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Coexistence of superconductivity and structural distortion in systems with degenerate bands[1]

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Abstract

The effect of the band Jahn-Teller distortion on superconductivity is studied for systems with orbitally degenerate bands using a simple theoretical model. The model assumes a two-fold degenerate band coupled to lattice strain and an attractive interaction mediated by some boson producing BCS pairing superconductivity. It therefore, incorporates two competing physical processes involving the removal of degeneracy by lattice distortion and the formation of the condensate state of the cooper pairs. It is found that as superconductivity sets in the growth of the lattice distortion is arrested. The magnitude of the distortion decreases with decreasing electron density, while the superconducting order parameter increases. Our observations agree with the anamalous structural behaviour of the superconducting compound $La_{1.85}Ba_{0.15}CuO_4$ as detected experimentally.

Keywords : Jahn-Teller Distortion, Doubly Degenerate band, Superconductivity.

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1 Introduction

Compounds which exhibit superconductivity are often prone to undergo structural instability [1]. Recently, in high T_c cuprates [2, 3] and in many intermetallic compounds [4, 5, 6], the structural transition associated with the lowering of crystallographic symmetry has been observed. The existence of orbital degeneracy in the ground state with the Fermi level (FL) lying within a degenerate band is a common feature to all these systems. The distortion (which is a measure of the orthorhombic splitting in the tetragonal to orthorhombic transition) lifts the degeneracy of the band and the electron redistribution between the shifted bands lowers the electronic energy provided the lowering in electronic energy outweighs the cost in elastic energy due to distortion. With such transition there is an associated change in the density of states around the FL and therefore, it is expected that the band Jahn-Teller (J-T) distortion would strongly influence the superconductivity in such a system. If the FL lies at the centre of the degenerate band then the density of states at FL is drastically reduced and the superconducting transition temperature T_c will go down. On the other hand, T_c can be higher as phonon softening due to J-T effect may increase the coupling constant which is inversely proportional to mean square phonon energy.

It is well known that some high temperature superconductors like the $Cu-O$ (e.g, La_2CuO_4) systems undergo structural transitions from the tetragonal to the orthorhombic phase. In the tetragonal phase, each Cu atom occupies a site of squared Bravais lattice and is surrounded by an octahedra of six neighbouring oxygen atoms, two of them lying above and below the plane and the four others occupying the sites inside the plane. The oxygen octahedra gives rise to a strong crystal field, the leading term of which is cubic and thus splits the five fold degenerate d-orbitals of Cu into a t_{2g} triplet (orbitals d_{xy}, d_{yz} and d_{zx}) which lies far below the Fermi energy and is thus completely occupied, and an e_g doublet (orbitals $d_{x^2-y^2}$ and $d_{3z^2-r^2}$) which is partially occupied. In this context, experimental observation of high resolution neutron diffraction experiments on the superconducting $La_{1.85}Ba_{0.15}CuO_4$ compound was reported [7]. A brief summary of their essential findings are presented below.

Their measurements [7] clearly exhibit a tetragonal to orthorhombic transition at 180 K together with further structural anomalies on approaching the onset of superconducting phase transition at 35 K. At temperatures greater than 185 K the tetragonal symmetry (as in the parent La_2CuO_4 compound above 500 K) is observed. Below this temperature, a symmetry breaking or-

thorhombic transition occurs with a splitting ratio that increases monotonically with decreasing temperature, reaching a maximum value at 75 K. Below 75 K a highly unusual and unexpected *decrease* in lattice distortion is observed which saturates at 35 K, coincident with the onset of superconductivity in this sample. Direct evidence of orthorhombic distortion is also detected from the splitting of the Bragg reflection peaks of the orthorhombic phase at 120 K which collapse at lower temperatures [7]. Most interestingly, the anomalous decrease in the orthorhombic splitting correlates with the plateau in resistivity and further, that the onset of superconductivity at 35 K corresponds to the saturation of the splitting at a very low label. One of the important experimental results, namely, the anamalous temperature dependence of the orthorhombic splitting which is defined as spontaneous strain is displayed in fig.1.

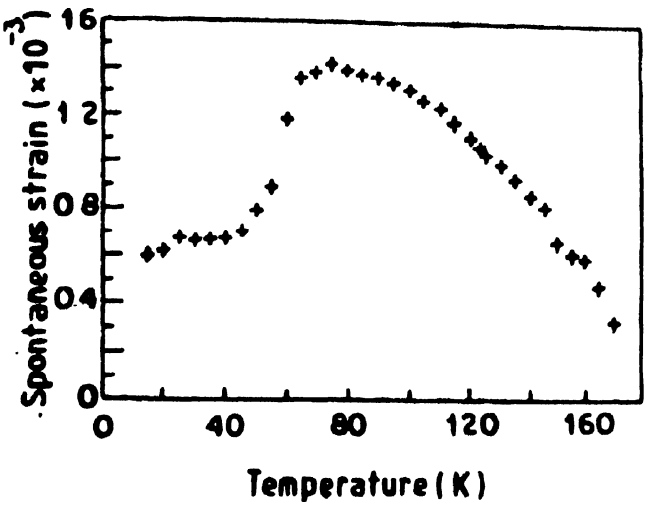

Fig.1 The temperature variation of the spontaneous strain as a function of temperature, obtained from the neutron diffraction experiment Ref.[7].

