561 Fall 2005 Lecture 11a

Solution of the Anderson Impurity Model and the Kondo Problem
See Phillips, Ch. 6 and 7. Also Mahan, Sec. 1.4, Ch. 11.

1. Exact solutions

Here we list the fact that there are exact solutions using the numerical renormalization group[1], the Bethe Ansatz[2] and quantum Monte Carlo[3]. Because problem is one dimensional (radial) it can be solved exactly by the Bethe Ansatz and the renormalization group. (We will describe the general idea and "poor man's scaling".) Quantum Monte Carlo is very general and in the case the Fermion sign problem can be treated well enough that that thermal, equilibrium properties are essentially exactly described.

The main results are that the exact solution is a non-magnetic single ground state and there is a characteristic energy scale T_K governing the properties as a function of energy and temperature. There is a logarithmic dependence on T/T_K and there is a *crossover* from high T spin fluctuations to low T coherent spin-quenched behavior. *There is no sharp phase transition.*

Solution of the Anderson Impurity Model in the Large Degeneracy Limit

The key idea of this approach is to identify a limiting case in which an analytic solution can be found that has the correct symmetry. The argument is that this captures the qualitative effects and that changing the hamiltonian to the actual one is an analytic continuation that preserves the symmetry and leads to the true solution.

Consider a problem in which the both the localized state and the host bands are N-fold degenerate; each of the $\nu = 1, \ldots, N$ localized states couples to the continuum band of states with labelled ν through a term that conserves ν, $V_{kL}[c^+_{k\nu} c_{L\nu} + c^+_{L\nu} c_{k\nu}]$, where V_{kL} is independent of ν. This the generalization of the spin problem and it is quite reasonable for a d state (N = 10) or an f state (N = 14). The problem can be solved exactly in the $N \to \infty$ limit.

The hamiltonian can be written exactly as for the Anderson model by replacing the spin index σ with an index $\nu = 1, \ldots, N$.

$$\begin{aligned} H &= H_{band} + H_{impurity} + H_{hybridization} \\ &= \sum_{k\nu} \left[\epsilon_k c^+_{k\nu} c_{k\nu} + \epsilon_L c^+_{L\nu} c_{L\nu} + \frac{U}{2} \sum_{k\nu' \neq \nu} n_{L\nu} n_{L\nu'} + V_{kL}[c^+_{k\nu} c_{L\nu} + c^+_{L\nu} c_{k\nu}] \right] \end{aligned} \tag{1}$$

All the step proceed as in the $N = 2$ case for $U = 0$ (N degenerate bands) and for the Hartree-Fock solution, except that now the case of one electron per site is not symmetric for $N > 2$. The sum rules require that the filled states integrated over energy summed over $\nu = 1, \ldots, N$ total one electron, and the empty states sum to $N - 1$ electrons.

This may seem a complication, but arguments for the $N \to \infty$ limit lead to a simple analytic solution that displays the key points.

The solution is given in Mahan (First Ed. gives the T=0 form and the second edition the finite T solution) and my handwritten notes (available). The interesting region is the case where $\epsilon_L << 0$ (where we set $E_F = 0$) and $\epsilon_L + U >> 0$, so that the occupation is approximately $n_L \approx 1$. The main results are that the ground state is an equal linear combination of the $\nu = 1, \ldots, N$ states, and that the energy is lowered by an amount

$$\delta = We^{-\frac{\pi}{N\Delta}|\epsilon_L|} \tag{2}$$

where

$$\Delta \equiv \pi|V|^2\rho(E_F) \tag{3}$$

is the resonance width for the each of the N impurity states in the non-interacting $U = 0$ case.

Note that the combination $N\Delta$ appears in teh formula. This is the key step in understanding the simplification in the large N limit: allow N to become large while keeping the combination $N\Delta$ fixed.

The result is a spectrum like that shown in the figure. Note the asymmetry and the fact that the lower band has width $N\Delta$. Note the sharp peak with narrow width that is required to be at the Fermi energy. This feature leads to the satisfaction of the Friedel sum rule!

The key point is that no matter how small is the coupling V, it leads to the strongly coupled ground state with nonmagnetic character. The energy scale is set by δ which determines T_K, and δ depends *exponentially* upon the "bare" parameters of the problem. *A new collective energy scale in the strongly interacting system!*

As stated in the previous notes, the characteristic temperature T_K varied wildly - from 300 K for V in Au (even higher but hard to observe at high T where many other effects obscure the Kondo effect) to 10^{-4} K for Mn in Au.

Transformation of Anderson Impurity Model in large U limit to the impurity spin model

See Phillips, Ch. 7.

Schrieffer-Wolfe transformation to an effective spin model with antiferromagnetic coupling J of a localized spin and the band elactrons.

Poor Man's scaling

See Phillips, Ch. 7.

The key idea is to integrate out the effects of high energy band states and work ones way down to a renormalized problem with large coupling J_{eff} even if the bare starting J was small.

References

[1] K. G. Wilson, 'The renormalization group: Critical phenomena and the kondo problem', *Rev. Mod. Phys.* 47:773–840, 1975.

[2] N. Andrei, K. Furuya, and J. H. Lowenstein, 'Solution of the kondo problem', *Rev. Mod. Phys.* 55:331–402, 1983.

[3] J. E. Hirsch and R. M. Fye, 'Monte Carlo Method for magnetic impurities in metals', *Phys. Rev. Lett.* 56:2521–2524, 1986.