Zero Temperature Series Expansions for the Kondo Lattice Model at Half Filling

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We present new results for the Kondo lattice model of strongly correlated electrons, on the simple cubic lattice, obtained from high-order linked-cluster series expansions. Results are given for various ground state properties at half-filling, and for spin and charge excitations. Estimates for the location of the quantum critical point are made.

The Kondo lattice model, described by the usual Hamiltonian

$$H = -t \sum_{<ij>\sigma} (c_{i\sigma}^{+} c_{j\sigma} + h.c.) + J \sum_{i} \mathbf{S}_i \cdot \mathbf{s}_i \quad (1)$$

represents a band of conduction electrons, interacting via a spin-exchange term with a set of immobile $s = \frac{1}{2}$ spins $\mathbf{S}_{\mathrm{i}}$ (f electrons). This is illustrated schematically in Figure 1.

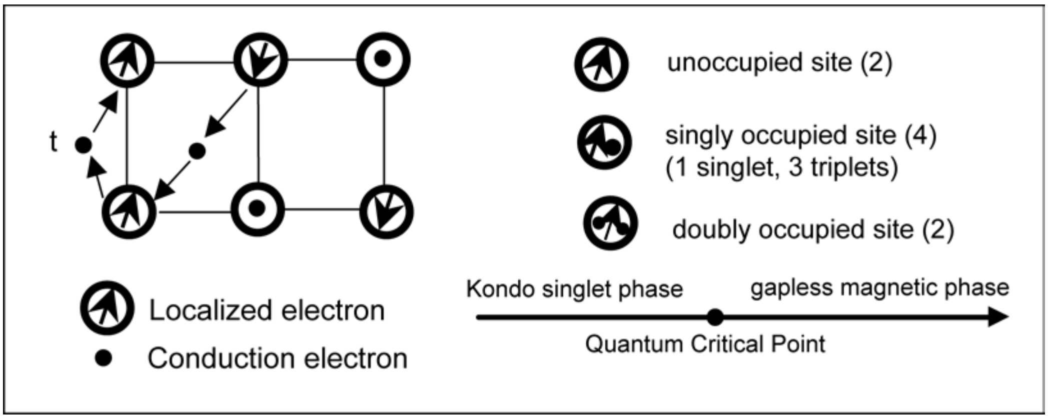

Fig. 1. Schematic illustration of the Kondo lattice model.

The model has been extensively studied in connection with a class of materials known as "Kondo insulators" [1,2] ($J > 0$), and in connection with the manganites ($J < 0$) [3]. Despite the apparent simplicity of the model, in which neither the conduction electrons nor localized spins interact directly among themselves, the spin exchange leads to a strongly-correlated many-body system. No exact results are known for either ground state or thermodynamic properties for general J/t, in any dimension.

The model incorporates two competing physical processes. In the strong-coupling (large J) limit, the conduction electrons are "frozen out" via the formation of local singlets ($J > 0$) or triplets ($J < 0$). In either case there will be a gap to spin excitations and spin correlations will be short ranged. On the other hand, at weak coupling, the conduction electrons can induce the usual RKKY interaction between localized spins, giving rise to possible magnetically ordered phases with no spin gap and long-range correlations. In one dimension there will be a smooth crossover from large J to small J behaviour, but in higher dimension a quantum phase transition is expected.

In this work we use linked cluster series expansion methods [4] to investigate the ground state properties of the Kondo lattice model on the simple cubic lattice, extending previous work [5] by several terms, as well as calculating, for the first time, the energies of elementary excitations. Further details of this work, including results for the linear chain and square lattice, are given in a full paper [6].

The linked cluster method expresses the bulk property, say the ground state energy E_0, as a sum over contributions from connected clusters of sites on the lattice, e.g.

$$E_0 / N = \sum_g c_g \varepsilon_g \quad (2)$$

where c_g is the embedding factor of cluster g in the lattice and ε_g is a "proper" or "cumulant" energy, which can be obtained recursively for larger and larger clusters. If we write the Hamiltonian in generic form as $H_0 + \lambda V$, where H_0 is a solvable unperturbed part and V is treated perturbatively, then (2) allows a perturbative expansion of E_0 / N in powers of the parameter λ. Similar expressions can be obtained for other quantities.

The most obvious choice is to take the exchange term in (1) as H_0, and to treat the hopping term perturbatively. This yields an expansion

$$E_0 / NJ = \sum_{s=0}^{\infty} e_s (t/J)^s \quad (3)$$

where we have computed terms to order $(t/J)^{12}$. The coefficients of this, and also series for the minimum triplet gap and antiferromagnetic susceptibilities for both local and conduction electrons, are given in Table 1.

