Anharmonicity of oxygen vibrations and formation of highly correlated state in a high-T_c superconductor

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(Submitted 21 January 1991)
Pis'ma Zh. Eksp. Teor. Fiz. **53**, No. 5, 242–245 (10 March 1991)

A state of a pseudo-Kondo lattice in the normal phase of a high-T_c superconductor is analyzed. This state would form because of an interaction of conduction electrons with highly anharmonic atomic displacements. Magnetic correlations in this state and the effect of defects on it are discussed.

The role played by correlation effects is one of the central questions in the problem of the high-T_c superconductivity of metal oxide compounds.[1] A number of opinions have been expressed, ranging from assertions that band theory holds[2] to the postulate that the standard quasiparticle description is totally inadequate (the theory of a Luttinger liquid,[3] a marginal Fermi liquid,[4] etc.). The proximity of high-T_c superconductors to a metal–semiconductor transition, their pronounced sensitivity to doping, and several other anomalies sharply distinguish them from ordinary metallic compounds and seem to imply strong correlations. The correlations are linked with both Hubbard correlations and a magnetism,[1] on the one hand, and charge fluctuations[4] and an electron–lattice interaction under highly anharmonic conditions,[5,6] on the other. Recent EXAFS studies of $YBa_2Cu_3O_{7-\delta}$ have provided direct proof that displacements of oxygen in O4 sites play an important role for superconductivity[7] and that the oxygen vibrations are highly anharmonic.[8] Anomalies of the vibrations in the CuO_2 layers and in T_c had been observed previously[9] in experiments on ion channeling. In this letter we wish to propose a picture of a "pseudo-Kondo lattice," which ties these results together with several known features of these superconductors.

As in Refs. 6 and 10, we assume a degeneracy of the electron spectrum $\epsilon_{\vec{k}}$, which is lifted by an interaction with ion displacements q_i (a band Jahn-Teller effect). We write the Hamiltonian of this model in the form

$$H = \sum_{k\tau} \epsilon_{\vec{k}} c^+_{\vec{k}\tau} c_{\vec{k}\tau} + H_l - \sum_{i\tau\tau'} U_{\tau\tau'}(q_i) c^+_{i\tau} c_{i\tau'} \,, \qquad (1)$$

where the operator $c^+_{\vec{k}\tau}$ creates an electron with a band index (a pseudospin projection) $\tau = \pm$ (for brevity, we omit the spin indices), H_l is the Hamiltonian of the system of interacting ions in the anharmonic potential $V(q_i)$, and $\hat{U}(q_i)$ is the matrix of the electron–lattice interaction at site i. In calculating the electron Green's function $G_{\vec{k}\tau}(E)$ in a perturbation theory in $\hat{U}$, we find "pseudo-Kondo" terms on the order of $U^2 \ln|D/(E-\omega_{\mu\nu})$, where D is the width of the electron band, E is reckoned from E_F, and $\omega_{\mu\nu}$ are the frequencies of transitions between the levels of the potential $V(q)$. We assume that the frequency of the transition from the ground state $|0\rangle$ to the first excited state is much lower than the other frequencies $\omega_{\mu\nu}$. This case is possible in two-well potentials (for O4 ions, we have $\omega_{10} \sim 10^2$ K and $\omega_{21} \gtrsim 10^3$ K according to Ref. 8). At an energy scale $\omega_{10} \lesssim |E| \ll \omega_{21}$ we can thus go over to a pseudospin model, introducing the operators $S_i^+ = |i0\rangle\langle i1|$, $S_i^z = 1/2(|i0\rangle\langle i0| - |i1\rangle\langle i1|)$, and reducing the last term in (1) to the form

$$H_{int} = -I_{\alpha\beta} \sum_{i\tau\tau'} c^+_{i\tau} \sigma^\alpha_{\tau\tau'} c_{i\tau'} S^\beta_i \,, \qquad (2)$$

where $\hat{I}$ is the matrix of "exchange" parameters, which is expressed in terms of $\hat{U}$, and $\hat{\vec{\sigma}}$ are the Pauli matrices. Analyzing model (1), (2) in the parquet approximation, we can show that a perturbation theory breaks down at a characteristic energy $|E| = T_K$ (the "Kondo temperature"), which is determined by the condition for a pole in the scattering matrix:

$$\det \| \delta_{\tau\tau'} \delta_{\alpha\beta} + i\epsilon_{\lambda\alpha\beta} I_{\gamma\lambda} \sigma^\gamma_{\tau\tau'} \rho \ln(D/T_K) \| = 0, \qquad (3)$$

where $\epsilon_{\alpha\beta\gamma}$ is the Levi-Civita density, and R is the density of states at E_F. For an isotropic s–d model ($I_{\alpha\beta} = I\delta_{\alpha\beta}$), Eq. (3) gives us the usual results $T_K = D\exp(1/2I\rho)$. It is legitimate to ignore the dynamics of the pseudospins if T_K

$>\overline{\omega}$, where $\overline{\omega}$ is a characteristic frequency of ion excitations (ω_{10}, renormalized by the ion–ion interaction).

