KONDO IMPURITY IN A METALLIC GRAIN: PARITY EFFECTS*

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The problem of a spin-1/2 impurity placed at the center of a small metallic sphere and contact exchange is reduced to the Bethe *Ansatz* solution of the Kondo model in a finite box. The average level spacing is an additional energy scale competing with $T_{\rm K}$. We obtain the energy levels as a function of $T_{\rm K}$ for two s-states, as well as the T-dependence of the entropy and the susceptibility. The results depend on the parity of the number of s-states.

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The main difference of a Kondo impurity placed at the center of a nano-sized sphere with the standard Kondo problem is that the energy spectrum of the host is now discrete. Two main approximations are adopted *(i)* the contact exchange interaction, which restricts the interaction of the impurity to s-waves, and *(ii)* the equal spacing of the s-wave energy levels (properties are expected to depend only on the average energy spacing at the Fermi level), which reduces the model to an effective one-dimensional one with a linear dispersion. Both approximations are usually also adopted in the thermodynamic limit, the latter corresponding to a constant density of states. In addition we consider only forward moving particles to avoid the degeneracy of states with momentum k and $-k$. The Hamiltonian is then

$$\begin{aligned} H_{\rm K} &= \sum_\sigma \int dx\ c^\dagger_\sigma(x) \left(-i\frac{\partial}{\partial x}\right) c_\sigma(x) \\ &+ J\sum_{\sigma\sigma'} \boldsymbol{S}\cdot \int dx\ \delta(x)\ c^\dagger_\sigma(x)\ \boldsymbol{s}_{\sigma\sigma'}\ c_{\sigma'}(x)\,, \end{aligned} \tag{1}$$

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with periodic boundary condition in the interval $(-L/2, L/2)$, and $\boldsymbol{S}$ and $\boldsymbol{s}$ are spin $1/2$ operators for the impurity and the host. The scaling of the energy with large L leads to the conformal towers for the excitations.

In nanoscale systems the properties depend on the parity of the number of s-electrons. If an s-state pins the Fermi level (odd N) the ground state is Kondo spin compensated. This case has been extensively discussed in Ref. [1] for $N = 3$ and $N = 5$. In this paper we study the situation of a non-s-state level pinning the Fermi level (even N). Here a thermally activated Kondo effect [2] can take place in which the ground state is magnetic, but the spin compensation occurs at intermediate temperatures.

The Kondo effect in an ultra-small metallic grain has been studied previously using the noncrossing diagram approximation within the framework of an Anderson impurity [3]. It was found that the Kondo resonance is strongly affected when the mean level spacing is comparable to T_{K} and it also depends on the parity of the number of electrons. An Anderson impurity like model in a finite size system was also studied by Büttiker and Stafford [4] in the context of tunneling into a quantum dot embedded or as a side-branch to a small metallic ring.

Model (1) is identical to the Kondo Hamiltonian solved by Andrei [5] and Wiegmann [6] by means of two nested Bethe *Ansätze* in terms of a set of N charge rapidities $\{k_j\}$ and a set of M spin rapidities $\{\lambda_\alpha\}$, which satisfy

$$\begin{aligned} \exp\left[i\left(k_j L - \frac{J}{4}\right)\right] &= \prod_{\alpha=1}^{M} e_1(\lambda_\alpha)\,, \\ e_1\left(\lambda_\alpha + g^{-1}\right)\left[e_1(\lambda_\alpha)\right]^N &= -\prod_{\beta=1}^{M} e_2(\lambda_\alpha - \lambda_\beta)\,, \end{aligned} \tag{2}$$

where $e_m(\lambda) = (\lambda + im/2)/(\lambda - im/2)$, $j = 1, \ldots, N$, and $\alpha = 1, \ldots M$. Here g is an effective coupling related to the Kondo exchange via $g = \tan(J/2)$. Rapidities within one set have to be all different. The magnetization and the energy are given by $S_z = \frac{1}{2}(N+1) - M$ and $E = \sum_{j=1}^{N} k_j$.

The second set of equations (2) is independent of the charge rapidities k_j because the impurity spin does not couple to the charges. It arises from the second (nested) Bethe *Ansatz*, which is essentially a generalized Heisenberg chain of length $N+1$ (N electrons and the impurity) with M flipped spins from the ferromagnetic vacuum state. There are, however, two important differences with the usual Heisenberg chain: (1) the expression of the energy is different, and (2) the symmetries of the Heisenberg ring are broken. The latter is evident from the factor involving g^{-1}, which in the thermodynamic limit gives rise to the Kondo temperature, $T_{\mathrm{K}} \propto \exp(-\pi/g)$. In the thermodynamic limit the rapidities form strings. The string hypothesis, however, is not valid for small systems. Here the rapidities can have real values or be pairs of complex conjugated numbers.

The partition function Q is a product of three factors, $Q = Q_{l\neq s} Q_q Q_{\rm K}$: *(i)* Since s-waves can be split off, $Q_{l\neq s}$ arises from all electron states other than s-waves, *(ii)* the charges of the s-states are free and decoupled from the spin degrees of freedom, Q_q, and *(iii)* the spin contribution of the s-waves and the impurity yields $Q_{\rm K}$. Here we study the effects of the last factor.