Table 1. Series coefficients for dimer expansions for the ground energy per site E_0 / N, the minimum triplet spin gap Δ_s / J, and the antiferromagnetic spin susceptibilities for both local and conduction spins (χ_l and χ_c). Nonzero coefficients $(t/J)^n$ up to order n = 12 for simple cubic lattice are listed.

n	E_0 / JN	Δ_s / J	χ_c	χ_l
0	-0.750000000	1.000000000	0.500000000	0.500000000
2	-2.000000000	-20.00000000	2.666666667	9.777777778
4	0.666666667	306.3111111	12.91555556	84.43753086
6	7.834807760	1060.237771	51.32587514	239.9390035
8	-71.14791245	-276065.8123	351.0946982	1684.588635
10	349.8368486	3860398.011	1354.232378	12172.47537
12	160.3723348	555719090.0	2797.156237	-25148.75289

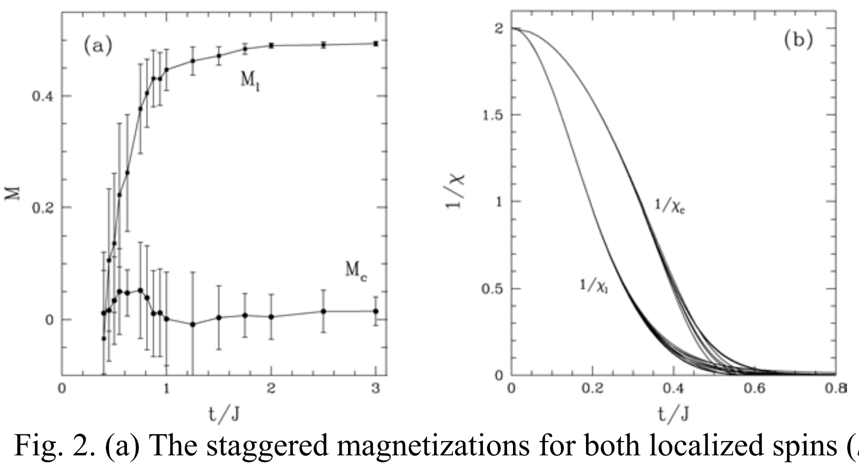

Fig. 2. (a) The staggered magnetizations for both localized spins (l) and conduction electrons (c); (b) the inverse antiferromagnetic spin susceptibilities for the simple cubic lattice.

We consider only the "half-filled" case where the number of conduction electrons is equal to the number of sites. To estimate the location of the **quantum phase transition** between the nonmagnetic (small *t/J*) and magnetic (large *t/J*) phases we first use Padé approximant methods to analyse the energy series. This results in the estimate

$$(t/J)_c = 0.46 \pm 0.01$$

This is consistent with, but more precise than, previous work.

An alternative approach is to evaluate the staggered magnetization directly via integrated different approximants. These results are shown in Figure 2. These results confirm the presence of a quantum phase transition around $t/J \approx 0.5$.

Finally we consider elementary excitations from the ground state, of which there are three kinds,

Triplet spin excitations which, in the large *J* limit, correspond simply to a Kondo singlet excited to Kondo triplet, which can then propagate.

One-hole or "quasiparticle" excitations which correspond to a removal of one electron from the half-filled band and hence, in the strong coupling limit, to a single localized spin at one site and Kondo singlets on all other sites.

Charge excitations, in which the system remains half-filled but with a doubly filled site and an empty site.

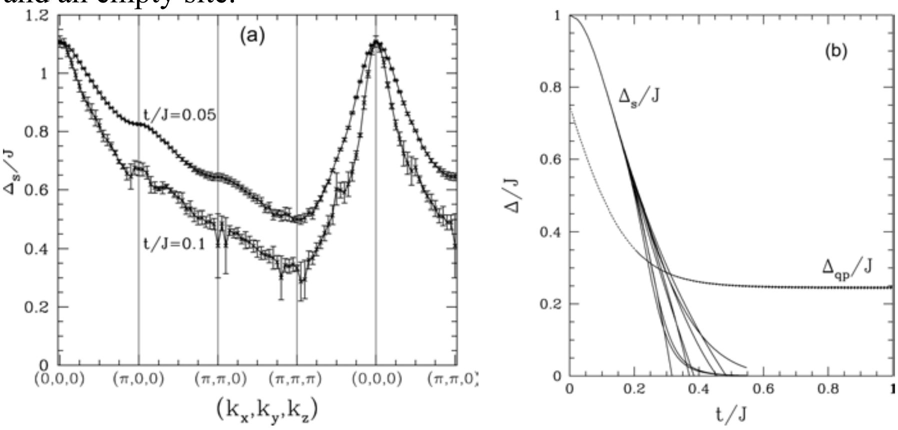

Fig. 3. The triplet spin excitation spectrum (a) and the triplet spin gap Δ_s / J and quasiparticle gap Δ_{qp} / J as function of *t/J* (b) for the simple cubic lattice.

Figure 3 shows the triplet spin excitation spectrum, and the triplet spin gap and the quasiparticle gap as functions of *t/J.* This figure shows clearly the quantum phase transition between the gapped phase ($\Delta_s > 0$) and the gapless phase ($\Delta_s = 0$). There appears to be no anomaly in the quasiparticle gap at this point.

Acknowledgments

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