D} dF_{K''} \qquad ... (8)$$

We obtain with the help of equation (1) and (2) as follows:

$$\frac{N(\omega)}{N(o)} = \frac{\left(\omega + M_{K''(-\omega)}\right)}{\sqrt{\left(\omega^2 - M_{K''(-\omega)}^2 - (Z + \Delta)^2\right)}} \qquad \dots (9)$$

Equation (9) may be written as:

$$\frac{N(\omega)}{N(0)} = \frac{\left(\omega + g^2 m^2 v_0 (\hbar \omega_D) / (2\pi)^2 2\hbar^3\right)}{\sqrt{\left[\omega^2 - \left(\frac{g^2 m^2 v_0 (\hbar \omega_D)}{(2\pi)^2 2\hbar^3}\right)^2 - \left\{\left(\frac{-g^2 v(0) 2m(\hbar \omega_D)^2}{3(2\pi)^2 \hbar^2}\right) - \Delta\right\}^2\right]}} \qquad \dots (10)$$

In the limit $V \rightarrow 0$ equation (10) reduces to

$$\frac{N(\omega)}{N(0)} = \frac{\omega}{\sqrt{\omega^2 - \Delta^2}} \qquad \text{for } \omega > \Delta \\ = 0 \text{ otherwise} \end{cases} \qquad .. (11)$$

Which is same as described by the BCC theory.

DATA ANALYSIS

From equation (10), we rewrite it as :

$$\frac{N(\omega)}{N(0)} = \frac{\left(\omega + g^2 m^2 v_0(\hbar\omega_D)/(2\pi)^2 2\hbar^3\right)}{\sqrt{\omega^2 - \left(\frac{g^2 m^2 v_0(\hbar\omega_D)}{(2\pi)^2 2\hbar^3}\right)^2 - \left\{\left(\frac{g^2 v(0)2m(\hbar\omega_D)^2}{3(2\pi)^2 \hbar^3}\right) - \Delta\right\}^2} \quad \dots (12)$$

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Table 1

Values of various Paramers for the System

[YBa₂Cu₃O_{7-δ}]

1.	Density of states N (0)	4.1×10^{12}
		per erg-copper atom
2.	Phonon energy $(\hbar \omega_{\rm D})$	$1.6 \times 10^{-14} \text{ erg}$
3.	Number of atoms per unit volume (N)	$5 \times 10^{22} \text{ per cm}^3$
4.	Critical Temperature (T _C)	90 k
5.	Velocity of phonon (v_0)	4×10^4 cm/sec
6.	Polaron binding energy (g ²)	$2 \times 10^{-5} \text{ erg}$
7.	Boltzman constant (k _B)	1.38×10^{-16} arg/k
8.	BCS attractive interactive strength	$0.4512 \times 10^{-12} \text{ erg}$
9.	Structure type and	Orthorhombic with an extended
	Cell parameter (123 phase)	C-axis 11.686 A and a-and b-axis
		annost
		b = 3.8895 A
10.	Phonon frequency $(\hbar\omega_0)$	$80 \times 10^{-6} \text{ erg}$
11.	Mass of electron (m _e)	$9.1 \times 10^{-28} \text{gm}$
12.	Planck constant (\hbar)	$6.62 \times 10^{-27} \text{ erg sec}$
13.	Coulomb potential V(0)	$0.2 \times 10^{-14} \text{ erg}$

Using $\omega = y \times 10^{-14}$ erg and Table 1, we can write

$$\frac{N(\omega)}{N(0)} = \frac{\left(y \times 10^{-14} + 0.925 \times 10^{-14}\right)}{\sqrt{\left\{\left(y \times 10^{-14}\right)^2 - \left(.925 \times 10^{-14}\right)^2 - \left(x \times 10^{-14}\right)^2\right\}}}$$
$$= \frac{y + 0.925}{\sqrt{\left(y^2 - 0.855 - x^2\right)}} \qquad \dots (13)$$

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Solving equation (13), the variation of $N(\omega)/N(0)$ with ω for a particular value of x is given in Table 2.

S.	W=Y×10 ⁻¹⁴	x ² =5.4289	x ² =1.7424	x ² =0.0064
No.	erg	$\Delta^2 = 5.4289 \times 10^{-28}$ erg ²	Δ ² =1.7424×10 ⁻²⁸ erg ²	$\Delta^2 = 0.0064 \times 10^{-28}$ erg ²
		$\Delta = 2.334 \times 10^{-14}$	Δ=1.320×10 ⁻¹⁴ erg	Δ =0.080×10 ⁻¹⁴ erg
		u g	N(ω) / N(0)	N(ω) / N(0)
		N(ω) / N(0)		
1.	10	1.1285	1.1069	1.0283
2.	20	1.0545	1.0496	1.0068
3.	30	1.0344	1.0323	1.0030
4.	40	1.0251	1.0239	1.0017
5.	50	1.0197	1.0190	1.0010
6.	60	1.0163	1.0157	1.0007
7.	70	1.0138	1.0134	1.0005
8.	80	1.0120	1.0117	1.0004
9.	90	1.0106	1.0104	1.0003
10.	100	1.0095	1.0093	1.0002
11.	110	1.0086	1.0085	1.0002

Table 2

The variation of N(ω)/N(0) with ω for superconducting order parameter (Δ) is shown in fig. 1. The dotted curve is that obtained from BCS theory and correspond to $\Delta = 10^{-14} \times 2.334$ from equation (11), it may rewritten as:

$$\frac{N(\omega)}{N(0)} = \frac{y}{\sqrt{y^2 - x^2}}$$
... (14)

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Density of States N(ω)



CONCLUSION

In the foregoing chapters we have presented the theoretical study of high temperature superconductivity in newly discovered high - T_Ccuprates. Starting with the one band Hamiltonian, including the Frohlich electron-phonon U and Coulomb V interactions and following Green's functions technique and equation of motion method, we have obtained expressions for superconducting order parameter (Δ), superconducting transition temperature (T_C), electronic specific heat (C_s^e), Density of states N(w), Free energy difference (F_S - F_N), and critical field (H_C). We have applied this model to the system YBa₂Cu₃O_{7-δ}. In the absence of experimental data, it is not possible to compare all the results from our model.

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