

Finite temperature static susceptibility of the Anderson lattice*

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The static magnetic susceptibility of the Anderson lattice in the symmetric Kondo case is calculated within an approach that leads to exact results in the limits of zero bandwidth, zero hybridization or zero Coulomb repulsion. The susceptibility agrees with the expected behavior of a Kondo system for high and intermediate temperatures. At low temperatures a partially compensated magnetic moment is obtained, which is probably an artifact of the approximation.

The low-temperature behavior of some heavy-fermion rare-earth compounds, like CeAl₃, CeCu₂Si₂, etc., has been extensively studied in the last few years [1]. At such temperatures these compounds show anomalies in a series of physical properties. In particular, the static susceptibility indicates the existence of a large effective magnetic moment [2, 3] and deviates from Curie's law at very low temperatures.

Heavy-fermion behavior is usually explained on the basis of a mixing between localized, strongly correlated f-states and extended conduction states. Here, we calculate the static homogeneous susceptibility for a system described by the Periodic Anderson Model (PAM). Our approach, as described in previous works [4–6], consists in solving exactly the atomic part (zero-bandwidth limit) and introducing the hopping term as a perturbation, within a temperature Green's function technique. The homogeneous susceptibility is calculated from a spin–spin correlation function as described below.

We write down the periodic Anderson Hamiltonian in the form,

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

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where the atomic term is

$$H_0^i = \sum_{\sigma} E f_{i\sigma}^{\dagger} f_{i\sigma} + E_B c_{i\sigma}^{\dagger} c_{i\sigma} + V(f_{i\sigma}^{\dagger} c_{i\sigma} + c_{i\sigma}^{\dagger} f_{i\sigma}) + U n_{i\uparrow}^f n_{i\downarrow}^f \quad (2)$$

and the band term is

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

The parameters of the Hamiltonian are: $E(E_B)$ is the energy of the atomic f (c -)level, V the hybridization, U the Coulomb repulsion for f -electrons in the same site, and t_{ij} the hopping matrix element.

The homogeneous static susceptibility is

$$\chi = \frac{1}{N} \sum_{ij} \chi_{ij}, \quad (4)$$

with

$$\chi_{ij} = \langle S_{iz} S_{jz} \rangle / T, \quad (5)$$

where S_{iz} is the z -component of the total (f plus c) spin operator on site i . Writing S_{iz} in terms of fermion operators, eq. (5) becomes

$$\begin{aligned} \chi_{ij} &\equiv \sum_{\alpha\beta} \chi_{ij}^{\alpha\beta} \\ &= \frac{1}{4T} \sum_{\alpha\beta} [\langle n_{i\uparrow}^{\alpha} n_{j\uparrow}^{\beta} \rangle - \langle n_{i\uparrow}^{\alpha} n_{j\downarrow}^{\beta} \rangle], \end{aligned} \quad (6)$$

where α and β stand for either f or c .

In the absence of local Coulomb repulsion, the averages in eq. (6) may be decoupled [7] and the homogeneous susceptibility can be evaluated from

$$\chi = -\frac{T}{4N} \sum_{\alpha\beta} \sum_{nm} \sum_{\mathbf{k}} G^{\alpha\beta}(\mathbf{k}, \omega_n) G^{\alpha\beta}(\mathbf{k}, \omega_n + \varepsilon_m), \quad (7)$$

where ω_n and ε_m are fermionic and bosonic Matsubara frequencies, respectively, and $G^{\alpha\beta}(\mathbf{k}, \omega_n)$ is a one-particle Green's function, calculated within an approximate diagrammatic expansion described in refs. [4–6]. However, inclusion of the Coulomb interaction leads to the breakdown of Wick's theorem [8] and, consequently, the correlation functions appearing in eq. (6) cannot be decoupled in terms of one-particle Green's functions. Taking into account that the correlation U is local, we use a decoupling scheme like that of eq. (7) only for the non-local contribution to the susceptibility, while the local part,

