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Interlayer coupling in peroxitonic model of superconductivity

R RAI
National Physical Laboratory, New Delhi 110012, India

Abstract. The unusual ESR spectra of $YBa_2Cu_3O_{7-x}$ is ascribed to a Cu^{2+} ion, whose one ligand in CuO_2 plane is involved in a peroxiton O^-–Cu^+–O^- bond. The analysis shows that the presence of a ligand in O^- substantially increases the energies of d-hole orbitals. Since this increase for $d_{x^2-y^2}$ orbital is much larger than that for $d_{3z^2-r^2}$ orbital, their separation is drastically reduced and there occurs a significant orthorhombic mixing between the two. This charge transfer from a planar $d_{x^2-y^2}$ orbital to a $d_{3z^2-r^2}$ orbital, which lies mainly perpendicular to the plane, provides a mechanism for interlayer coupling. The effect of this coupling on superconducting transition temperature is discussed.

Keywords. Interlayer coupling; peroxitonic model.

1. Introduction

Nearly isotropic ESR spectrum of $YBaCu_3O_{7-x}$ observed by Meheran *et al* (1988) was recently explained (Rai 1989) by ascribing it to a Cu^{2+} ion, whose one ligand in CuO_2 plane is involved in a O^-–Cu^+–O^- peroxiton bond with an oxygen and copper of neighbouring CuO_2 unit (figure 1). The analysis shows that the presence of a ligand in O^- form, instead of O^{2-}, drastically reduces the separation between $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ orbitals and causes a significant orthorhombic mixing between the two. Thus there occurs an oxygen hole-assisted charge transfer from a planar $d_{x^2-y^2}$ orbital to a $d_{3z^2-r^2}$ orbital, which lies mainly in a direction perpendicular to the plane. A simultaneous charge transfer of this type at the nearest copper sites on two adjacent CuO_2 planes will affect an out-of-phase displacement of bridge O_4 oxygen atoms in the direction perpendicular to the planes (figure 1). This provides a mechanism for interlayer coupling. Our aim in the present paper is to investigate the effect of this coupling on superconducting transition temperature.

2. Theory

The appropriate hamiltonian can be written as

$$H = H_0 + H', \tag{1}$$

$$H_0 = \sum_{K\sigma} [(t_k^\varepsilon + E_\varepsilon) n_{k\sigma}^\varepsilon + t_k^\pi \pi_{k\sigma}^+ \pi_{k\sigma}] + \sum_{\substack{\langle i\alpha\rangle\langle ij\rangle \\ \sigma\sigma'}} \Bigg[u \sum_{\substack{(rr') \\ =(\varepsilon\theta)}} n_{\alpha\sigma}^r n_{\alpha\sigma'}^{r'} + U_\pi n_{i\uparrow}^\pi n_{i\downarrow}^\pi - J \pi_{i\uparrow}^+ \pi_{j\downarrow}^+ \pi_{j\uparrow} \pi_{i\downarrow} + h(\varepsilon_{\alpha\sigma}^+ \pi_{i\sigma} + \pi_{i\sigma}^+ \varepsilon_{\alpha\sigma}) + Q_{ij} n_{i\sigma}^\pi n_{j-\sigma}^\pi \Bigg], \tag{2}$$

$$H' = \sum_{\substack{\langle i\alpha\rangle\langle\alpha\alpha'\rangle_\perp \\ \sigma\ \ \sigma'}} \Bigg[E_\theta \theta_{\alpha\sigma}^+ \theta_{\alpha\sigma} + (V_\varepsilon n_{\alpha\sigma}^\varepsilon + V_\theta n_{\alpha\sigma}^\varepsilon) n_{i\sigma'}^\pi + d_i n_{i\sigma'}^\pi (\varepsilon_{\alpha\sigma}^+ \theta_{\alpha\sigma} + \theta_{\alpha\sigma}^+ \varepsilon_{\alpha\sigma}) + \left\{ \hbar w b_{\alpha\alpha'}^+ b_{\alpha\alpha'} + \lambda_\perp \left(\frac{\hbar}{2\mu_\perp w_\perp} \right)^{1/2} (b_{\alpha\alpha'}^+ + b_{\alpha\alpha'}) \right\} n_{\alpha\sigma}^\theta n_{\alpha'\sigma'}^\theta \Bigg]. \tag{3}$$

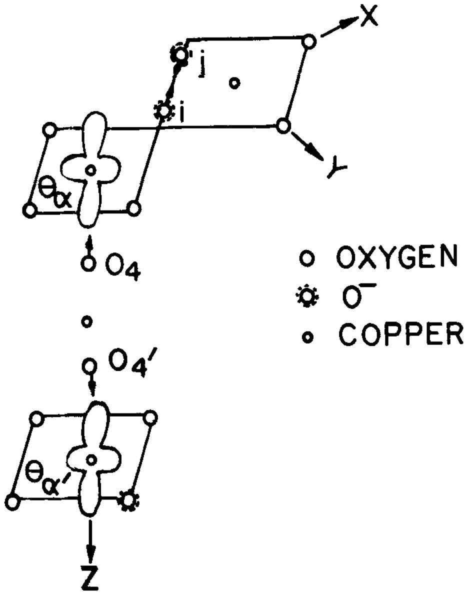

Figure 1. Occupancy of $d_{3z^2-r^2}$ orbital affected by a O^- ligand and an out-of-these displacement of bridge O_4 and $O_{4'}$ oxygen atoms due to simultaneous occupancy of $d_{3z^2-r^2}$ orbitals on sites α and α', the nearest neighbours on two adjacent CuO_2 planes.

