Interaction of conduction electrons with "ferroelectric" displacements in high-T_c superconductors and titanium alloys: pseudospinons

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A model of a conducting "pseudospin ferromagnet" is proposed. It describes the interaction of electrons with coherent atomic displacements. Nonquasiparticle current-free states (pseudospinons) can contribute a component of the electron specific heat which is linear in T. The possibility of a restructuring of the spectrum near E_F, accompanied by the formation of a new energy scale of the Kondo-temperature type, is demonstrated.

Recent experimental data point to the existence of a ferroelectric polarization (i.e., corrlated lattice distortions) over large regions in the high-T_c superconductors[1,2] and also in Ti- and Zr-based alloys.[3] The closest results in this connection is the observation of a huge absorption of a microwave field.[1,3] A dipole polarization coexists with a metallic conductivity. This circumstance may lead to a radical restructuring of the electron spectrum, as we will show below.

A "local" dipole moment arises because the effective potential goes through several minima as a function of the displacements. For the high-T_c superconductors the existence of such potentials follows from a band calculation of La_2CuO_4 (Ref. 4) and a model-based analysis of $YBa_2Cu_3O_7$ (Ref. 5). For the alloys of Ti and Zr, it follows from experiments which indicate local distortions (Mössbauer spectra of $Ti_{1-x}Fe_x$;

Ref. 6) and also two-level systems.[7] The latter are described on the basis of a pseudospin formalism, while the dipole polarization in large regions is described as a "pseudoferromagnetism." We will discuss here a situation which corresponds to a Jahn-Teller band effect,[8] which has a degeneracy in the conduction band which is described by a projection of the electron pseudospin, $\tau = \uparrow, \downarrow\ (\pm)$, and which is lifted by atomic displacements; this is the actual situation in La_2CuO_4 (Ref. 4). Taking into account pseudospin-flip processes, which make the singular contributions in which we are interested here, we can then write the Hamiltonian of the model in the form

$$H=\sum_{\mathbf{k}\tau}\epsilon_{\mathbf{k}}c^+_{\mathbf{k}\tau}c_{\mathbf{k}\tau}+H_s-\sum_i[(J_\perp s^+_i c^+_{i\downarrow}c_{i\uparrow}+\tilde{J}_\perp s^+_i c^+_{i\uparrow}c_{i\downarrow})+\text{Herm. adj.}$$
$$+J_\parallel s^z_i(c^+_{i\uparrow}c_{i\uparrow}-c^+_{i\downarrow}c_{i\downarrow})]$$

(H_s is the Hamiltonian of the pseudospin subsystem). We will not discuss the term with $\tilde{J}_\perp$ below, since it makes additive contributions $(J_\perp\to\tilde{J}_\perp,\ \tau\to-\tau,\ J_\parallel\to-J_\parallel)$. A calculation of the one-electron retarded Green's function in second order in $J_\perp$ yields

$$\langle\langle c_{\mathbf{k}\tau}|c^+_{\mathbf{k}\tau}\rangle\rangle_E=[E-\epsilon_{\mathbf{k}\tau}-\Sigma^\tau_{\mathbf{k}}(E)]^{-1},\qquad \epsilon_{\mathbf{k}\tau}=\epsilon_{\mathbf{k}}-\tau J_\parallel\langle s^z\rangle,$$

$$\Sigma^\tau_{\mathbf{k}}(E)=J_\perp^2\sum_{\mathbf{q}}\int_{-\infty}^{\infty}d\omega K^{-\tau,\tau}_{\mathbf{q}}(\omega)\frac{N_B(\omega)+f(\epsilon_{\mathbf{k}+\mathbf{q},-\tau})}{E-\epsilon_{\mathbf{k}+\mathbf{q},-\tau}+\omega},\quad K^{-\tau,\tau}_{\mathbf{q}}(\omega)=-\frac{1}{\pi}\,\mathrm{Im}\,\langle\langle s^\tau_{\mathbf{q}}|s^{-\tau}_{-\mathbf{q}}\rangle\rangle_\omega,$$

