Possible analogies between perovskite superconductors and heavy-fermion superconductors

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The coupling of electrons with anharmonic phonons in high-temperature superconductors is described by a Kondo-lattice Hamiltonian.

Calculations of the phonon spectra of Y–Ba–Cu–O and La–Cu–O compounds from first principles indicate that their orthorhombic phase contains an unstable phonon mode which is coupled with sliding motions of ions in the *xy* plane and which has an extremely slight dispersion.[1] All of these calculations have been confirmed well experimentally for La_2CuO_4 (Ref. 2). Evidence in favor of a phonon mode with a slight dispersion comes from the structural disorder which is observed[3] in Y–Ba–Cu–O down to $T = 4.2$ K. Neutron-diffraction studies indicate a pronounced anharmonicity in these compounds.[4] On the basis of these calculations and experimental data, it was assumed in Refs. 1, 5, and 6 that some of the oxygen ions in these compounds are in two-well potentials which overlap each other slightly. Judging from the pronounced anharmonicity, a slightly split lower phonon level in this well is not far from the central hill of the well—perhaps a hundred degrees away. It was suggested in Refs. 5 and 6 that the high value of T_c in perovskite superconductors results from a strong electron-phonon coupling, which in turn arises because of a pronounced deformation susceptibility of two-well oscillators.

I agree completely with this point of view, but I would like to clarify several details and point out some far-reaching analogies. The effect of electrons on the tunneling of an ion from well to well was ignored in Refs. 5 and 6. Without such an effect, the tunneling would be exceedingly slight, because of the large mass of the oxygen ion, and there would be no pronounced response. Since the height of the barrier is apparently small, however, the conduction electrons may substantially "assist" the tunneling, by lowering the barrier. This circumstance dramatically changes the entire physical picture of the effect.

I will describe a high-temperature superconductor with the model which was proposed in Ref. 7 to describe the electron-phonon coupling in a strongly anharmonic crystal, but I will add to that model a term which describes a tunneling of an ion from well to well in a process involving conduction electrons. In this form, the model has been used to describe the interaction of electrons with two-level systems in metallic glasses.[8] The Hamiltonian of the model is

$$\mathcal{H} = \mathcal{H}_e + \mathcal{H}_{ph} + \mathcal{H}_{ph-e}, \tag{1a}$$

$$\mathcal{H}_{ph} = \Omega \sum_n S_n^x, \tag{1b}$$

$$\mathcal{H}_e = \sum_{k,\sigma} \epsilon_k c^+_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \tag{1c}$$

$$\mathcal{H}_{ph-e} = \sum_{n,\sigma,k_1,k_2} V^\alpha(\mathbf{k}_1 - \mathbf{k}_2) S_n^\alpha c^+_{\mathbf{k}_1\sigma} c_{\mathbf{k}_2\sigma}, \tag{1d}$$

where S_n^α ($\alpha = x,y,z$) are spin-1/2 matrices at site n. These matrices act in the space of those states of an ion which correspond to its presence in one well or the other of a two-well potential.

From the requirement that Hamiltonian (1) be invariant under time reversal we find $V^y = 0$. The presence of two noncommuting terms, V^x and V^z, in the interaction Hamiltonian makes the scattering a nontrivial matter. As was shown in Ref. 9, the single-ion problem reduces to a two-channel Kondo model in which electrons with a pseudospin of 1/2 carry an additional index, which corresponds to ordinary spin, which is conserved during scattering. Model (1) is thus a model of a Kondo lattice, but one with an anisotropic interaction. We know that dense Kondo systems are frequently superconductors (see, for example, the review by Stewart[10]). The superconducting transition temperature in them is lower than the Kondo temperature by a factor of only a few units. I think that perovskite superconductors differ from heavy-fermion superconductors in that they have a high Kondo temperature. The large electrical resistance in the normal phase of a perovskite superconductor can be attributed to a pronounced Kondo scattering, and the absence of a minimum on the temperature dependence of the resistance can be attributed to a high Kondo temperature.

A picture of the low-energy behavior of model (1) can be drawn on the basis of the single-ion version of this model. In this case the model simplifies dramatically,[8,9] effectively reducing to a one-dimensional model. It is necessary to expand the fermion operators in a basis chosen in a certain way and consisting of linear combinations of spherical harmonics. It then turns out that only two vectors of this basis interact with an ion (this situation corresponds to an electron pseudospin of 1/2). Hamiltonian (1) takes the form

$$\mathcal{H} = \Omega S^x + \sum_{k,\sigma,a} k c^+_{k\sigma a} c_{k\sigma a} + \sum_{k,p,\sigma} v_0^\alpha S^\alpha c^+_{ka\sigma} \sigma^\alpha_{ab} c_{pb\sigma} . \tag{2}$$

Model (2) is integrable if $v_0^x = v_0^y$ and $\Omega = 0$. In our case we have $v_0^y = 0$, but a renormalization-group analysis shows[8] that the constant v_0^y, which arises from the renormalization, becomes comparable to v^x as early as $(1/\pi)\ln \Lambda/T \sim 1/v_0^z$ (Λ is the high-energy cutoff). Because of the renormalization, the effective splitting $\Omega(T)$ also decreases:

$$\Omega(T) = \Omega \exp\left(-\frac{(v_0^x)^2}{4\pi v_0^z}\left(\frac{\Lambda}{T}\right)^{2v_0^z/\pi}\right). \tag{3}$$

[As we mentioned earlier, a direct tunneling from well to well could hardly lead to a value of Ω greater than a fraction of a degree. Expression (3) shows that even if there is some seed value of Ω, stemming from some nonelectronic mechanisms which I have not considered here, it would be suppressed in the limit $T \to 0$.]

The susceptibility of the ion increases in the limit $T \to 0$:

$$\chi = \frac{1}{\pi^2 T_K} \ln(T_K/T) \tag{4}$$

[this expression also follows from an exact solution of model (2) and is written here without derivation]. This growth intensifies the electron-phonon coupling and thus the electron-electron coupling. The Kondo temperature T_K is expressed in terms of the coupling constants in the following way:

$$T_K = \Lambda v_0^x (v_0^x / v_0^z)^{\pi/2v_0^z} , \tag{5}$$

where v_0^x and v_0^z are dimensionless constants, i.e., the interactions multiplied by the state density at the Fermi surface. Since we have $v_0^z \sim d$ (d is the distance between wells), and since we have the estimates $d \sim 0.2$–0.3 Å from Ref. 5 for a perovskite superconductor, the value of v_0^z may be ~ 1. The constants cannot be estimated in greater detail until detailed calculations of the electron-phonon coupling have been carried out.

The overall picture of the establishment of superconductivity seems to be as follows: At $T \lesssim T_K$ a polaron band of width $\sim T_K$ forms near the Fermi surface. Excitations in this band interact with each other through the polarization of ion centers. Since the interaction is a local one, it does not depend strongly on the purity or degree of order of the sample. The effective electron coupling constant is apparently $\lambda \sim 1$, as in a heavy-fermion superconductor. A high value of T_c is reached by virtue of the high value of T_K.

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