Possible mechanism for a nonphonon superconductivity in Kondo lattices

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A possible nonphonon mechanism for superconductivity in materials of the $CeCu_2Si_2$ type is described. This mechanism is based on a combination of a Kondo effect and an indirect exchange interaction.

For the past few years, physicists have been studying unusual superconducting systems with heavy fermions.[1] Interpretations of the properties of these superconductors have been proposed in several papers.[2–4] Anderson[2] and others have called attention to the possibility of a nonphonon mechanism for the effective attraction of electrons in these systems. So far, there has been no description of a microscopic origin of a nonphonon mechanism in these systems. Our purpose in the present letter is to partially fill this void.

The localization and delocalization of f electrons and the appearance of heavy quasiparticles and a local magnetic moment in a system such as $CeCu_2Si_2$ are conveniently described by the Anderson lattice model. We consider two bands of valence

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electrons and f electrons, for which we ignore the orbital degeneracy for simplicity:

$$H = \sum_{\mathbf{k},j,\sigma} \epsilon_{\mathbf{k}j} c^{+}_{\mathbf{k}j\sigma} c_{\mathbf{k}j\sigma} + \sum_{\mathbf{k},j,\sigma,n} V_{\mathbf{k}nj}(c^{+}_{\mathbf{k}j\sigma} f_{n\sigma} + \text{h.c.}) + U \sum_{n} n_{n\uparrow} n_{n\downarrow} + E_f \sum_{n,\sigma} n_{n\sigma}, \tag{1}$$

where $\epsilon_{\mathbf{k}j}$ is the energy of the jth band, $c^{+}_{\mathbf{k}j\sigma}$ and $c_{\mathbf{k}j\sigma}$ are the operators that create and annihilate valence electrons, $f^{+}_{n\sigma}$ and $f_{n\sigma}$ are the corresponding operators for f electrons at the n-th f atom, the $V_{\mathbf{k}nj}$ are mixing parameters, U is the energy of the Coulomb repulsion of the f electrons, and E_f is the energy of their local level. A Schrieffer-Wolff canonical transformation[5] converts this Hamiltonian into the Hamiltonian of a Kondo lattice. We ignore the other terms of the new Hamiltonian. Here and below, we assume that the parameter values in (1) are such that localized spins exist at f atoms, i.e., such that these spins correspond to an integer valence of the f ions. This assumption is probably valid[6] for $CeCu_2Si_2$; the valence in UBe_{13} and UPt_3 is probably not an integer value.[7] The Kondo lattice for the spins at f atoms is described by the following Hamiltonian for the case with two valence electron bands:

$$H' = \sum_{\mathbf{k},j,\sigma} \epsilon_{\mathbf{k}j} c^{+}_{\mathbf{k}j\sigma} c_{\mathbf{k}j\sigma} + \frac{1}{2} \sum_{j,n,\alpha,\beta} J_j \mathbf{S}_n \, (c^{+}_{njx} \vec{\sigma}_{\alpha\beta} c_{nj\beta}), \tag{2}$$

where $J_j \cong |V_{k_{Fj}}|^2 [U/|E_f|(E_f + U)] > 0$ for momenta at the Fermi surface, and $V_{\mathbf{k}nj} \equiv e^{i\mathbf{k}\mathbf{R}_n} V_{\mathbf{k}j}$. As was shown in Ref. 3 (and several other papers), in the case of a single band there is a critical value J_c such that for a system with $J > J_c$ the ground state at low temperatures is a singlet Kondo state. At $J < J_c$ this state is antiferromagnetic. We assume here that these results can be extended to the case of the Kondo lattice, with two valence electron bands. If the mixing parameter $V_{K_F 1}$ for the first band has a magnitude corresponding to $J_1 > J_c$, while that for the second band has a magnitude corresponding to $J_2 < J_c$, then even at very low temperatures the effective value of J_1 increases, to $J_1 \gg J_c$, while that of J_2 decreases, so that we have $J_2 \ll J_c$. Photoemission spectra indicate the presence of pronounced hybridization.[9] Consequently, the conduction electrons of the second band are responsible for the magnetic interaction (indirect exchange between localized spins at f atoms) in our model, and the electrons of the first band are scattered by these localized spins. The effective Hamiltonian describing this behavior of the system is found in the standard way from (2); it is