where $N_B(\omega)$ and $f(E)$ are Bose and Fermi functions. The contribution to the spectral density $\delta K^{-+}_q(\omega)=2\langle s^z\rangle\delta(\omega-\omega_q)$, which corresponds to a collective "pseudomagnon" mode $\omega_{\mathbf{q}}$, gives rise to a singular contribution $\delta\mathrm{Re}\Sigma(E)\sim\ln(E^2+\bar{\omega}^2)$ and to a one-sided "nonquasiparticle" contribution to the state density which changes sharply near E_F (over an interval on the order of the characteristic $\bar{\omega}$) (cf. the discussion of the *s-d* model in Ref. 9):

$$\delta N_\tau(E)=-\frac{1}{\pi}\sum_{\mathbf{k}}(E-\epsilon_{\mathbf{k}\tau})^{-2}\,\mathrm{Im}\Sigma^\tau_{\mathbf{k}}(E),$$

$$\delta N_\tau(E\to0,T=0)\sim2\langle s^z\rangle J_\perp^2\rho_{-\tau}|E|^{1+\alpha}\theta(-\tau E).$$

Here ρ_τ is the density at E_F in the Hartree-Fock approximation, and the quantity α is determined by the behavior of the spectral density averaged over $\mathbf{q}$ as $\omega\to+0[K^{-+}(\omega)\sim\omega^\alpha]$. Although we have $\delta N_\tau(0)=0$ at $T=0$, this contribution gives rise to a correction to the linear term in the specific heat because of the temperature dependence of the Fermi function in Σ:

$$\delta C(T)=\frac{\partial}{\partial T}\int dEEf(E)N(E)-\frac{\pi^2}{3}N(0)T=\int dEEf(E)\frac{\partial N(E)}{\partial T}.$$

Only nonquasiparticle states with $\tau=\uparrow$ contribute to the linear term, since they are filled. At $J_\parallel<0$, for example, we have the following result in the "saturated" case $[2|J_\parallel|\langle s^z\rangle>E_F$, so that $N_\uparrow(0)=0]$:

$$\delta C(T) = C_{\uparrow}(T) \approx \frac{2\pi^2}{3} T\rho_{\downarrow} J_{\perp}^2 \langle s^z \rangle \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}\uparrow} - E_F)^{-2}.$$

When the potential impurity scattering is taken into account, the sharply altered contribution $\delta N_{\tau}(E)$ makes corrections to the resistance and the thermal emf which are proportional to $T^{1+\alpha}$. Nonquasiparticle states are current-free, since the corresponding correction to the distribution, $\langle c_{k\tau}^{+} c_{k\tau} \rangle$ depends only weakly on $\mathbf{k}$ (Ref. 10). The states which we are discussing here, and which are described by a cut of the Green's function (these states were discussed in Ref. 11 in the Hubbard model with strong correlations), thus play a role which is largely analogous to the role played by Anderson spinons.[12] They might be called "pseudospinons." One can show that in a superconducting phase there pseudospinons would give rise to a gapless superconductivity at finite T; this effect could explain data on nuclear spin-lattice relaxation in the high-T_c superconductors (Ref. 13, for example).

At small values of $\bar{\omega}$, higher orders in $\hat{J}$ must be taken into account. A summation of the "parquet" sequence to the following results if we ignore the pseudospin dynamics:

$$\Sigma_{\mathbf{k}}^{\tau}(E) = \frac{2\tau \langle s^z \rangle J_{\perp}^2 R_{\tau}(E)}{1 + J_{\parallel} R_{\tau}(E)}, \qquad R_{\tau}(E) = \sum_{\mathbf{q}} \frac{f(\epsilon_{\mathbf{q}\tau - \tau}) - \delta_{\tau\downarrow}}{E - \epsilon_{\mathbf{q}\tau - \tau}}.$$