$$\chi_{ii} = \frac{1}{4T} \sum_{\alpha\beta} [\langle n_{i\uparrow}^\alpha n_{i\uparrow}^\beta \rangle - \langle n_{i\uparrow}^\alpha n_{i\downarrow}^\beta \rangle], \quad (8)$$

is evaluated by means of new local Matsubara Green's functions

$$A_{\sigma\sigma'}^{\alpha\beta\gamma}(\tau) \equiv \langle\langle n_\sigma^\alpha(\tau) a_{\sigma'}^\beta(\tau); a_{\sigma'}^{+\gamma} \rangle\rangle, \quad (9)$$

where a_σ^α stands for either c_σ or f_σ .

The averages in eq. (8) can be calculated through the limit

$$\begin{aligned} \langle n_\sigma^\alpha n_{\sigma'}^\beta \rangle &= \lim_{\tau \rightarrow 0^-} A_{\sigma\sigma'}^{\alpha\beta\beta}(\tau) \\ &= \lim_{\tau \rightarrow 0^-} T \sum_n A_{\sigma\sigma'}^{\alpha\beta\beta}(\omega_n) e^{i\omega_n \tau}. \end{aligned} \quad (10)$$

Using the same approximate diagrammatic method as in refs. [4–6], one obtains

$$A_{\sigma\sigma'}^{fff}(\mathbf{k}) = A_{\sigma\sigma',0}^{fff} + A_{\sigma\sigma',0}^{ffc} E(\mathbf{k}) G^{cf}(\mathbf{k}), \quad (11a)$$

$$A_{\sigma\sigma'}^{fcc}(\mathbf{k}) = A_{\sigma\sigma',0}^{fcc} + A_{\sigma\sigma',0}^{fcc} E(\mathbf{k}) G^{cc}(\mathbf{k}), \quad (11b)$$

$$A_{\sigma\sigma'}^{eff}(\mathbf{k}) = A_{\sigma\sigma',0}^{eff} + A_{\sigma\sigma',0}^{efc} E(\mathbf{k}) G^{cf}(\mathbf{k}), \quad (11c)$$

$$A_{\sigma\sigma'}^{ecc}(\mathbf{k}) = A_{\sigma\sigma',0}^{ecc} + A_{\sigma\sigma',0}^{ecc} E(\mathbf{k}) G^{cc}(\mathbf{k}), \quad (11d)$$

In the numerical calculations, the k -dependence in eqs. (7) and (11) is eliminated through the transformation

$$\begin{aligned} &\frac{1}{N} \sum_{\mathbf{k}} \Phi(E(\mathbf{k})) \\ &= \frac{1}{N} \int dE \sum_{\mathbf{k}} \delta(E - E(\mathbf{k})) \Phi(E(\mathbf{k})) \\ &= \int dE \rho^0(E) \Phi(E), \end{aligned} \quad (12)$$

$\rho^0(E)$ being a model density of states for the unhybridized conduction band. Here we adopt

$$\rho^0(\omega) = \begin{cases} \frac{3}{4W} \left(1 - \frac{\omega^2}{W^2}\right), & |\omega| < W, \\ 0, & |\omega| > W, \end{cases} \quad (13)$$

where W is the half-width of the conduction band.

We present in figs. 1 and 2 typical results for the dependence of the susceptibility on temperature in the symmetric (Kondo) case with two electrons per site. Figure 1 shows the exact results for the atomic limit [9], and fig. 2, the finite bandwidth case. The susceptibility decreases at high temperatures in both cases. As

