

LOCAL SPIN SCREENING IN THE HIGH T_C SUPERCONDUCTORS

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We point out that parallels can be drawn between the metallic state of the cuprate superconductors and that of heavy fermion materials. To gain intuition about the effectiveness of the Kondo spin-screening mechanism in this situation we investigate the single (Cu) impurity limit.

A popular model for the electronic structure of the high T_c superconducting oxides (HTSO) is the $J - t$ -model. One assumes that the local spins, showing up at half-filling, persist in the metallic state. Further, the $O2p$ -like holes introduced by doping would bind to a Cu -spin, forming a so-called Zhang-Rice (or local) singlet [1], which hops as an entity through the spin lattice. It is far from clear if this is the relevant model for the HTSO. According to this model, the effective bandwidth would be $O(J) \simeq 0.1eV$, leading to large mass-enhancement effects, while the effective mass is actually quite low. Also, in the truly High T_c materials apparently no low energy spin-degrees of freedom can be detected. Furthermore, evidence is accumulating pointing at an appreciable overlap between the quasiparticles at E_f and the bare electrons [2]. Finally, it is obvious that if the correlation gap disappears, it is no longer possible to think in terms of local spins and a low concentration of holes. According to XAS-data, this gap does not seem to persist in metallic HTSO [3].

How then to imagine the transition from the strongly localized anti-ferromagnet at half filling to this rather 'normal' metallic state? One plausible scenario is offered by renormalized band theory. Using the Gutzwiller approximation for the two band model it can be shown that the gap and the moments disappear at $\simeq 10\%$ doping [4] using realistic parameters. A complementary approach is to consider the usual two-band model with one 3d-(Cu) site (impurity model)

$$H = \sum_{\sigma} \epsilon_d d_{\sigma}^{\dagger} d_{\sigma} + \sum_{\epsilon, \sigma} (\epsilon_p + \epsilon) c_{\epsilon\sigma}^{\dagger} c_{\epsilon\sigma} + \sum_{\epsilon, \sigma} V(\epsilon) (d_{\sigma}^{\dagger} c_{\epsilon\sigma} + h.c.) + U n_{d\uparrow} n_{d\downarrow}$$

In this model the undoped system (half filling) has one hole, which is largely localized on the Cu site. An additional hole may get bound to the impurity spin forming the local singlet (LS). However, the LS is not invariably

formed. For instance, in the localized limit (large Δ/V) the LS binding energy (E_0) follows from the relation $1 = I \sum_{\epsilon} |V(\epsilon)|^2 / (\epsilon - E_0)$ with $I = 2/(U - \Delta) + 1/\Delta$ and assuming a semielliptical band and constant V , the LS is only stable if $2V^2 I > W_p$. An interesting problem is how the LS renormalizes the Fermi-liquid at higher carrier density. We show elsewhere that this gives rise to similar physics as in the Kondo problem.

If the carrier density is increased, fluctuations appear which lead to screening of the impurity spin by the Kondo mechanism. This may be seen from Fig. 1 where we show the basis states of the variational $1/N$ approach up to $O(1/N^2)$ [5] (for $Cu < d^9 |H| d^{10} \epsilon \rangle = V(\epsilon)$ and $\langle d^{10} |H| d^9 \epsilon \rangle = NV(E)$). Neglecting the conduction band, the hybridization is $O(1/N)$ at half filling ($|d^9 \rangle \Leftrightarrow |d^{10} \epsilon \rangle$, or (b) \Leftrightarrow (c) with the band fully occupied). Half filling with one hole added is described by (d) \Leftrightarrow (e). In order to find a bound LS, it turns out that in the standard diagrammatic approach one has to include the $O(1/N^2)$ vertex corrections, i.e. the non-crossing approximation (NCA [6]) breaks down. At finite hole concentrations, also fluctuations

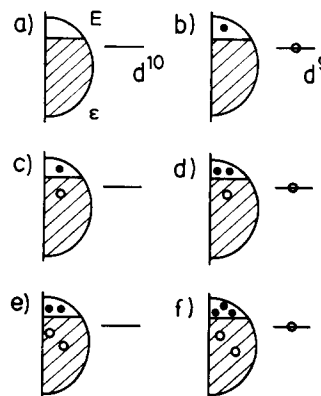


Fig. 1: Basis states in the variational $1/N$ approach

$|d^{10} \rangle \Leftrightarrow |d^9 E \rangle$ (a-b), (c-d), etc.) start to contribute and these lead to the formation of the Kondo-singlet (KS).

