Finite Temperature Strong-Coupling Expansions
For the Kondo Lattice Model

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Strong-coupling expansions, to order $(t/J)^8$, are derived for the Kondo lattice model of strongly correlated electrons, on the simple cubic lattice at arbitrary temperature. Results are presented for the specific heat and spin susceptibility, for varying electron density and temperature.

This paper studies the thermodynamic properties of the Kondo lattice model, described by the Hamiltonian

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

The first term describes a single band of conduction electrons, the "Kondo coupling" term represents an exchange interaction between conduction electrons and a set of localized $S = \frac{1}{2}$ spins, and the final term allows for variable conduction electron density via a chemical potential. The antiferromagnetic model is believed to be relevant to heavy-electron systems such as $CeCu_{6-x}Au_x$ [1] where non-Fermi liquid behaviour is observed near a quantum critical point. A popular scenario [2] is that low energy spin fluctuations, as represented by the Kondo lattice model, are an essential part of the physics of these systems.

The Kondo lattice model combines two competing physical effects. In the strong coupling (large $|J|$) limit, the conduction electrons will form local singlets ($J > 0$) or triplets ($J < 0$) with the localized spin at each site. 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, leading to magnetic order.

Despite the apparent simplicity of the model, no exact results are known, either at $T = 0$ or at finite temperatures, in any spatial dimension. We know of only a few previous studies of this model at finite temperature. Röder *et al.* [3] considered the ferromagnetic model in the limit $J \to -\infty$, on the simple cubic lattice, via a high temperature expansion. Here we treat the general J case and focus on the antiferromagnetic model. Haule *et al.* [4] have treated the 2D case, primarily via a numerical finite temperature Lanczos method. We compare our results with this work wherever possible. Haule *et al.* have also considered the atomic limit ($t = 0$), and the order t^2 correction terms.

Our approach treats the single site terms exactly and treats the hopping term perturbatively. It is, thus, an expansion about the "atomic limit". The calculation starts from an expansion of the grand partition function

$$\mathrm{Z} = \mathrm{Tr}\{e^{-\beta(H_0+V)}\} = z_0^N \left\{ 1 + \sum_{r=1}^{\infty} (-1)^r \int_0^{\beta} d\tau_1 \cdots \int_0^{\tau_{r-1}} d\tau_r \left\langle \widetilde{V}(\tau_1) \cdots \widetilde{V}(\tau_r) \right\rangle \right\} \qquad (2)$$

where $z_0 = 2 + (e^{3K} + 3e^{-K})\zeta + 2\zeta^2$, $K = \beta J / 4$, and $\zeta = e^{\beta\mu}$, $\beta = 1/k_B T$. The V operators are the hopping terms, in the interaction representation.

The free energy (grand potential) is then given by

$$-\beta F / N = \ln z_0 + \sum_{\{G\}} C_G W_G(t, K, \zeta)$$

where the sum is over a set of finite clusters or "graphs", with C_G being a numerical embedding factor, and W_G the "graph weight". This latter quantity can be expressed in the form

$$W_G(t,\zeta) = z_0^{-p}(t/J)^l \sum_{i,j,k} a_{i,j,k} K^i e^{jK} \zeta^k$$

where *p, l* are the number of points and lines in the graph, and the $a_{i,j,k}$ are numerical constants. Evaluation of these expressions is a lengthy procedure, involving a trace over a space of 8^p states and evaluation, for each terms in the trace, of an *r*-fold multiple integral. Figure 1 shows an example of a graph, and its corresponding weight.

$$W = z_0^{-2}(t/J)^2 X$$

$$X = (\zeta+\zeta^3)[\tfrac{1}{2}K^2(e^{3K}+9e^{-K})+\tfrac{3}{4}K(e^{3K}-e^{-K})] + \zeta^2 K(\tfrac{1}{6}e^{6K}+3e^{2K}+\tfrac{9}{2}e^{-2K}+\tfrac{4}{3})$$

Fig. 1. The lowest order graph for the free energy and its corresponding weight.

We have computed the series to order $(t/J)^8$. From the free energy we compute the internal energy and average particle number. Inversion of the latter series allows quantities to be evaluated for fixed temperature and electron density.

In our full paper [5] we present and discuss results for the linear chain, square lattice, and simple cubic lattice. Here we consider only the simple cubic lattice.

Figure 2 shows the specific heat at temperature *T* for the simple cubic lattice, at half-filling (n = 1) for various ratios of *t/J.*

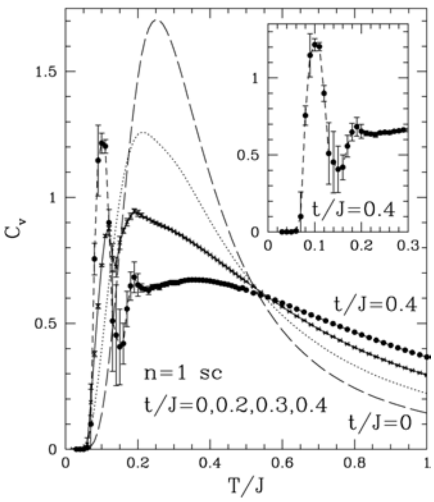

Fig. 2. The specific heat C_v versus *T/J* for the simple cubic lattice at n = 1 for *t/J* = 0, 0.2, 0.3, 0.4. The inset enlarges the small *T/J* region for *t/J* = 0.4.