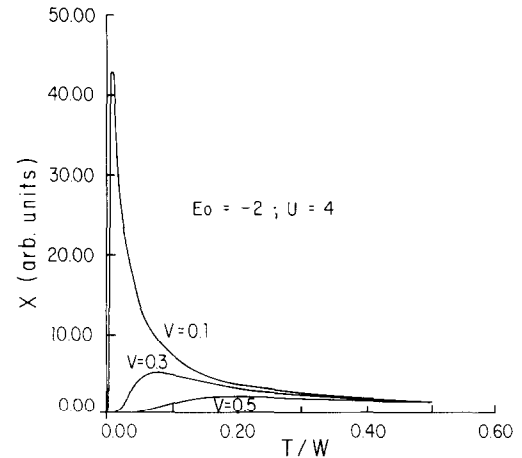


Fig. 1. Atomic susceptibility vs. temperature in the symmetric Kondo case for three different values of the hybridization parameter, $V = 0.1$, $V = 0.3$, $V = 0.5$. The bare f -level energy $E = -2.0$ and the Coulomb repulsion $U = 4.0$. All energies are measured in units of the unhybridized conduction band.

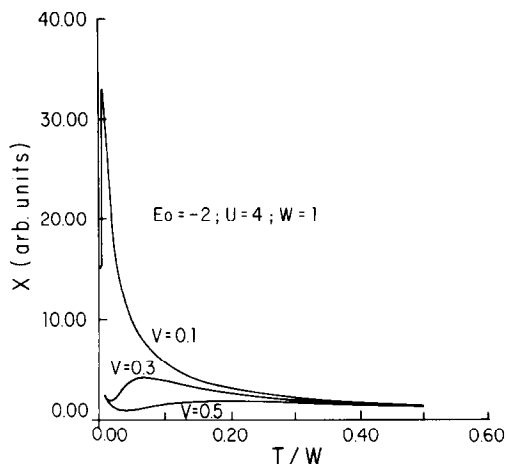


Fig. 2. Same as fig. 1 but taking the band into account.

the temperature is lowered it presents a maximum, and while the atomic susceptibility goes to zero with T , the band susceptibility initially decreases but eventually turns up and diverges as $1/T$ at very low temperatures.

For a more detailed analysis, we plot in fig. 3 an effective Curie constant versus temperature. We can distinguish three different regimes [10]:

(i) A high-temperature one, in which all states contribute to the susceptibility and the effective Curie constant tends to the value $\frac{1}{4}$ (characteristic of a pair of free orbitals) independently of hybridization.

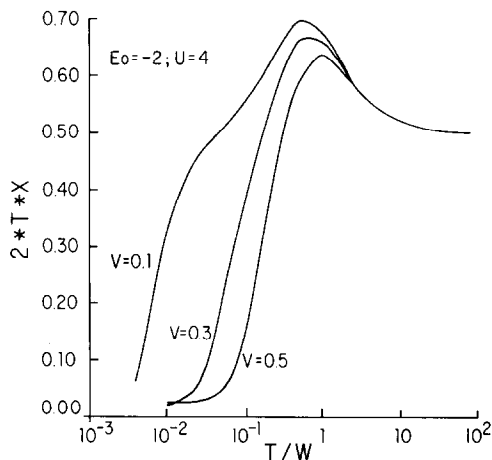


Fig. 3. Twice the effective Curie constant as a function of temperature, with the same set of parameters of fig. 2.

(ii) An intermediate temperature regime in which the main contribution comes from levels with energy just about the ground state. In this situation, a maximum value for the Curie constant is obtained and a dependence on the hybridization is observed.

(iii) A low-temperature regime, which is reached as the singlet ground-state progressively dominates and the effective Curie constant tends to zero.

We can conclude that the exact results for the atomic susceptibility agree with the idea of compensation of localized magnetic moments. However, when the band effects are taken into account we observe that the effective Curie constant does not go to zero, apparently indicating an incomplete compensation of the local moments. We believe that this result is an artifact of the approximation, since important correlations have been neglected in this scheme.

Finally, we want to remark that the present approach is exact in the limits $V=0$ and/or $U=0$. New results for the susceptibility and for the electronic specific heat within a slightly different treatment will be reported soon.

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