H_0 is essentially the hamiltonian proposed by Chakraverty *et al* (1987). Here E refers to the hybridized $d_{x^2-y^2} - p_\sigma$ antibonding orbital, θ to $s_{3z^2-r^2}$ and π to oxygen p_π. The operators $\varepsilon^+(\varepsilon)$ etc are the corresponding band or site hole creation (annihilation) operators. Q_{ij} involves the $O_i - O_j$ bond fluctuation in a CuO_2 plane due to the presence or absence of a hole on each of these two oxygen atoms.

The quantities V_ε and V_θ in H' are respectively the increase in Coulomb energies of ε and θ hole orbitals due to the presence of a hole on a nearest neighbour oxygen site in CuO_2 plane, $d_i = d$ or $-d$ depending upon whether the site i is on x or y axis (figure 1) and d is an orthorhombic parameter (Rai 1989). The notation $\langle\alpha\alpha'\rangle_\perp$ indicates that α and α' are the nearest copper sites on two adjacent CuO_2 planes. The presence or absence of a hole on each of the two θ_α and $\theta_{\alpha'}$ orbitals is responsible for the out-of-phase oscillation of the two bridge O_4 oxygen atoms (figure 1) and $b^+_{\alpha\alpha'}$ $(b_{\alpha\alpha'})$ are the phonon creation (destruction) operators corresponding to this oscillation.

Using a unitary transformation

$$\bar{H} = u^+ H u, \tag{4}$$

with

$$u = \prod_{\langle\alpha i\rangle\sigma\sigma'} \exp[\Phi_i(\varepsilon^+_{\alpha\sigma}\theta_{\alpha\sigma} - \theta^+_{\alpha\sigma}\varepsilon_{\alpha\sigma})n^\pi_{i\sigma'} \tag{5}$$

and

$$\tan 2\Phi_i = 2d_i/E_\theta + V_\theta - E_\varepsilon - V_\varepsilon]. \tag{6}$$

Neglecting the interactions between three or more sites in the same CuO_2 plane we notice that, excepting the terms with h and $\lambda_\perp$ as coefficients, the mixing between ε and θ orbitals is eliminated. The h and $\lambda_\perp$ dependent terms are modified as

$$\sum_{\langle\alpha i\rangle\sigma} h[1+(1-\cos\Phi_i)n^\theta_{\alpha\sigma}](\varepsilon^+_{\alpha\sigma}\theta_{\alpha\sigma}+\theta^+_{\alpha\sigma}\varepsilon_{\alpha\sigma}), \tag{7}$$

and

$$\sum_{\substack{\langle\alpha\alpha'\rangle_\perp\langle i\alpha\rangle\\ \sigma\sigma'\sigma'}} \lambda_\perp\left(\frac{\hbar}{2\mu_\perp w_\perp}\right)^{1/2}(b^+_{\alpha\alpha'}+b_{\alpha\alpha'})n^\theta_{\alpha'\sigma'}\{n^\varepsilon_{\alpha\sigma}n^\pi_{i\sigma'}\sin^2\Phi_i$$
$$+n^\theta_{\alpha\sigma}\cos^2\Phi_i-\tfrac{1}{2}\sin 2\Phi_i(\varepsilon^+_{\alpha\sigma}\theta_{\alpha\sigma}+\theta^+_{\alpha\sigma}\varepsilon_{\alpha\sigma})n^\pi_{i\sigma'}\}. \tag{8}$$

Neglecting the last term in the curly bracket in (8), dropping all terms in $\bar{H}$ which involve only θ-dependence, and using the Lange–Firsov transformation operator

$$S=\exp\left[-\sum_{\substack{\langle\alpha\alpha'\rangle\langle\alpha i\rangle\\ \sigma\ \sigma'\ \sigma''}}\lambda_\perp\left(\frac{\hbar}{2\mu_\perp w_\perp}\right)^{1/2}\frac{1}{hw_\perp}(b^+_{\alpha\alpha'}-b_{\alpha\alpha'})n^\theta_{\alpha'\sigma'}n^\pi_{i\sigma''}n^\varepsilon_{\alpha\sigma}\sin^2\Phi_i\right] \tag{9}$$