For $N = 2$ there are three spins (including the impurity) such that the spin space consists of 8 states, classified according to their S_z projection. The $S_z = 3/2$ state is the Bethe *Ansatz* vacuum with zero energy. There are three $M = 1$ states characterized by a real spin rapidity that satisfies

$$2\arctan(2\lambda_\alpha) + \arctan[2(\lambda_\alpha + g^{-1})] = \pi J_\alpha \,, \tag{3}$$

where periodic boundary conditions require that $J_\alpha = -1/2, 1/2$ or $3/2$ and

$$E(J_\alpha) = -L^{-1}[2\arctan(2\lambda_\alpha) + \pi] \tag{4}$$

is the energy. Note that $J_\alpha = -3/2$ yields a non-physical solution, firstly because it has the same energy as the vacuum, but a spin-flip allows the particles to rearrange, reducing the energy. Secondly, in the limit of a decoupled impurity ($g \to 0$) it does not have a solution for the same branch of the arctan function. For $J_\alpha = 3/2$ we have $\lambda_\alpha = \infty$. Two limits are of special interest: *(i)* for $g \to \infty$ the impurity is strongly coupled to the host and the system acts like a ring of three sites ($E = -2\pi n/3L$, with $n = 1,\ 2,\ 3$), and *(ii)* for $g \to 0$ the impurity is decoupled and the behavior is that of two sites ($E = -\pi n/L$, with $n = 0,\ 1,\ 2$). The energy spectrum as a function of g^{-1} is shown in Fig. 1(a). Here F is the ferromagnetic vacuum state and J denote the states with one real rapidity. The remaining four states are obtained by reversing all the spins.

The partition function for the spin sector is

$$Q_{\rm K} = 2\cosh\left(\frac{3H}{2T}\right) + 2\cosh\left(\frac{H}{2T}\right)\sum_J \exp\left[\frac{-E(J)}{T}\right] . \tag{5}$$

The Curie constant (χT) and the entropy as a function of TL for $g = 0$, 1 and ∞ are displayed in Fig. 1(b) and 1(c), respectively. The discrete spectrum yields an exponential activation at low T. Note that, since N is even, the ground state has a remaining spin 1/2. In contrast to the infinite system it is not possible to extract the impurity contribution in the present case.

The gaps decrease with increasing particle size and in the thermodynamic limit the finite size corrections to the energy are given by the conformal towers. The gaps are then infinitesimal and the system is a Fermi liquid, *i.e.*

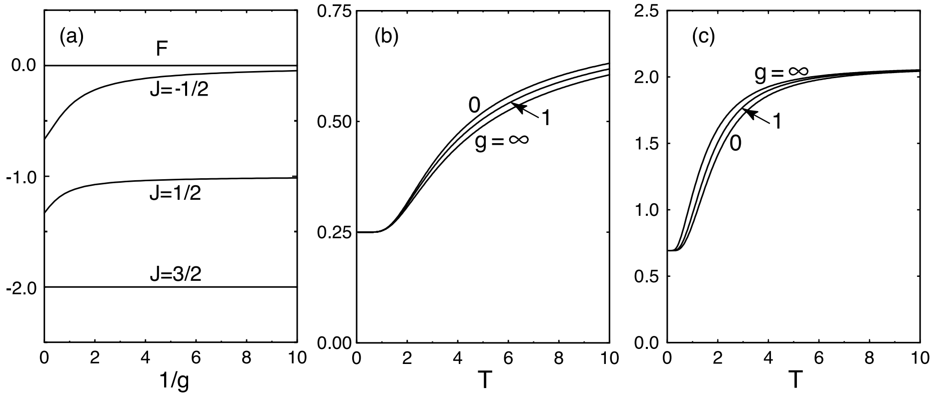

Fig. 1. (a) Energy levels, EL/π, as a function of g^{-1}, (b) Curie constant, χT, and (c) entropy, S, as a function of TL (for $L = 1$) for $g = 0$, 1 and ∞.

χ is finite and the specific heat is proportional to T. In this limit the effects of the impurity can be separated from those of the host (L^{-1} corrections).

The competition of T_{K} with the finite size of the system is best seen in the dependence of the energy levels on the coupling constant, $g^{-1} = \pi^{-1}\ln(D/T_{\mathrm{K}})$. The variation of the energies with g^{-1} is largest for small g^{-1}, corresponding to large T_{K}. For large g^{-1} the Kondo temperature is much smaller than the level spacing and the effect of the Kondo coupling is only weak. This crossover is similar to the one found in Ref. [3].

A Kondo impurity embedded into a small particle is equivalent to a single electron quantum dot in the Coulomb blockade regime coupled to a short quantum wire. Due to the quantization of the energy levels the system at low T is rather stable to electric and magnetic fields. Small changes in the bias voltage do not affect the quantum dot, because the spin and charge sectors are decoupled. The $T = 0$ magnetization shows plateaus as a function of field and can be changed with a magnetic tip. The steps are rounded off at low T, but the step structure remains, such that the system could be used as a magnetic storage device.

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