By analogy with the *s–d* model, we would expect the formation of a highly correlated state of the pseudospin-liquid type below T_K. The properties of this state, including its superconductivity, can be described by (for example) the functional-integration method.[11] The basic results are a hybridization of conduction electrons with Abrikosov pseudofermions which arise upon the "dismantling" of the pseudospins and the appearance of peaks in the density of states in the energy spectrum near E_F, with a scale value T_K. The residue of the Green's function of the Fermi excitations at the pole is $Z \sim (T_K/D) \ll 1$. Much of the spectral density is determined by cuts and in this sense is of a nonquasiparticle nature. By analogy with the RVB theory, the pseudofermions may be pertinent to the problem of the anomalous linear term in the specific heat of the high-T_c superconductors.

A value of T_K for $YBa_2Cu_3O_{7-\delta}$ can be estimated[6] from the behavior of the thermoelectric power $\alpha(T)$; the result is $T_K \gtrsim 10^2$ K at $\delta \simeq 0.5$. Assuming that the interaction of the current carriers in the CuO_2 plane with O4 ions is important, and taking account of the decrease in the ion–plane distance with decreasing δ (Ref. 7), we are forced to conclude that T_K is even higher for compositions with $T_c \simeq 90$ K ($\delta \simeq 0$). At temperatures below room temperature, we are thus dealing with a highly correlated pseudo-Kondo state. The interaction with electrons weakens the original two-well shape of $V(q)$ (as in the Kondo cancellation of magnetic moments). The on-center distance between the wells should decrease as T is lowered to T_c and should then rise because of a suppression of the Kondo effect by the superconducting gap at E_F. Specifically, this behavior was observed in Ref. 8.

A distinctive feature of this state is its pronounced lability. Small changes in $V(q_i)$ cause an ion to acquire a non-Kondo nature, since an increase in the frequency ω_{10}, which depends very strongly on the barrier between the wells, cuts out the Kondo divergences, while a decrease in this frequency implies a simultaneous decrease in the parameters $I_{\alpha\beta}$, which are responsible for scattering with tunneling. Accordingly, one defect can suppress the Kondo effect throughout the region, by working through long-range elastic distortions. At the same time, a replacement of the Kondo center by an ordinary center would create the strongest local perturbation of the electron system (the phase shift for Kondo scattering at E_F is $\pi/2$).

These arguments explain the pronounced sensitivity of the properties of $YBa_2Cu_3O_{7-\delta}$ to nonmagnetic impurities and irradiation. In particular, the growth in the linear term in the specific heat to values comparable to those characteristic of heavy-fermion systems upon doping with zinc[12] can be interpreted as a decrease in the "average" T_K. The thermoelectric power increases, as would be expected.[13] We also note that there is a sharp decrease in the anisotropy of the resistivity, ρ_c/ρ_{ab}, upon neutron bombardment near the metal–semiconductor transition,[14] where ρ_c is determined by hopping between planes. In a highly correlated state, the probability for such hops contains a factor $Z^2 \propto (T_K/D)^2$ ($Z^{1/2}$ represents a renormalization of the wave function). This suppression is a consequence of Anderson's orthogonality catastrophe (the decrease in the probability for the disappearance or appearance of an electron in the plane as a result of the relaxation of a many-electron system). During bombardment, the pseudo-Kondo state is destroyed, and ρ_c/ρ_{ab} approaches the value determined exclusively by the bare electron spectrum.

The restructuring of the electron spectrum, accompanied by the formation of an energy scale $T_K \ll D$, radically changes in the way the current carriers affect magnetic interactions in the system. The exchange interaction in CuO_2 planes is strong ($J \sim 10^3$ K), and we can assume $T_K \lesssim J \ll D$. In the ordinary Hubbard situation, the current carriers would lead to a "double exchange" and would cause a tendency toward a ferromagnetism, but no such tendency is actually observed in the high-T_c superconductors. The renormalization of the spectrum causes the current carriers to become slow (an "antiadiabatic" regime), and it may lead to a change in the sign of certain exchange integrals (e.g., it may convert the antiferromagnetic superexchange into a ferromagnetic one upon a "static" change in the oxygen valence). In other words, they may lead to frustrations. "Slow" electrons of this sort should promote the formation of an RVB state in the t–J model (Ref. 15, for example).

Analysis of the entire set of experimental data reveals several analogies among the high-T_c superconductors, heavy-fermion superconductors, and compounds with the A 15 structure.[16] The implication is that the final state in all these systems is highly correlated and has features of a Kondo lattice, which arises as a result of either magnetic interactions (as in the heavy-fermion superconductors) or electron–lattice interactions (as in the A 15 superconductors[10]). We believe that the high-T_c superconductors are distinguished by the coexistence and mutual effects of the two types of correlations. The latter circumstance is seen, for example, in the ease with which "free" magnetic moments form during irradiation[14] or doping,[17] i.e., upon a disruption of the pseudo-Kondo state.

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Translated by D. Parsons