Effect of Anderson impurities with a strong local electron-phonon coupling on the superconducting transition temperature

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Quasistationary impurity electronic states which are coupled with local lattice vibrations are analyzed in the Anderson model. The theory of a Fermi liquid is used to calculate T_c. If the coupling constant describing the coupling of the impurity states with the vibrations is sufficiently large, even a small impurity concentration may cause a significant increase in T_c. The isotopic effect does not correspond to the BCS theory. Some consequences of the model for high-temperature superconductors are discussed.

The Hamiltonian of an individual impurity is

$$H = \Sigma \epsilon_k n_{k\sigma} + \Sigma \epsilon n_\sigma + \Sigma (V C^+_{k\sigma} a_\sigma + \text{H.a.}) + U n_\uparrow n_\downarrow + \alpha \Sigma n_\sigma q + \frac{M g^2}{2} + M \omega_0^2 \frac{q^2}{2}. \quad (1)$$

The first four terms in H are the standard Anderson Hamiltonian.[1] The fifth describes

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the coupling of electrons with local vibrations. For simplicity, only a single vibrational degree of freedom has been taken into account. The impurity level is assumed to be nondegenerate.

Let us assume $\Gamma \gg \omega_0$, where $\Gamma = \pi|V|^2 N(0)$ is the width of the quasistationary impurity level [$N(0)$ is the state density at the Fermi surface]. As was shown in Ref. 2, an oscillator experiences an instability in the adiabatic approximation with $\xi \equiv \alpha^2/M\omega_0^2\Gamma = \xi_c$. The quadratic term disappears from the potential energy, and a two-well adiabatic term forms as ζ is increased further. Depending on the value of ϵ, the potential well may be either symmetric or asymmetric. The value of ζ_c is determined by the charge susceptibility at zero frequency. It is easy to show that we have $-4\xi_c\chi_{ch}(\epsilon_0) = 1$ and that ϵ_0 is the point at which $\chi_{ch} = -(1/4)d\langle n\rangle/d\epsilon$ reaches its maximum ($\langle n\rangle = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle$). An exact solution[1] of the Anderson model yields the values of χ_{ch} for large values of U, which are always characteristic of states with an atomic localization scale. To the extent that a two-well term forms, the adiabatic approximation breaks down, because of the Kondo effect which results from a tunneling of the system between two states and the low-frequency response of the electron subsystem to this motion. The situation is analogous to that which was studied in Ref.3, although the initial Hamiltonian there is not the same as (1). In the symmetric case, the electron subsystem undergoes quantum oscillations between two degenerate states, which differ in the number of electrons in a local level. Under the condition $U \gg \Gamma$, the behavior of the system is determined by a competition between the fluctuations in the charge and those in the spin, which suppress each other. The single-particle state density is characterized by the presence of a narrow ($\sim T_K$) resonance near E_F. If $T \lesssim T_K \ll \omega_0$ (T_K is the Kondo temperature), we can ignore the delay in the response of the vibrational subsystem, whose role reduces to the appearance of an attractive two-electron interaction $U_{ph} = 2\zeta\Gamma$. At $U_{ph} > U$, the system is described by Hamiltonian (1) with $U = U_{\text{eff}} < 0$. A so-called negative U center forms (see Ref. 4 regarding the situation in the Hubbard model).

The effect of impurities with a strong local electron-phonon coupling on T_c was studied in Ref. 5 at $\zeta < \zeta_c$ and also in Refs. 6 and 7, in the Anderson model with $U_{\text{eff}} < 0$. A question which has remained open is the correct way to deal with both the Coulomb repulsion in Ref. 5 and a strong electron attraction in Refs. 6 and 7. A numerical simulation carried out in Ref. 8 with $U = 0$ yielded the derivative $dT_c/dc|_{c=0}$ (c is the impurity concentration) Below we discuss two cases: a) The relation $\zeta < \zeta_c$ holds, and there is no localized spin at the impurity. b) The relation $\xi - \xi_c \gtrsim \xi_c$ holds for $2\zeta\Gamma - U > 0$ and $T \ll T_K \ll \omega_0$. Both cases correspond to the region $T \ll T_K$ (in the first case, to $T_K \sim \Gamma$). We can thus use the theory of a Fermi liquid to calculate the vertex of the electron-electron coupling, which appears in the equation for the gap. Using the Ward identities, we can express the vertex in terms of the charge and spin susceptibilities of the impurity, χ_{ch} and χ_{sp}, respectively. We carry out an ordinary averaging over the positions of the impurities.[9]

In case a) we have $T_c \approx \omega_D \exp(-1/f)$, where

$$f = \frac{\lambda - N(\chi_{sp} - \chi_{ch})/a + 4N\xi^*\chi_{ch}^2}{1 + N(\chi_{sp} + \chi_{ch} + 4\xi^*\chi_{ch}^2)}, \qquad (2)$$

