A POSSIBLE MECHANISM FOR THE RECENTLY DISCOVERED HIGH T_C SUPERCONDUCTORS

R. JAGADISH and K. P. SINHA*

Division of Physics and Mathematical Sciences, Indian Institute of Science, Bangalore 560 012, India.

ABSTRACT

A possible mechanism for high T_C superconductivity in the recently discovered systems ($La_{2-x}M_xCuO_4$, where M is Ba, Sr or Pb) is discussed. It involves virtual exchange of electronic excitations by pairing electrons.

The recent discovery of high T_c (~ 36 K or more) in doped lanthanum copper oxide systems (e.g. $La_{2-x}M_xCuO_4$, where M = Ba, Sr or Pb)[1-4] has posed a theoretical challenge towards the possible mechanisms. The usual acoustic phonon-mediated pairing mechanism sets an upper limit of 28 K[5]. In the past, various equilibrium and non-equilibrium mechanisms involving phonons, excitons, plasmons etc have been suggested[6-9]. For oxides, the polarons and bipolarons have been invoked by many authors[10, 11]. However, for understanding the mechanisms of high T_c in $La_{2-x}M_xCuO_4$ systems, we must note some special features of their structure[12]. These systems have K_2NiF_4-type structure having planes of CuO_6 octahedra which share corners. These planes are separated by (La, M) layers.

In the pure La_2CuO_4 (with copper in Cu^{2+} state, a Jahn-Teller ion) the structure has slight orthorhombic distortion. It is a semiconductor with low magnetic susceptibility (suggesting antiferromagnetic correlation). Further, $LaSrCuO_4$ is an insulator with Cu^{3+} ions in the diamagnetic state[12]. This would suggest the stabilization of the low spin state by the ligand field (or on-site bipolaron formation). The metallic behaviour of $La_{2-x}M_xCuO_4$ is thus related to the presence of both Cu^{2+} and Cu^{3+} ions. The system is anisotropic in the sense that metallic behaviour occurs only in two dimensions, comprising planes of CuO_6 octahedra.

We visualize the following energy level diagram (for notation see ref. 13). The manifolds t_2^6 and $e^2\,(3z^2-r^2)$ are localized and σ^* (derived from $e(x^2-y^2)$ and appropriate anion p orbitals) are itinerant but the band is very narrow. However, above the Fermi level (lying in the σ^* band) there are localized empty orbitals of La^{3+}, M^{2+} ions and defects. This situation can lead to an additional pairing mechanism besides the usual phonon-induced superconductivity. For this we consider the Hamiltonian,

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}\, C^+_{\mathbf{k}\sigma}\, C_{\mathbf{k}\sigma} + \sum_{m\alpha\sigma} E_{m\alpha}\, C^+_{m\alpha\sigma}\, C_{m\alpha\sigma}$$

$$+ \sum_{m_\alpha m'_\alpha \mathbf{k}\mathbf{k}'\sigma\sigma'} \Big[g^{m_\alpha m'_\alpha}_{\mathbf{k}\mathbf{k}'} C^+_{\mathbf{k}'\sigma}\, C_{\mathbf{k}\sigma}$$

$$\times\, C^+_{m'_\alpha\sigma'}\, C_{m_\alpha\sigma'} + \text{h.c.} \Big]$$

$$+ H_c + H_{\text{ph}} + H_{\text{int}}(\text{BCS}), \tag{1}$$

where ($C^+_{\mathbf{k}\sigma}$, $C_{\mathbf{k}\sigma}$) are creation and annihilation operators for conduction electrons in the Bloch state $|\mathbf{k}\sigma>$, having single particle energy $\varepsilon_{\mathbf{k}}$, wave vector $\mathbf{k}$ and spin σ; ($C^+_{m\alpha\sigma}$, $C_{m\alpha\sigma}$) and $E_{m\alpha}$ represent the corresponding entities for localized states, α being the orbital index, and m the site index. The third term is the scattering of conduction electrons along with orbital transitions of the localized electrons; $g^{m_\alpha m'_\alpha}_{\mathbf{k}\mathbf{k}'}$ is the corresponding matrix element. Further, H_c is the Coulomb interaction between conduction electrons, H_{ph} is the phonon Hamiltonian and H_{int} (BCS) is the BCS pairing interaction which is taken to be very weak for the present system.