Therefore, we emphasize that it is extremely important for high T_c superconductors like La_2CuO_4 to have a detailed and acurate knowledge of structural instabilities which may throw light about the origin of superconductivity in such materials. Also, such observed anamalous structural behaviour will have stringent constraint to any realistic theoretical model for high T_c superconductors. Hence, our main aim in this paper is to present a detailed study of the coexistence of superconductivity and band J-T distortion in the two-fold degenerate e_g band as a function of the electron concentration.

2 Model for coexistence of superconductivity and lattice distortion

We consider a model system in which the electrons are in a two fold degenerate band and interact with the lattice as well as between themselves, the later via a BCS pairing interaction. Therefore, the total Hamiltonian H consists of four terms,

$$H = \sum_{k,\alpha\sigma}(\epsilon_k - \mu)C^{\dagger}_{\alpha k\sigma}C_{\alpha k\sigma} + \sum_{k,\sigma} Ge\{C^{\dagger}_{1k\sigma}C_{1k\sigma} - C^{\dagger}_{2k\sigma}C_{2k\sigma}\} + \frac{3}{4}(C_{11} - C_{22})e^2 - \sum_{k,k',\alpha,\alpha',\sigma,\sigma'} V_{kk'\alpha\alpha'}C^{\dagger}_{k\alpha\uparrow}C^{\dagger}_{-k\alpha\downarrow}C_{-k'\alpha'\downarrow}C_{k'\alpha'\uparrow}. \quad (1)$$

The first term in the hamiltonian represents the non-interacting electrons in a two-fold degenerate (e_g) band ($\alpha = 1, 2$; is the orbital index) with single-particle energy ϵ_k. The coupling between the electron density in the degenerate electron band and the static elastic strain in presence of tetragonal distortion is described by the 2nd term of equation (1). The third term is the elastic energy in absence of strain. The pairing hamiltonian described by the 4th term of (1) assumes that the BCS pairing exists only within the same orbitals and the strength of interaction is same for both the orbitals [8].

Therefore, the interaction of the electrons in the degenerate conduction band with the lattice acts as external perturbation to the free electrons in the band which tries to creat a population difference between the two bands. As the population difference increases, the strain builds up [10] in the system resulting in a splitting of the single degenerate band into two with band energies $\varepsilon_\alpha(k) = \epsilon_k - (-1)^\alpha Ge$, provided there is a net gain in the electronic energy due to the redistribution of electrons between the splitted subbands in comparison to the cost in the elastic energy.

In order to study the actual nature of the superconducting condensate state in the distorted orthorhombic phase one has to understand the superconducting gap equation, the associated gap equation for the strain mode and the position of the chemical potential. The respective gap equations as well as an equation for the chemical potential can be obtained from equation (1) within the mean field approximation [8]. For example the equation for the SC gap is given as usual by,

$$1 = \sum_{k,\alpha} \frac{V}{2E_\alpha(k)} \tanh(\beta E_\alpha(k)/2) \quad (2)$$

where the superconducting quasi particle energies $E_\alpha(k)$ are obtained as, $E_\alpha(k) = \pm\sqrt{(\varepsilon_\alpha(k) - \mu)^2 + |\Delta|^2}$ for a chemical potential μ.

Similarly, the gap equation corresponding to the strain order parameter is given by,

$$e = -\frac{G}{C}\sum_{k,\alpha}(-1)^\alpha \frac{\epsilon_\alpha(k)}{2E_\alpha(k)} \tanh\frac{\beta E_\alpha(k)}{2} \tag{3}$$

and the total number of electrons determines the chemical potential.

It is to be noticed that the above equations are coupled integral equations in the sense that the equation for the superconducting gap function Δ is a functional of itself, the splitting in the band due to strain as well as the chemical potential μ i.e, $\Delta \equiv \Delta(\Delta, e, \mu)$. Similarly we have the strain $e \equiv e(\Delta, e, \mu)$ and the number conservation equation $n \equiv n(\Delta, e, \mu)$. Therefore, in order to determine the temperature variation of any of these quantities which is important to understand the nature of the system, we solve these three equations numerically self-consistently for different band fillings [8].