NCA is not unreasonable if the LS is not formed (or at high carrier concentration, elsewhere we study the cross-over LS-KS) and we calculated in this approximation the Kondo temperature (T_K , derived from the position of the Kondo peak) for the following model: the valence and conduction bands are represented by square bands with widths W_v and W_c and the virtual bound state width is Γ . These bands are separated by a gap (E_g) and we place the d-level at ϵ_d^0 relative to the top of the valence band and under doping, μ is placed T_F below the top of the valence band. Using parameters representative for HTSO ($N = 2, V_{dps} = 1eV$, $W_v = 4eV$, $W_c = W_v/3$, and strong mixed valency $\langle n_d \rangle \simeq 0.5$) we find T_K as a function of E_g and T_F as indicated in Fig. 2. The $N \rightarrow \infty$ limit (only fluctuations a-b) is instructive: for $N\Gamma/|\epsilon_d^0| \ll 1$ we find for the Kondo temperature

$$T_K = T_F \frac{(T_F + W_c + E_g)}{(T_F + E_g)} \exp\left(-\frac{\pi(|\epsilon_d^0| + T_F)}{N\Gamma}\right)$$

This equation describes qualitatively the trends in Fig. 2. E_g and T_F enter in the prefactor and if $E_g \rightarrow 0$ we obtain the familiar large N expression ($W \rightarrow W_c + T_F$). However, for $E_g \rightarrow \infty$ (or $W_c \rightarrow 0$) $T_K \propto T_F$ i.e. the Kondo temperature is limited by the Fermi-temperature and roughly inversely proportional to the magnitude of the gap.

Although for Ce systems the single impurity limit describes the physics quite well down to temperatures $< T_K$, it might be risky to extrapolate the above results

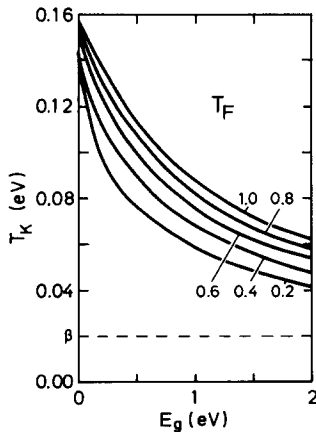


Fig. 2: The Kondo temperature (T_K) as a function of the Fermi temperature (T_F) and the gap magnitude (E_g) according to NCA ($\beta = 1/k_B T$).

in the case of the HTSO. One problem is that in the latter case band formation effects may be more important (small degeneracy and $W_v/\Gamma \simeq 1$). Another problem is the 'shortage' of screening electrons compared to the number of local spins, at least as long as the correlation gap persists. Nevertheless, also in this case Kondo screening may be relevant. If no LS is formed, one would expect a cross-over from a state dominated by collective spin dynamics to a Fermi-liquid (with confined spins) as T_K becomes larger than the spin-spin exchange. If the system is strongly mixed-valent, it is probably better to think in terms of a rather broad band which, if undoped, has a gap at 3/4 filling; the strong $Cu - O$ covalency results in appreciable $O2p$ character in the unoccupied $d_{x^2-y^2}$ band [3] and the gap can close under doping, i.e. the situation we mimicked in the model. As can be seen from Fig. 2, a decreasing gap will lead to a strong increase of the Kondo temperature. According to our calculations T_K would be relatively high (order 0.1 eV) if the gap is closed and therefore rather hard to detect experimentally. In this respect, recent I.R. spectroscopy data are interesting. If these data are interpreted in a generalized Drude framework, a similar picture is obtained for $YBa_2Cu_3O_7$ and $CePd_3$ [7]. For $CePd_3$ a natural explanation is offered by the Kondo effect [8], suggesting that the same physics is relevant for HTSO. If so, T_K is of the order expected from theory. From this picture one expects rather modest mass- and susceptibility enhancement because T_K is large. In order to see if this concept of local spin screening applies, more direct experimental information is needed, e.g. k-independent spin fluctuations should show up in neutron scattering and one would expect a relatively broad-Kondo resonance in photoemission.

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