Localized and delocalized states and the properties of the normal phase of recently discovered superconductors

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The principal characteristics of the magnetic interactions have been determined in a two-band model for metal-oxide superconductors.

The extent of the relationship between the normal and superconducting properties of the recently discovered materials has not yet been clarified. Experimental studies of $La_{2-x}Sr_xCuO_y$ and $YBa_2Cu_3O_{6.5+x}$ have shown that in a "stoichiometric" composition strong Coulomb correlations leading to electron localization are present.

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Most of the theoretical studies have therefore used the Hubbard model. Since this model alone, however, could not explain the body of experimental data, in particular, the metallic nature of the conductivity in doped LaSrCuO compounds, Emery[1] suggested that the oxygen p orbitals, in addition to the $d_{x^2-y^2}$ Cu states, should be taken into account. For definiteness, we will consider below the properties of lanthanum systems and regard holes as the carriers.

The crucial factor, from our viewpoint, is the sharp change in the number of carriers in $La_{2-x}Sr_xCuO_4$, with $x \sim 0.15$, below the values corresponding to one hole per unit cell.[3] The interpretation of such a transition will be sought on the basis of the hole-spectrum model[2] which contains both localized and delocalized states. Gor'kov and Sokol[2] postulated the existence of a phonon degree of freedom Q, whose interaction $V_Q Q$ with a certain level ϵ' is strong. If a hole is situated in this level ϵ', the level will descend (the Jahn-Teller pseudoeffect) and the resultant position of the trapped electron will be $\epsilon_0 = \epsilon' - V_Q^2/2M\Omega^2(x)$. Here ϵ' corresponds to the d^{10} configuration at the Cu atom ($Q = 0$). The stiffness of the system $M\Omega^2(x)$ generally depends on the doping x. We believe that delocalized band states associated with the motion along the oxygen are present in the system. In the case of the d^{10} configuration at the Cu atom this band is half full. The hole spectrum is reckoned from the minimum at the point $p = 0$.

Since stoichiometric La_2CuO_4 is, from the experimental standpoint, an antiferromagnet, we assume that ϵ_0 lies below the conduction band, that each level is singly occupied, and that the self-trapped states are the analogs of the Hubbard centers.[4] If $\Omega(x)$ decreases with the doping, the level rises, crosses the conduction band, and may escape from it. In the last case it is entirely irrelevant. The lanthanum compounds have a phonon peak of 250 cm^{-1} for metallic samples and a phonon peak of 150 cm^{-1} in the magnetic dielectric phase (see, e.g., Ref. 5). A situation in which ϵ_0 lies above the bottom of the oxygen band was discussed by Gor'kov and Sokol.[2] Let us now consider in greater detail the case in which the electrons remain trapped, a situation which in this model would correspond to the properties of La_2CuO_4.

If the probability for the escape of an electron from the level at which it is trapped is low, this model would be equivalent to the Anderson periodic Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{p}\sigma} \epsilon_{\mathbf{p}} a^+_{\mathbf{p}\sigma} a_{\mathbf{p}\sigma} + \sum_n \{\epsilon_0 \sum_\sigma d^+_{n\sigma} d_{n\sigma} + U d^+_{n\uparrow} d^+_{n\downarrow} d_{n\downarrow} d_{n\uparrow}\}$$

$$+ \frac{V}{N^{1/2}} \sum_{\mathbf{p}n\sigma} \{a^+_{\mathbf{p}\sigma} d_{n\sigma} \exp(-i\mathbf{p}\mathbf{R}_n) + d^+_{n\sigma} a_{\mathbf{p}\sigma} \exp(i\mathbf{p}\mathbf{R}_n)\}, \qquad (1)$$

($N^{-1/2}$ is the normalization constant). According to Gor'kov and Sokol,[2] the hybridization term V is small to the extent that the formation of the local level is linked with the rearrangement of the ion subsystem. We assume that the interaction U at the center is strong.