Because of the logarithmic divergence of $R_{\tau}(E \rightarrow 0)$, the quantity Σ diverges at

$$|E| = T_K^{\tau} \approx W \exp(1/J_{\parallel}\rho_{-\tau}), \quad J_{\parallel} < 0$$

(W is on the order of the band width). As $E \rightarrow \tau T_K^{\tau}$ we have

$$\Sigma_{\mathbf{k}}^{\tau}(E) = (V_{\tau}^{ef})^2/(E - \tau T_K^{\tau}), \qquad (V_{\tau}^{ef})^2 = 2\langle s^z \rangle (J_{\perp}/J_{\parallel})^2 T_K^{\tau}/\rho_{-\tau},$$

so a gap forms in the spectrum. This gap corresponds to an effective hybridization parameter V_{τ}^{ef}. Depending on the ratio $J_{\perp}/J_{\parallel}$, this gap may either go to E_F or lie near E_F. Like the criterion for the suppression of the RKKY interaction in lattice Kondo theory, the condition for the occurrence of a divergence is of the form $T_K^{\tau} > \bar{\omega}$.

The narrow peaks of a many electron but nonmagnetic nature which appear at the edges of the gap explain the large values ($\sim 100\,\mu V/K$) and nonmonotonic dependence of the thermal emf $S(T)$ in $YBa_2Cu_3O_{6+x}$ $(0.45 < x < 0.65)$ (Ref. 14) and $La_{2-x}Sr_xCuO_4$ (Ref. 15). The energy scale of the peak which would be required to explain the $S(T)$ behavior is very small (~ 100 K; Ref. 14), and the Pauli part of the magnetic susceptibility $\gamma(x)$ in $YBa_2Cu_3O6 + x$ exhibits no anomalies in this region of compositions.[16] The peak thus could not be of one-electron origin [the many-electron amplification factor $(1 - \partial\Sigma/\partial E)$ appears in S but not in χ]. On the other hand, the renormalization of the spectrum could not be a conseqence of spin fluctuations, since if it were, then χ would take on huge values, as S does. Also indicating a nonmagnetic nature of the peak is the weak field dependence of S (Ref. 15).

In our analysis we include, in addition to the states $c_{\mathbf{k}\tau}^{+}$ "normal" electron states $a_{\mathbf{k}}^{+}$ and the matrix elements representing the hybridization between these groups of states, V_τ. Under conditions corresponding to a restructuring of the spectrum, the Green's function of the a-electrons takes the form characteristic of the ordinary hybridization model, with the substitution $V_\tau^2 \to Z_\tau V_\tau^2, Z_\tau \sim T_K^\tau |E_F \ll 1$. The hybridization of the a-electrons and the c-electrons is thus suppressed. This suppression can be explained in a graphic way in terms of Anderson's orthogonality catastrophe[17]: A transition of an electron from a c-state which is strongly coupled with pseudospins to a weakly coupled a-state causes a sharp restructuring of the entire electron system. The existence of essentially independent electron subsystems in high-T_c superconductors is indicated by data on the thermal conductivity at $T \lesssim 1$ K (Ref. 18), according to which some of the electrons do not participate in superconducting pairing even in the ground state.

It is possible that the restructuring of the electron spectrum of titanium alloys as the result of a transition to a "Kondo" regime corresponds to an electronic phase transition (e.g., at 7% Fe in the $Ti_{1-x}Fe_x$ system).[19,20] Such a transition would be characterized , in particular, by a sharp increase in the resistence, the appearance of a "pseudogap" near E_F, and the appearance of an anomalous magnetoresistance $\Delta R(h)/R \sim \pm (\mu_B h |/E^*)^2$, where E^* is a scale value for the energy dependence of the conductivity. From the experimental data of Ref., 20 we reach the estimate $E^* \sim 10^2$–10^3 K. An even more important consequence of the model is the suppression of hybridization, which apparently underlines the "coexistence" of localized and delocalized states in Ti alloys.[20,21]

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