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Electron-fluctuating distortion interaction in the new high T_c superconductors

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Abstract. A mechanism involving interaction of conduction electrons with the distortion field and the phonon modes is considered for the newly discovered high T_c superconducting materials. This is capable of explaining the observed range of T_c.

Keywords. Structural distortion; superconductivity; Jahn-Teller polarons.

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Intense research activities have started at many centres in the world after the discovery of high T_c (36 K or more) superconductivity in doped lanthanum copper oxide systems, e.g. $La_{2-x}M_x CuO_4$, M = Ba, Sr, etc (Bednorz and Müller 1986; Uchida *et al* 1987; Chu *et al* 1987; Cava *et al* 1987). Regarding possible mechanisms, it is felt that the usual acoustic phonon-mediated processes may not give high enough transition temperatures. Accordingly, one should look for new mechanisms which may involve exchange of electronic excitations (Jagadish and Sinha 1987), bipolaronic mechanisms (Chakraverty 1979; Alexandrov and Ranninger 1981), interfacial excitonic mechanisms (Allender *et al* 1973; Ginzburg and Kirzhnits 1982), antiferromagnetic correlation as in the Hubbard model (Nozieres 1984; Anderson 1987) and mechanisms emanating from local distortions and structural instabilities in the system (Phillips 1976; Ngai and Reinecke 1977; Vujicie *et al* 1981).

At this stage it is desirable to note some special features of the $La_{2-x}M_xCuO_4$ systems. They have K_2NiF_4-type structure having planes of CuO_6 octahedra which share corners. These planes are separated by (La, M) layers. The structure of pure La_2CuO_4 (with copper in Cu^{2+} state, a Jahn-Teller ion) has a slight orthorhombic distortion. It is a semiconductor with low magnetic susceptibility (Rao *et al* 1985). $LaSrCuO_4$ is an insulator with Cu^{3+} ions in the diamagnetic state (Rao and Ganguly 1987). This low spin state appears to us to be stabilized by on-site bipolaron formation owing to strong electron-phonon interaction. It also leads to the splitting of e_g electronic states (at Cu^{2+}) leading to J-T polaron formation. The metallic behaviour of $La_{2-x}M_xCuO_4$ arises from the presence of Cu^{2+} and Cu^{3+} ions in the system wherein the J-T polarons become mobile and form a very narrow conduction band. It is confined to the two-dimensional planes of CuO_6 octahedra. Further, these oxide superconductors lie near the metal insulator transitions arising from the J-T polaron formation.

The crucial point, in the context of the model that we shall develop here, is that the system in question exhibits structural instabilities due to tetragonal to orthorhombic distortion when it is very rich in Cu^{2+} ions. Our stipulation is that even in the M^{2+} ion stabilized tetragonal phase local structural instabilities towards orthorhombic distortions exist. This is akin to a pseudo Jahn-Teller-induced local lattice distortion. This mechanism was first suggested by Sinha and Sinha (1964) for displacive ferroelectrics (e.g. $BaTiO_3$) and the full dynamical aspect leading to phonon softening worked out by Shukla and Sinha (1966). The model involves a two-level system of configurational local distortions. This was transcribed to a pseudo-spin ($S = 1/2$) formalism for protonic ferroelectrics (see Blinc and Zeks 1974).

Thus the Hamiltonian of a system of conduction electrons (in a narrow band) interacting with phonons and a distortion field described by the two-level system can be written as

$$H = H_e + H_c + H_{\mathrm{Ph}} + H_{e-\mathrm{Ph}} + H_{df} + H_{e-df}, \tag{1}$$

where

$$H_e = \sum \varepsilon_{\mathbf{k}} C^{\dagger}_{\mathbf{k}\sigma} C_{\mathbf{k}\sigma} \tag{2}$$

($C^{\dagger}_{\mathbf{k}\sigma}\, C_{\mathbf{k}\sigma}$) are (creation, annihilation) operators for conduction electrons in the Bloch state $|\mathbf{k}\sigma\rangle$, having single particle energy $\varepsilon_{\mathbf{k}}$ wave vector $\mathbf{k}$ and spin σ; H_c is the screened coulomb interaction between conduction electrons, H_{ph} is the standard phonon Hamiltonian and $H_{e-\mathrm{ph}}$ represents the electro-phonon interaction. In the pseudo-spin representation, we can write

$$H_{df} = -E_{as} \sum S^z_m - \frac{1}{2} \sum_{l,m} J_{lm} S^x_l S^x_m, \tag{3}$$

where $E_{as} = E_a - E_s > 0$ is the energy difference between the two levels at site m; and J_{lm} represents the interaction energy between distortions at site l and m. Further,

$$H_{e-df} = \sum_{\mathbf{k}-\mathbf{k}=\mathbf{q}} V_d(\mathbf{k}, \mathbf{k}')\, C^{\dagger}_{\mathbf{k}'\sigma}\, C_{\mathbf{k}\sigma}\, S^x_{\mathbf{q}}, \tag{4}$$

which involves the scattering of a conduction electron along with a change in state of the distortion field. The effective electron-electron interaction λ_d analogous to the phonon-mediated process, can be calculated by the Eliashberg procedure. We get

$$\lambda_d = N(0) \langle I_d^2 \rangle E_{as} \langle S^z \rangle / \omega_d^2, \tag{5}$$

where ω_d is the average frequency of the distortion field mode; the average $\langle I_d^2 \rangle$ being defined in the standard way. This expression should be compared with the phonon-mediated coupling constant

$$\lambda_{\mathrm{ph}} = N(0)\, \langle I^2_{\mathrm{ph}} \rangle \langle 1/M\omega^2_{\mathrm{ph}} \rangle, \tag{6}$$

ω_{ph} being the usual phonon frequency and M the mass in question. Following Vujicic *et al* (1981) the expression for T_c can be written as

$$T_c = 1{\cdot}14\, \omega_d \exp(-1/\lambda) \tag{7}$$

where

$$\lambda = \lambda_d + \frac{\lambda_{ph}}{1 - \lambda_{ph} \ln(\omega_{ph}/\omega_d)}.$$

Note that the Coulomb repulsion has been neglected inasmuch as it will be negligible owing to onsite and intersite bipolaron effects.

At this stage it is difficult to give a quantitative estimate of T_c. For a rough idea the following should be noted. We expect $\langle I_d^2 \rangle$ and $\langle I_{ph}^2 \rangle$ to be comparable. But the distortion modes are low-frequency modes and hence λ_d will be much larger than λ_{ph} (cf equations (5) and (6)). Thus this interaction via the distortion field mode will strengthen the pairing of electrons further and enhance T_c. We give below a few values calculated for a choice of parameters.

$$T_c = 36\,\text{K for } \lambda_d = 1{\cdot}5, \quad \lambda_{ph} = 0{\cdot}3, \quad \omega_d = 50\,\text{K}, \quad \omega_{ph} = 300\,\text{K},$$
$$T_c = 44\,\text{K for } \lambda_d = 1{\cdot}7, \quad \lambda_{ph} = 0{\cdot}3, \quad \omega_d = 60\,\text{K}, \quad \omega_{ph} = 300\,\text{K},$$
$$T_c = 94\,\text{K for } \lambda_d = 1{\cdot}7, \quad \lambda_{ph} = 0{\cdot}6, \quad \omega_d = 100\,\text{K}, \quad \omega_{ph} = 400\,\text{K}.$$

The last entry is appropriate for the system Y–Ba–Cu–O (Wu *et al* 1987). Thus the mechanism used in the present paper is capable of explaining the observed T_c. It should, however, be noted that the system may involve electronic and bipolaronic mechanisms also.

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