it is seen that the zero phonon expectation value of $(S^+\bar{H}S)$ regains the form of the original hamiltonian (Chakraverty *et al* 1987) with renormalized functions E_ε and h given by

$$E'_\varepsilon=E_\varepsilon+\frac{\delta}{2}\{E_\theta+V_\theta+V_\varepsilon-E_\varepsilon-[4d^2+(E_\theta+V_\theta-E_\varepsilon-V_\varepsilon)^2]^{1/2}\}, \tag{10}$$

$$h'=h[1+a_1\delta+a_2\delta^2+a_3\delta^3], \tag{11}$$

$$\delta=(1-2x)=\langle n^\pi_{i\sigma}\rangle=\frac{1}{2\sin^2\Phi}\langle n^\theta_{\alpha\sigma}\rangle, \tag{12}$$

$$\begin{aligned}a_1&=2\sin^2\Phi(1-\cos\Phi)\\ a_2&=2q_-\sin^2\Phi(1-4\sin^2\Phi-2\sin^2\Phi\cos\Phi),\\ a_3&=4q_+\sin^4\Phi(4-2\cos^2\Phi)+4q_-\sin^4\Phi(1-\cos\Phi),\end{aligned} \tag{13}$$

$$q_-=\exp\left(-\frac{2\sin^4\Phi}{2\hbar\mu_\perp w_\perp 3}\right)-1, \tag{14}$$
$$q_+=\exp\left(\frac{\lambda^2_\perp\sin^4\Phi}{2\hbar\mu_\perp w_\perp 3}\right)-1.$$

In writing (12) we have noted that the expectation value of a hole at any oxygen site in a CuO_2 plane is $\frac{1}{2}(1-2x)$. The expectation value of $n^\theta_{\alpha\sigma}$ is non-zero only if one ligand of Cu^{2+} ion at α is in O^- form so that there is an orthorhombic mixing between $|\varepsilon_{\alpha\sigma}\rangle$ and $|\theta_{\alpha\sigma}\rangle$ orbitals resulting in a combined orbital of the form $(\cos\Phi|\varepsilon_{\alpha\sigma}\rangle\pm\sin\Phi|\theta_{\alpha\sigma}\rangle)$ (Rai 1989). Since there are two oxygen sites per copper in a CuO_2 unit $\langle n^\theta_{\alpha\sigma}\rangle=\sin^2\Phi\,(1-2x)$.

Noting that the superconducting transition temperature in a peroxiton model is proportional to h^2 a relation between T_c and the doping parameter δ can readily be written as

$$T_c=T_0[1+a_1\delta+a_2\delta^2+a_3\delta^3]^2. \tag{15}$$

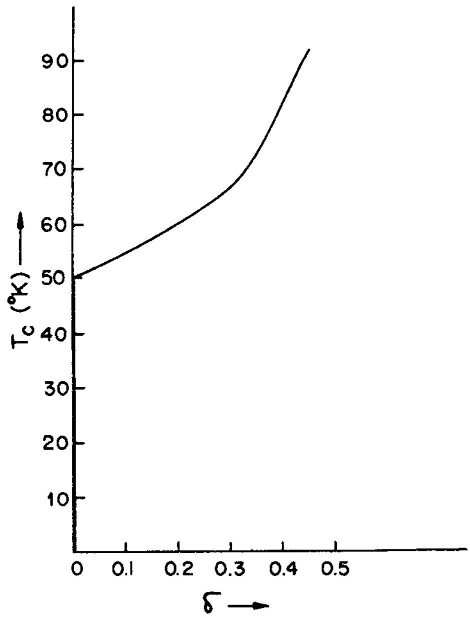

Figure 2. Variation of superconducting transition temperature T_c versus doping parameter $\delta = 0{\cdot}5 - x$ for $YBa_2Cu_3O_{7-x}$.

3. Discussion

Figure 2 shows a plot of T_c versus δ for the value of $T_0 = 50°K, (\lambda_{\perp}/(2h\mu W_{\perp}^3))^{1/2} = 1{\cdot}208$ and $\Phi = 55{\cdot}2°$. These parameter values are chosen to simulate the experimental T_c versus δ curve (Goucharov *et al* 1988) as best as possible. Even though the curve near $\delta \approx 0{\cdot}2$ does not resemble the experimental 60°K plateau the slope in this region is much slower than that above $\delta = 0{\cdot}3$. Above $\delta = 0{\cdot}3$ the present plot resembles the experimental curve (figure 2). The present value of $\Phi = 55{\cdot}2°$ is close to the value of $\Phi = 49°$ obtained after a phase correction of the value required to explain the ESR result (Rai 1989). The present calculation clearly brings out the importance of oscillation of O_4 bridge oxygen atoms in interlayer coupling. The importance of these oscillations is also emphasized in experimental infrared and Raman spectroscopic results (Goncharo *et al* 1988; Yonggang *et al* 1988).

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