The Kondo-Hubbard model at half-filling

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We have analyzed the antiferromagnetic ($J > 0$) Kondo-Hubbard lattice with the band at half-filling by means of a perturbative approach in the strong coupling limit, the small parameter is an arbitrary tight-binding band. The results are valid for any band shape and any dimension. We have obtained the energies of elementary charge and spin excitations as well as the magnetic correlations in order to elucidate the magnetic and charge behaviour of the Kondo lattice at half-filling. Finally, we have briefly analyzed the ferromagnetic case ($J < 0$), which is shown to be equivalent to an effective antiferromagnetic Heisenberg model.

We consider here the Kondo lattice model first introduced to describe heavy-fermion systems [1], but studied here for the particular half-filled case with one band electron per site so that the model can describe an insulator with Kondo like properties [2]. The Hamiltonian consists in a periodic lattice of magnetic atoms in a metallic background modelled by f orbitals and a tight-binding band respectively. The two systems interact through an exchange coupling constant J between the spin density of the band electrons and the spin of the magnetic atoms. Additionally, we introduce a Coulomb intra-site repulsion between the electrons of strenght U. The model Hamiltonian is,

$$H = \sum_{i,j,s} t_{ij} c^\dagger_{is} c_{js} + J \sum_i \mathbf{s}_{ci} \cdot \mathbf{S}_{fi} + U \sum_i c^\dagger_{i\downarrow} c_{i\downarrow} c^\dagger_{i\uparrow} c_{i\uparrow} = H_t + H_0.$$

The first term is the tight-binding band where $t_{ij} = t_{ji}$ is an unrestricted hopping parameter ($t_{ii} = 0$). The second term is the spin-spin interaction where $\mathbf{s}_{ci} = \frac{1}{2} c^\dagger_{is} \sigma_{ss'} c_{is}$ is the spin density of the conduction electrons, σ^a are the Pauli matrices and $\mathbf{S}_{fi}$ ($S_f = 1/2$) is the spin of the magnetic impurities.

In the $t_{ij} = 0$ limit the sites are uncorrelated and we have just to obtain the eigenvalues and eigenvectors of the one-site Hamiltonian $h_{0i} = J\mathbf{s}_{ci} \cdot \mathbf{S}_{fi} + U n_{i\downarrow} n_{i\uparrow}$. We obtain the complete solution, eigth eigenstates: a singlet state $|s_i\rangle$ with energy $-3J/4$, two doublets $\{|d^\pm_{0i}\rangle, |d^\pm_{2i}\rangle\}$ with energy 0 and U respectively, and finally a triplet $\{|t^0_i\rangle, |t^\pm_i\rangle\}$ with energy $J/4$.

From the one site solution we can build and classify by inspection all the eigenstates of the complete Hamiltonian H_0. We restrict the analysis to the half-filled band in any dimension. The ground state in this limit is a non degenerate singlet which describes an insulator without any magnetic structure. This limit seems appropiate to describe qualitatively some of the properties of the FeSi [2] at zero temperature.

When we introduce the band term the sites are correlated and the physical picture can be modified. We are interested in the magnetic and insulating behavior of the system and therefore we have obtained the spin and charge energy gaps and the spin-spin correlations. The spin gap is defined as the difference between the energies of the ground state and the triplet state, $\Delta_S = E_0(N, S = 1) - E_0(N, S = 0)$. The zero order ($t_{ij} = 0$) value of Δ_S is J and it corresponds to the difference between the energy of the first excited state, a triplet, and the singlet state. The triplet is N-fold degenerate in absence of hopping. Hence, we need to apply the perturbation formalism corresponding to the degenerate case, then obtain an effective Hamiltonian in the $S = 1$ subspace (see [6] and [7] for details) and finally, we get the following expression for the spin excitation energy,

$$\Delta_S(\mathbf{q}) = J + (-2B_1^{S=1} + 2B_2^{S=1})\sigma_1 - 2B_2^{S=1}\tau^{(2)}(\mathbf{q}). \qquad (1)$$

where, $\sigma_1 = \int \frac{d^d\mathbf{q}}{(2\pi)^d}[\tau(\mathbf{q})]^2$, $\quad \tau^{(2)}(\mathbf{q}) = \int \frac{d^d\mathbf{q}'}{(2\pi)^d}\tau(\mathbf{q}' + \mathbf{q})\tau(\mathbf{q}')$, $B_1^{S=1} = -1/(3J+U)$ and $B_2^{S=1} = -1/(J + 2U)$ and $\tau(\mathbf{q})$ is the band dispersion.