A two-peak structure is evident for the larger values of *t/J*. We believe that the broad high-temperature peak is due to the conduction electrons, while the emerging low temperature peak arises from fluctuating local spins, which become correlated with increasing *t*. To display the effect of conduction electron density we have chosen a fixed intermediate value *t/J* = 0.3 and show, in Figure 3, the specific heat as a function of temperature for various values of band filling n = 0.25, 0.5, 0.75, 1.

The decrease in the high-temperature with decreasing *n* confirms the assignment of this peak to conduction electrons. To explore the magnetic properties we have computed the magnetic susceptibility χ_S. Fig. 4 shows χ_S as a function of temperature in two ways: for half-filling and various values of *t/J,* and for fixed *t/J* = 0.3 for various electron densities.

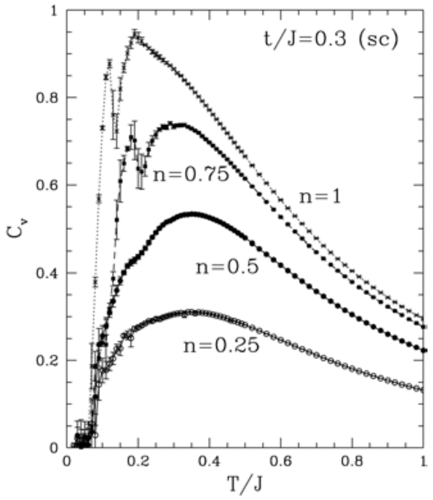

Fig. 3. The specific heat C_v versus *T/J* for simple cubic lattice at *t/J*=0.3 for various electron densities *n*.

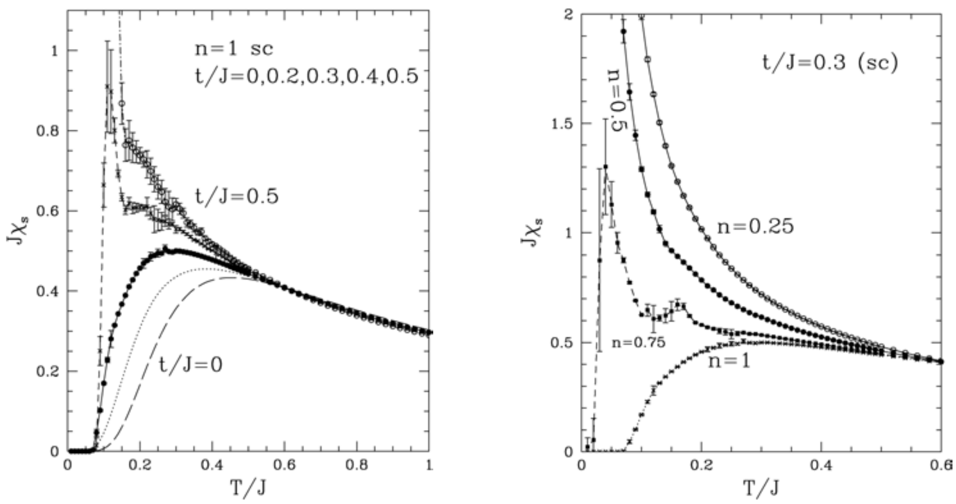

Fig. 4. Magnetic susceptibility versus temperature for the simple cubic lattice, showing the effects of varying *t/J* at *n* = 1 (a), and *n* at *t/J* = 0.3 (b).

For *n* = 1, at low-temperature, we see the development of a sharp peak for increasing *t/J*, consistent with increasing spin fluctuations. For fixed *t/J* = 0.3 the susceptibility shows a striking crossover from *n* = 1, where χ_S is structureless and vanishes as $T \to 0$, to lower densities n = 0.5, 0.25 where χ_S appears to diverge. Evidently *n* = 0.75 is near the critical concentration. A mean-field treatment [6] suggests the existence of a finite-temperature phase transition to a ferromagnetic phase for small *n*. The results of Fig. 4(b) support this conclusion.

Acknowledgments

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References

[1] H. von Löhneysen, J. Phys. Condens. Matter **8**, 9689(1996).
[2] M. Lavagna and C. Pepin, Phys. Rev. B**62**, 6450(2000).
[3] H. Röder, R.R.P. Singh and J. Zang, Phys. Rev. B**56**, 5084(1997).
[4] K. Haule, J. Bonca, and P. Prelovsek, Phys. Rev. B**61**, 2482(2000).
[5] J. Oitmaa and W. Zheng, Phys. Rev. B, to be published.
[6] H. Tsunetsugu, M. Sigrist, and K. Ueda, Rev. Mod. Phys. **69**, 809(1997).