The third term of equation (1) can be transformed using the standard method[14] to yield a BCS type pairing interaction. We get

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* For correspondence

$$-\sum \frac{2\,E_{m_\alpha m'_\alpha}\,(g_{\mathbf{kk'}}^{m_\alpha m'_\alpha})^2\langle n_{m\alpha\sigma}\rangle}{[E^2_{m_\alpha m'_\alpha}-(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k'}})^2]} \times C^+_{\mathbf{k'}\uparrow}\,C^+_{-\mathbf{k'}\downarrow}\,C_{-\mathbf{k}\downarrow}\,C_{\mathbf{k}\uparrow}\,, \qquad (2)$$

where $E_{m_\alpha m'_\alpha} = E_{m'_\alpha} - E_{m_\alpha} > 0$,

and $\langle n_{m\alpha\sigma}\rangle$ is the occupation number of the localized occupied states. As $(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k'}}) \ll E_{m_\alpha m'_\alpha}$, the pairing interaction is attractive by this mechanism also. In this limit the interaction is

$$-\sum \frac{2(g_{\mathbf{kk'}}^{m_\alpha m'_\alpha})^2}{E_{m_\alpha m'_\alpha}} C^+_{\mathbf{k'}\uparrow}\,C^+_{-\mathbf{k'}\downarrow}\,C_{-\mathbf{k}\downarrow}\,C_{\mathbf{k}\uparrow}\,, \quad (3)$$

where we have taken $\langle n_{m\alpha\sigma}\rangle = 1$. We expect $\langle E_{m_\alpha m'_\alpha}\rangle \sim 0.5$ to 1 eV and

$$\langle 2(g_{\mathbf{kk'}}^{m_\alpha m'_\alpha})^2 / E_{m_\alpha m'_\alpha}\rangle \equiv V_{\mathrm{el}}$$

exchange integral of the order of 0.1 eV. Owing to the two-dimensional nature of the band, the density of electronic states $N(\varepsilon)$ is likely to have logarithmic singularity. If the peak lies near the Fermi level, it will yield an effective $\lambda_{\mathrm{el}} = N(\mathrm{O})V_{\mathrm{el}}$, to be sufficiently strong say in the range 0.5 to 1. The expression for the superconducting temperature T_c from this mechanism is similar to the exciton mechanism. It will have the form

$$T_c \sim \theta_{\mathrm{el}} \exp\left[-\frac{1+\lambda_{el}}{\lambda_{el} - \mu^*(1+\lambda_{el})}\right], \qquad (5)$$

where $\theta_{\mathrm{el}} = \langle E_{m_\alpha m'_\alpha}\rangle / k_B$. It will be in the range of 10^3 to 10^4 K. With the Coulomb parameter μ^* around 0.1, T_c can easily reach 10^2 K or more with this mechanism.

In the present paper, we have discussed an electronic mechanism for the high T_c superconductors. The role of strong electron-phonon interaction has been taken to produce local splitting of e_g electronic states (at Cu^{2+}) and bipolaron formation at Cu^{3+} (onsite). It also reduces the intersite Coulomb interaction. The systems in question lie near metal insulator transitions arising from J-T polaron formation. The systems also show further structural instabilities, namely, from tetragonal to orthorhombic distortion when it is richer in Cu^{2+} ions. That such instabilities exist in the incipient state in the M^{2+} ion stabilized tetragonal phase can lead to yet another mechanism for high T_c superconductivity and will be discussed in another paper.

A model of a resonating valence band superconductor has also been suggested[15].

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1. Bednorz, J. G. and Müller, K. A., *Z. Phys.*, 1986, **64**, 189.
2. Uchida, S., Takagi, H., Kitazawa, K. and Tanaka, S., *Jpn. J. Appl. Phys.*, 1987, **26**, L1.
3. Chu, C. W., Hor, P. H., Meng, R. L., Gao, L., Huang, Z. J. and Wang Y. Q., *Phys. Rev. Lett.*, 1987, **58**, 405.
4. Cava, R. J., Van Dover, R. B., Batlogg, B. and Rietman, E. A., *Phys. Rev. Lett.*, 1987, **58**, 408.
5. McMillan, W. L., *Phys. Rev.*, 1968, **167**, 331.
6. Kumar, N. and Sinha, K. P., *Phys. Rev.*., 1968, **174**, 482.
7. Ginzburg, V. L. and Kirzhnits, D. A., (eds), High temperature superconductivity, Consultants Bureau, New York, 1982.
8. Sinha, K. P., *Indian J. Cryogen*, 1978, **3**, 181.
9. Sinha, K. P., *J. Low. Temp. Phys.*, 1980, **39**, 1.
10. Chakraverty, B. K., *J. Phys. (Paris) Lett.*, 1979, **40**, L99.
11. Alexandrov, A. and Ranninger, J. *J. Phys. Rev.*, 1981, **B24**, 1164.
12. Rao, C. N. R. and Ganguly, P., *Curr. Sci.*, 1987, **56**, 47.
13. Goodenough, J. B., In: *Progress in solid state chemistry*, (ed) H. Reiss. Pergamon Press, 1971. Chapter 4, Vol. 5.
14. Schrieffer, J. R., *J. Appl. Phys.*, 1967, **38**, 1143.
15. Anderson, P. W., (Preprint).