Here λ is the electron-phonon coupling constant (without impurities); $N = c/N(0)\Gamma$; and $\xi^* = \xi/(1 - 4\chi_{ch}\xi)$ The frequency region corresponding to a repulsion, $\chi_{sp} - \chi_{ch}$, is on the order of $\Gamma \gg \omega_0$. Related to this circumstance is the appearance of a parameter α: an ordinary logarithmic renormalization. In the case $\xi = 0$, expression (2) is the same as that in Ref. 10, and it describes a suppression of superconductivity by Anderson impurities. A numerical analysis of (2) with the help of the expressions for χ_{ch} and χ_{sp} from Ref. 1 shows that T_c can be raised substantially only in the region $\Delta \equiv (1 - 4\chi_{ch}\xi) \ll 1$. For example, with $\epsilon^*/2\Gamma = 0.3$ (ϵ is the renormalized value of ϵ; Ref. 1), $\lambda = 0.2, \Gamma/\omega_D = 20$, $N = 3$ and $\xi = 5$, we find $f \approx 0.3$, but even at $\xi = 4$ the value of f is considerably smaller. At small values of Δ there is a transition to a two-well potential energy of an oscillator, and anharmonic terms are naturally important. In the example above we have $\Delta \approx 0.1$, so we are right at the limit of the range of applicability of the harmonic approximation.

In case b) we can use the symmetry (pointed out in Ref. 11) of the susceptibilities under a change in the sign of U in a symmetric Anderson model. Specifically, the quantity $\chi_{sp} - \chi_{ch}$ is antisymmetric, while $\chi_{sp} + \chi_{ch}$ is symmetric, under $U \to -U$. Consequently, χ_{sp} and χ_{ch} exchange places. This is a consequence of the electron-hole symmetry which was pointed out in Ref. 1. With $\lambda = 0$ we have $T_c \approx T_K \exp(-1/f)$, where f is found from (2) through the replacements $\xi \to 0$, $\alpha \to 1$, and $\chi_{sp} \rightleftarrows \chi_{ch}$. At $T \ll T_K$ and $|U_{\text{eff}}| \gg \Gamma$ we have $\chi_{sp} \to \pi\Gamma/2T_K$ and $\chi_{ch} \to 0$. In this case χ_{sp} determines a fluctuation of the charge of the system, while χ_{ch} determines a fluctuation of the spin. In the ground state, the behavior of this system is governed by quantum oscillations between states with two electrons at an impurity and with an empty impurity level. As in the case $U > 0$, charge fluctuations are suppressed. In this case, spin fluctuations are suppressed. Since we have $\chi_{sp} \gg 1$, f reaches saturation, $f = 1$, even at comparatively small values of N. It should be recalled, however, that the theory is valid in the region $T_c \ll T_K$. According to Ref. 3, the value of T_K varies over a wide range. If we ignore the delay in the attractive part of U_{eff}, we can write[1]

$$T_K = \frac{(2|U_{\text{eff}}|\Gamma)^{1/2}}{\pi} \exp(-\pi|U_{\text{eff}}|/8\Gamma). \tag{3}$$

A question which remains open, however, is whether the parameter $T_K/\omega_0 \ll 1$ determines the range of applicability of expression (3) in the case $\omega_0 \ll \Gamma$. In the approach marked out in Ref. 3, ω_0 is essentially an ultraviolet cutoff parameter, and it appears explicitly in T_K at $T_K \ll \omega_0$. With high-temperature superconducting oxides in mind, we take account of the high frequency of the local vibrations of oxygen atoms, which reaches 0.08 eV. We thus see that, in any case, fairly large values of T_K are completely probable. The isotope effect is determined by the dependence of T_K on the frequency ω_0 (with $\lambda = 0$),and it thus exhibits a nontrivial behavior. If expression (3) holds, there is no isotope effect.

Because of the disorder which is characteristic of superconducting oxides, the level ϵ may be distributed over a fairly wide energy interval. Such a situation implies that there will also be wide distribution of the "magnetic" fields which create an asymmetry ΔE in the energies of the two possible impurity states. The presence of a wide distribution of energies of two-level systems should evidently cause these systems

to make a linear contribution to the resistance. A likely center (at least for the yttrium ceramics) at which a resonant state could form is an oxygen atom at the vertex of an octahedron. For specifically this configuration the mean square displacement characteristically has an anomalously large value.[12] Furthermore, it follows from band calculations[13] that the π level of oxygen makes a large contribution to a narrow band near E_F. An important point is that the vertex oxygen serves as a bridge for electrons in different CuO_2 planes. It is then clear that if there is a wide energy distribution of two-level systems, the transparency for a resonant tunneling of electrons between planes varies $\sim T$, while the resistance along the c axis varies $\sim T^{-1}$. These conclusions agree qualitatively with the observed anisotropy of the temperature dependence of the resistance. These arguments of course ignore the universal component of the resistance which is characteristic of Kondo systems, and they are valid only at $T > T_K$. It is accordingly important to extend the theory to the region $T_c \gtrsim T_K$.

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