This expression is $\mathbf{q}$-dependent. We could then define the absolute gap as the minimal value of (1), $\Delta_S(\mathbf{q}_{min})$, which corresponds to a value of the wave vector $\mathbf{q}_{min}$ which minimizes the energy. The nearest-neighbor case gives, $\Delta_S(\mathbf{q}) = J - 20t^2(3J)d$. From this result on one hand one could think that there exist a phase transition between the triplet and the singlet state. On the other hand it is believed that the

half-filled Kondo lattice in one dimension at zero temperature is a spin liquid [3, 8], so that the spin gap is non zero for any $J \neq 0$. The contradiction is due, of course, to the poor approximation to the true gap we have obtained. Nevertheless, if we accept the existence of the spin gap, we can deduce that our result is qualitatively good even for moderate values of J/t (at $J = 3$ the gap is always positive, so there is no transition). When more terms in the series in t/J for the spin gap will be available, an analysis of the series should tell us about the critical value $(t/J)_c$ at which the spin gap closes and a magnetic phase transition takes place. Another interesting point is that even when J is small and U is sufficiently large we get a non zero spin gap so that the Kondo insulator behavior could be obtained in a Kondo lattice system with small Kondo coupling if the conduction electrons are by themself strongly correlated: when $J \sim 0$ then $B_1^{S=1} = B_2^{S=1} = -1/(2U)$, so that $\Delta_S \sim t^2/U > 0$. The spin-spin correlations between the magnetic atoms have been also obtained for the nearest-neighbor hopping, $\langle S_{fi} \cdot S_{fj} \rangle = -(5/6)(t/J)^2$ (we write the result in the simple case U=0).

The insulating gap is defined as, $\Delta_I = \mu^+ - \mu^- = E_0(N+1, S=1/2) + E_0(N-1, S=1/2) - 2E_0(N, S=0)$. It can be seen as the difference between the chemical potential with $N+1$ particles, μ^+ and μ^-, the chemical potential at $N-1$ particles. With this definition, the gap is the second derivative of the energy with respect to the number of particles. In this sense the insulator gap could be considered as an order parameter of the insulator-metal transition. The total energy dispersion in the $N \pm 1$ subspace is,

$$E_0^{N\pm1}(\mathbf{q}) = -(N-1)\frac{3}{4}J + U \pm \frac{1}{2}\tau(\mathbf{q}) + 3(B_2^{N\pm1} - B_1^{N\pm1})\sigma_1 + 2NB_1^{N\pm1}\sigma_1 - B_1^{N\pm1}\tau^2(\mathbf{q}), \tag{2}$$

where $B_1^{N\pm1} = B_1^{S=1}/2$, $B_2^{N\pm1} = -1/(4J)$. The gap can be now explicitly written. It is interesting, however, to discuss the meaning of two different expressions for the gap. The first one is the $\mathbf{q}$-dependent generalization,

$$\Delta_I = \frac{3J}{2} + 6(B_2^{N\pm1} - B_1^{N\pm1})\sigma_1 - 2B_1^{N\pm1}\tau^2(\mathbf{q}), \tag{3}$$

where no first order term appear. The second expression of the gap can be obtained if we strictly follow the prescription given in (2), where the lowest energy value on the $N+1$ subspace and the highest energy value on the $N-1$ subspace are taken,

$$\Delta_I = \frac{3J}{2} + U - \frac{1}{2}(\tau(\mathbf{q}^+_{min}) - \tau(\mathbf{q}^-_{max})) + 6(B_2^{N\pm1} - B_1^{\pm})\sigma_1 - B_1^{N\pm1}(\tau^2(\mathbf{q}^+_{min}) + \tau^2(\mathbf{q}^-_{max})) \tag{4}$$

Both expressions are physically acceptable if one thinks, for example, in terms of excitations which can be created by direct or indirect absortion of a photon. The former will be piloted by (4) where the particle momentum does not change and the later by (3). The chemical potential expressions can be then taken as effective bands of the original Hamiltonian. If we explicitly write them as functions of q in one dimension and nearest-neighbor hopping (we take henceforth $U = 0$ in order to simplify) we obtain $\mu^+ = 3J/4 - t\cos q - t^2/(2J) + 2t^2\cos^2 q/(3J)$, $\mu^- = -3J/4 - t\cos q + t^2/(2J) - 2t^2\cos^2 q/(3J)$.

The direct gap (4) at each value of J/t, is graphically given by the difference between the two chemical potentials as functions of q. The indirect gap is the energy

difference between the absolute minimum of the μ^+ band and the absolute maximum of the μ^- band.

We have also considered the ferromagnetic interaction $J < 0$. In this case when the hopping term is zero the ground state is degenerate and there is a triplet $\{t^0, t^+, t^-\}$ on each site. When the band term is included the low energy excitations are described by an (insulating) antiferromagnetic Heisenberg Hamiltonian, $H = -(2t^2/J)\mathbf{S}_i \cdot \mathbf{S}_j$, where $\mathbf{S}_i$ represents the spin one on site i.

This work was supported in part by spanish DGICyT under contract no. PB95-0797.

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