3 Results and discussions

The equations (2,3) are numerically solved for a given set of the values of input parameters (V, G, ω_D, C and B) with varying electron concentration n. For all the results presented here the values of these parameters are chosen as follows : the dimensionless pairing potential $N(0)V = 0.11$, the Debye frequency $\omega_D = 0.038\ eV$, the elastic stiffness constant $C = 30\ eV$ and the half bandwidth $B = 0.1\ eV$ are kept fixed. The peak density of state (DOS) used has an energy dependence given by, $N(\epsilon) = N(0)\sqrt{1 - |\frac{\epsilon}{B}|}\ln|\frac{B^2}{\epsilon^2}|$;B being the half-bandwidth [9]. In fig. 2 (a, b) superconducting gap and strain are plotted as a function of temperature for different dopant concentrations ($\delta = 0.05$ and 0.1 respectively) with $G = 1.15\ eV$. We find that close to half filling (δ small) the structural transition takes place at higher temperatures and it increases with decreasing temperature till the onset of superconductivity where it attains the maximum magnitude, then decreases drastically and saturates to a lower magnitude (almost 50% of the maximum magnitude) at lower temperatures (cf. fig.2(b)). Such a behaviour is in complete agreement with the experimental observation (cf. fig.1). The structural transition temperature T_s as well as the maximum magnitude of the strain $e_{max}(T)$ reduces as the hole dopant concentration increases. To note, the $e_{max}(T)$ shifts towards higher temperatures with increasing dopant concentration. In contrast, experimentally the maximum in

the strain occurs at a temperature much higher than T_c whereas that from our results coincide exactly at T_c. Such experimental data may be an indication of the fact that there is large fluctuation in the high-T_c superconductors close to T_c so that the superconducting pairing exists even at a higher temperature than T_c and hence the suppression of strain starts at T > T_c. On the otherhand, ours is an exact mean field result which does not take into account fluctuation effects, resulting in such qualitative differences with experiment.

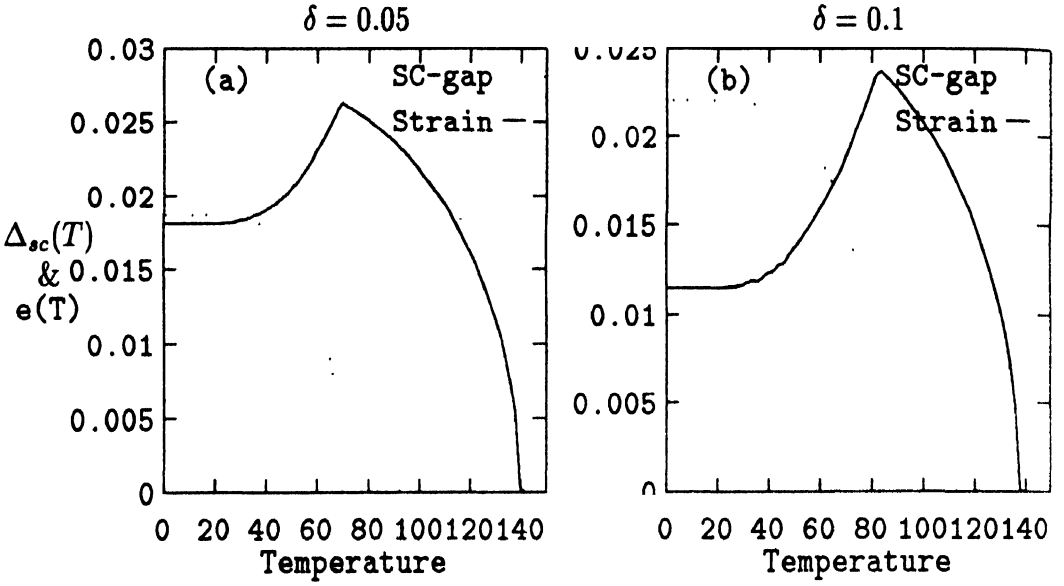

Fig. 2 The temperature variation of the SC and the strain order parameters for different hole concentrations (a) $\delta = 0.05$ and (b) $\delta = 0.1$, obtained from our model

In contrast, the SC T_c as well as the $\Delta(0)$ increases with increasing dopant concentration (δ). At half-filling, the lower splitted sub-band is fully occupied whereas the upper one completely empty, resulting in a maximum population difference between the bands and hence maximum splitting. Consequently, a large amount of electronic states are taken away from the Fermi level resulting in strong suppression of T_c for the half-filling case. On the other hand, a small doping (n<1) reduces the effect of strain and T_c increases rapidly. Such strong influence of distortion is intimately related to energy dependence of the density of states near the Fermi level [8].

However, the present model is too simplified because the strong electron correlation, which is known to play an important role in $Cu-O$ systems is not considered here. The effect of intra and inter-orbital correlation and exchange interaction has also not been incorporated in the present calculation partly for numerical simplification and partly for the well known difficulties in treating them. In systems like alkali doped fullerides (which shows no magnetism) such Jahn-Teller distortion is well es-

tablished. The strong correlation treated within the Slave Boson approach has been under study in order to make the applicability of our present model more appropiate for such systems [10].

4 Conclusion

Interplay between the band Jahn-Teller distortion and superconductivity in a narrow two-fold degenerate band has been found to be strongly dependent on band occupation and electron -lattice interaction strength. The transition temperature for the distorted phase goes down with hole doping and the coexistence phase appears at low temperatures. Observed temperature dependence of the lattice strain is in qualitative agreement with the experimental observation.

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