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FINITE TEMPERATURE PROPERTIES OF THE ANDERSON LATTICE

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Abstract. – Within an approximate diagrammatic solution the density of states of the Anderson Lattice exhibits Abrikosov-Suhl peaks and a gap near the Fermi level that decrease as a function of the temperature. The results can be compared with experimental ones for Ce-compounds that are assumed to be Kondo lattices.

It is well known [1] that low temperature anomalies in a series of physical properties of Cerium compounds (CeCu₂Si₂ [2], CeAl₃ [3]) are related to a large enhancement in the electronic density of states near the Fermi level (called Abrikosov-Suhl resonance [4]). The mixing between uncompletely filled localized f-states and itinerant conduction states is the guiding idea to explain this behaviour. In the description of these systems the two band Periodic Anderson Hamiltonian (PAH) has been largely used through different approaches [5, 6]. In the Alloy Anolog scheme [5], for example, the electrons are considered as "seeing" a binary alloy into the Coherent Potential Approximation (CPA) and the hybridization is treated as a perturbation. No Kondo peaks are observed.

The central point in our treatment of the PAH is that the local hybridization between f and c electrons is embodied in the exact solution of the atomic part of the PAH [7]. We solve exactly a system with two hybridized levels, one of them (f) with finite Coulomb repulsion U . The band is introduced through a perturbative hopping term. In the solution of the two hybridized levels system the lowest lying energy state is obtained for two particles and it is a singlet with zero spin [8]. Above this level we find one- and three-particle triplet states. As the temperature decreases the hybrid states with one and three particles are no more reached by the system, if one has an average of two electrons per atom, just the two-particle singlet state remains. This is the way one divides the magnetic moment suppression for zero band width. As the conduction band is introduced the hybrid levels become wider in energy and the position of the chemical potential must be set in order to preserve the average number of electrons. So, both band structure and chemical potential are temperature dependent.

We start writing the Periodic Anderson Hamiltonian:

$$H = \sum_i (H_0^i) + H' \quad (1)$$

where the atomic term is:

$$H_0^i = E \sum_{\sigma} f_{i\sigma}^{\dagger} f_{i\sigma} + E_B \sum_{\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} + V \sum_{\sigma} (f_{i\sigma}^{\dagger} f_{i\sigma} + \text{h.c.}) + \frac{U}{2} \sum_i n_{i\sigma} n_{i\bar{\sigma}} \quad (2)$$

being E (E_B) the energy of the pure f-(c-) electronic level, V the hybridization and U the Coulomb repulsion between f and conduction electrons. The perturbative band term H' is:

$$H' = \sum_{i \neq j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} \quad (3)$$

where t_{ij} is the hopping matrix element between i - and j -sites.

The atomic Green functions are

$$G_0^{AB} = \langle\langle A ; B \rangle\rangle_{\omega} \quad (4)$$

where A and B are the fermion field operators, i.e. c and f . The Green function can be calculated from the knowledge of the eigenvalues and eigenstates of H_0^i [9] using their spectral representation [10]:

$$\langle\langle A ; B \rangle\rangle = Q^{-1} \sum_{\mu, \nu} e^{-E_{\mu} / k_B T} \times \left[\frac{\langle \mu | A | \nu \rangle \langle \nu | B | \mu \rangle}{z - (E_{\nu} - E_{\mu})} + \frac{\langle \nu | A | \mu \rangle \langle \mu | B | \nu \rangle}{z - (E_{\mu} - E_{\nu})} \right] \quad (5)$$

where E_{μ} are the eigenvalues of the atomic Hamiltonian and Q is the grand partition function. The Green functions calculated through equation (5) are local propagators corresponding to sites with a variable number of particles. We assume that every site is in contact with a common particle reservoir, so the chemical potential determines the average number of particles at each site.

The complete Green function can be determined through a Dyson-like equation obtained from an ap-

proximate diagrammatic method [11]:

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \mathcal{W} \mathcal{G} \quad (6)$$

where $\mathcal{G}$ and $\mathcal{W}$ are

$$\mathcal{G} = \begin{pmatrix} G^{ff} & G^{fd} \\ G^{df} & G^{dd} \end{pmatrix} \quad \mathcal{W} = \begin{pmatrix} 0 & 0 \\ 0 & E(k) - E_B \end{pmatrix}. \quad (7)$$

In the numerical calculation we consider a model density of states for the unperturbed conduction band given by:

$$\rho^0(\omega) = \begin{cases} \frac{3}{4W} \left(1 - \frac{\omega^2}{W^2}\right) & |\omega| < W \\ 0 & |\omega| > W \end{cases} \quad (8)$$

where W is the half width of the conduction band. Furthermore, we choose the values: $E = -2W$, $U = 4W$ and $V = 0.25W$; that generates a symmetric density of states. For this set of parameters and two electrons per atom the chemical potential is into the hybridization gap at any temperature [12], so it is easier to analyse the modifications of the band structure with the temperature. It is clear from figure 1 that the area under the f peaks around the gap becomes thinner at higher temperatures. This is so because the two particle peaks lose their population to the neighbouring peaks of one and three particles.

Fig. 1. - Density of states near the Fermi level for $E = -2W$, $U = 4W$, $V = 0.25W$ and $W = 1.0$ for two values temperature $k_B T / W = 0.003$ and $k_B T / W = 0.03$. The two extra peaks correspond to one-and three-particles states excited at high-temperatures.

Choosing other value for the Coulomb repulsion, $U = 10W$, the bands are shifted to higher energies because the position of the atomic energy levels depends on U . As the temperature is increased the chemical potential also increases, crossing the f -peaks. These results are shown in figure 2. For values of $U < 4$ the chemical potential goes downwards showing a behaviour symmetric to the mentioned above.

Fig. 2. - Same as figure 1 but $U = 10W$.

Concluding, the density of states determined from a local point of view presents some characteristic features of a Kondo system: a) narrow peaks near or at the Fermi level; b) the number of states in those peaks decreases at higher temperatures; c) the weight of the peaks corresponding to one and three particles states increases with temperature. Then the model explains in a qualitative way the low temperature anomalies in some properties of rare earth compounds like CeAl_3 or CeCu_2Si_2 . Specific heat and static susceptibility calculations are in progress.

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