$$H'' = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}1} c^{+}_{\mathbf{k}1\sigma} c_{\mathbf{k}1\sigma} + \frac{J_1}{2} \sum_{n,\alpha,\beta} \mathbf{S}_n (c^{+}_{n1\alpha} \vec{\sigma}_{\alpha\beta} c_{n1\beta}) + \frac{K}{z} \sum'_{n,n'} \mathbf{S}_n \mathbf{S}_{n'}, \tag{3}$$

where $K \cong |J_2|^2 f_{RKKY}(k_F r_{spin\text{-}spin})$. In the last term in (3), we have considered only the interaction of nearest neighbors (f atoms). As we have already mentioned, we are assuming that at low temperatures the first band is in a singlet Kondo state and that we have $J_1 \gg J_c$. In this case, of all possible states of the system that are described by (3) only those occur for which the localized spin S_n is completely screened by the spins of the conduction electrons of the first band. For these states we can write $\mathbf{S}_n$

$\equiv -(1/2)(c^+_{n1\alpha}\sigma_{\alpha\beta}c_{n1\beta})$, and from (3) we find a paramagnetic effective Hamiltonian (here and below, we omit the index 1 specifying the first band):

$$H''' = \sum_{k,\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} + \frac{K}{4z} \sum_{n,n',\alpha,\beta,\gamma,\delta}{}' (c^+_{n\alpha} \vec{\sigma}_{\alpha\beta} c_{n\beta})(c^+_{n'\gamma} \vec{\sigma}_{\gamma\delta} c_{n'\delta})$$

$$= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^+_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2\nu} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\alpha,\beta,\gamma,\delta} V^{\alpha\beta\gamma\delta}(\mathbf{q})\, c^+_{\mathbf{k}\alpha} c_{\mathbf{k}+\mathbf{q}\beta} c^+_{\mathbf{k}'\gamma} c_{\mathbf{k}'-\mathbf{q}\delta}, \qquad (4)$$

where the interaction energy is

$$\gamma(\mathbf{q}) = \frac{1}{z} \sum_{n'}{}' \exp(i\mathbf{q}(\mathbf{R}_n - \mathbf{R}_{n'})), \quad V^{\alpha\beta\gamma\delta}(\mathbf{q}) = \frac{K\rho\gamma(\mathbf{q})}{2} \vec{\sigma}_{\alpha\beta} \vec{\sigma}_{\gamma\delta}, \quad \rho = \nu/N. \qquad (5)$$

The crystal symmetry of the system is incorporated here in the particular form of the function $\gamma(\mathbf{q})$. The interaction of phonon origin has been omitted from (5). In the weak-coupling approximation, and in the isotropic-medium approximation [in which we have $\gamma(\mathbf{q}) \to (1/4\pi) \int d\Omega_\delta \exp(i\delta\mathbf{q}) \equiv \gamma_i$] by the Gor'kov method[10] we find that a singlet phase occurs for the antiferromagnetic spin coupling ($K>0$). If we had $\gamma_1 K<0$ in the expansion $\gamma_i(\mathbf{p}_1 - \mathbf{p}_0) \approx \gamma_0 + \gamma_1 \hat{\mathbf{p}}_1 \hat{\mathbf{p}}_0 + \ldots$, the Anderson–Brinkmann-Morel model phase of the triplet state would be preferable. The high-temperature properties of the magnetic susceptibility are evidence[1] for $K>0$. In the isotropic approximation, using typical values for the constants of the materials $CeCu_2Si_2$, UBe_{13}, UPt_3, U_6Fe, and U_2PtC_2 from the literature,[1,11] we find $\gamma_0>0$ and $\gamma_1>0$. The superconducting gap for the singlet phase at $T=0$ is $\Delta_{\text{SING}}(0) = 2k_B T_K \times \exp[-(4/3K\rho\gamma_0 N_F)]$, where T_K is the Kondo temperature, $\rho = \nu/N$ is the volume per f atom, and N_F is the state density of electrons with $\epsilon \approx \epsilon_F$. Preliminary calculations outside the isotropic approximation, which explicitly incorporate the effects of the crystal symmetry, indicate that a superconducting gap of this type depends on the direction in the crystal: In certain directions, there is no superconducting gap. The gap and the critical temperature are very sensitive to the value of the exchange integral and also to a disorder in the arrangement of atoms.

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