Using this Hamiltonian and assuming the hybridization V to be small, we obtained several expressions which characterize the interactions in the localized-spin system. The s-d exchange operator is

$$\frac{V^2/N}{\epsilon_{\mathbf{p}'}-\epsilon_0}\left(\frac{1}{2}+\mathbf{S}\vec{\sigma}_{\sigma'\sigma}\right)\exp\{i\mathbf{R}_n(\mathbf{p}-\mathbf{p}')\}\,a^+_{\mathbf{p}'\sigma'}a_{\mathbf{p}\sigma}\,, \tag{2}$$

where S is the spin of the trapped electron, and $\vec{\sigma}$ are the Pauli matrices. In Eq. (2) the *s-d* coupling has an antiferromagnetic sign. The matrix element of the hop between the centers m and n is

$$t_{mn}=-\sum_{\mathbf{p}}\frac{V^2/N}{\epsilon_{\mathbf{p}}-\epsilon_0}\exp(i\mathbf{p}\mathbf{R}_{mn}). \tag{3}$$

The exchange interaction between the cells m and n $\mathscr{H}_{\text{exch}}=-\Sigma_{n\neq m}J(R_{mn})S_mS_n$,

$$J(R)=-2\sum_{\mathbf{p}}\frac{V^2/N}{\epsilon_{\mathbf{p}}-\epsilon_0}\exp(i\mathbf{p}\mathbf{R})\sum_{\mathbf{p}'}\frac{V^2/N}{(\epsilon_{\mathbf{p}'}-\epsilon_0)^2}\exp(-i\mathbf{p}'\mathbf{R})\,, \tag{4}$$

also has an antiferromagnetic nature.

The information on the properties of the ground state of the system can be obtained by refining the hole spectrum, which is assumed to be essentially two-dimensional with a minimum at the point $\mathbf{p}=0$ and a maximum at $\mathbf{p}=\mathbf{Q}_0$, where $\mathbf{Q}_0=(\pi/a,\pi/a)$; a is the lattice constant in the plane. The "effective masses" are near $\mathbf{p}=0$ and $\mathbf{p}=\mathbf{Q}_0-m_H$ and m_B, respectively, and the band width is D. The gap between the bottom of the oxygen band and the localized states is denoted by Δ. We will assume below that $V\ll\Delta\ll D\sim(a^2m_{H,B})^{-1}$.

We introduce the parameters

$$\lambda=\frac{V^2a^2m_H}{2\pi\Delta}\,,\qquad \eta=Da^2m_H/4,\qquad \nu=m_B/m_H \tag{5}$$

(for a $2D$ strong-coupling spectrum η and ν are equal to 1). For $R\gg R_0=(2m_H\Delta)^{-1/2}$ the hopping integral and the exchange integral are

$$t(R)=-\lambda\Delta(2\pi R_0/R)^{1/2}\exp(-R/R_0),\quad J(R)=-2\lambda^2\pi\Delta\exp(-2R/R_0). \tag{6}$$

The characteristic length R_0 can generally be greater than the atomic spacing. In a standard mean-field approximation, for the Néel point we find

$$T_N={}^1/_2(J(\mathbf{q}=\mathbf{Q}_0)-J(R=0))=\lambda^2\Delta(\ln(\pi^2D/8\eta\Delta)-\pi/2\eta) \tag{7}$$

[$J(\mathbf{q})$ is the Fourier component in (4)]. The logarithm in (7) stems from the assumed two-dimensional nature of the spectrum. The ground state was chosen in the form of an antiferromagnetic structure with the vector $\mathbf{Q}_0$. Above T_N the susceptibility behaves as $\chi^{-1}\sim T+\theta$, where

$$\theta=-{}^1/_2(J(\mathbf{q}=0)-J(R=0))=\lambda^2D\pi/4\eta. \tag{8}$$

In the case of small wave vectors $q\ll Q_0$ the magnon spectrum is

$$\omega(q) = (qa)\frac{\pi\lambda^2}{4\eta}\left[\frac{D\Delta}{\eta\nu}\right]^{1/2}. \tag{9}$$

The maximum magnon frequency is on the order of magnitude

$$\omega_{max} \approx \lambda^2\pi\Delta/\eta. \tag{10}$$

Assuming η and $\nu \sim 1$ (but $\Delta \ll D$), we see that the following relations hold in our case:

$$\omega_{max} < T_N < a^{-1}d\omega/dq|_0 < \theta, \tag{11}$$

in contrast with the nearest-neighbor approximation, where all these quantities are on the order of magnitude of the exchange integral, J.

The value of J was estimated experimentally to be $J \sim 1000$ K. Equations (7)–(10) thus have many parameters which can be chosen in such a way that V and Δ would still be small (and λ would be $\ll 1$). We recall that the small value of Δ is assumed to be important to the extent that the concentration interval of Sr in $La_{2-x}Sr_xCuO_4$ corresponds to $x < 0.15$.

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