The Anderson Lattice

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Abstract

In this lecture a review of the existing theories of the Anderson model for a single magnetic impurity and for the lattice case will be given. The basic physics of the model will be discussed and some of the theoretical methods used will be critically evaluated. New alternative approaches will be suggested.

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I. Introduction

In 1961 Anderson proposed a model for a magnetic impurity in a metallic matrix, which incorporates the basic ingredients of moment formation in metals: a localized atomic state with strong Coulomb correlations hybridizing with a band of conduction electrons. The Hamiltonian of this problem in its simplest form is given by

$$H = H_c + H_f + H_{mix} \qquad (1a)$$

where

$$H_c = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{+} c_{\mathbf{k}\sigma} \qquad (1b)$$

and

$$H_f = \epsilon_f^o \sum_{\sigma} n_{\sigma}^f + U n_{\uparrow}^f n_{\downarrow}^f \qquad (1c)$$

are the Hamiltonians for the conduction electrons (c) and the localized electrons (f), respectively, and

$$H_{mix} = V \sum_{\mathbf{k}\sigma} (c_{\mathbf{k}\sigma}^{+} f_{\sigma} + h.c.) \qquad (1d)$$

is the hybridization term. For an orbitally nondegenerate impurity level and allowing for the two spin states σ, the possible occupation numbers of the local level are $0, 1, 2$. We will later discuss models with $N = 2S + 1$ spin states, where the limit $N \to \infty$ is taken.

The part of parameter space relevant for moment formation is the one where the local level is well below the Fermi level $\epsilon_f^o << E_F$, and the Coulomb repulsion is strong such that the energy for the doubly occupied level is far above the Fermi level (see Fig. 1). In the limit $U \to \infty$ there will be at most one electron in the local state,

and for small hybridization the average number of electrons $< n^f >$ is close to one. One may then expect a local magnetic moment to be formed. At low temperatures the moment is screened by the conduction electrons via the socalled Kondo effect, and a spin singlet state is formed (Anderson 1973; Wilson 1975). The low temperature properties may be phrased in terms of a local Fermi liquid theory (Nozieres 1974). At temperatures above the energy of spin singlet formation perturbation theory in (V^2/ϵ_f^o) may be applied to give e.g. the famous Kondo minimum in the resistivity as a function of temperature (Kondo 1964). It turns out that the crossover between the two temperature regimes is difficult to describe. Although there exist exact results on the energy spectrum obtained by Bethe ansatz techniques (Andrei et al. 1983, Tsvelick and Wiegmann 1983), a controlled description of the excited states of the system, needed e.g. for the calculation of transport properties, is still lacking. This is even more so for the Anderson lattice, consisting of a regular array of Anderson impurity atoms. There, in particular the interplay between Kondo screening and conduction electron induced magnetic exchange (RKKY) interaction between the localized spins is not well understood.

2. Anderson Impurity Model

An important breakthrough in the theoretical formulation occurred in the early 80's when the concept of slave bosons (Barnes 1976) was applied (Coleman 1984). The idea is to represent the projection operator onto the part of the Hilbert space with no double occupancy (in the $U = \infty$ limit!) by a bose operator b, which describes the creation (b^+) or annihilation (b) of the empty local atomic level. Using these

operators the mixing term may be expressed as

$$H_{mix} = V \sum_{\mathbf{k},\sigma} (c_{\mathbf{k}\sigma}^+ b^+ f_\sigma + h.c.) \tag{2}$$

describing the annihilation of an f-electron and the simultaneous creation of a conduction electron and an empty site. The Coulomb interaction term may be dropped since the number of doubly occuped sites is exactly zero in this limit. The b bosons are "slaved" because the local level is either empty or singly occupied, i.e.

$$Q \equiv b^+ b + \sum_\sigma f_\sigma^+ f_\sigma = 1 \tag{3}$$

In other words, these bosons cannot form a macroscopic condensate as free bosons do, because of the local constraint (3).

It is now convenient to generalize the original Anderson model by allowing for $N = 2S + 1$ spin states, i.e. the spin index σ in (1) runs from $-S$ to S, describing a spin S local level coupled to N conduction bands. This model is referred to as the $SU(N)$ Anderson model. The model does not really describe a spin $S = 5/2$ or $S = 7/2$ impurity as encountered e.g. in the case of rare earth ions, because the number of conduction electron bands hybridizing with the local level is usually less than $2S + 1$, and only certain linear combinations of local substates are coupled to the conduction electrons (for a discussion of this point for the lattice model see Zou and Anderson (1986) and Zhang and Lee (1987)).

The N-state model is appealing because it can be solved exactly in the limit $N \rightarrow \infty$. For this limit to make sense the hybridization matrix element V has to scale with N as $V = \tilde{V} N^{-1/2}$. The solution is obtained from a mean field treatment of the

model Hamiltonian

$$H = H_c + \epsilon_f^o n^f + \frac{\tilde{V}}{\sqrt{N}} \sum_{\mathbf{k}\sigma}^{+} b^+ f_\sigma + h.c.)$$
$$+ \lambda(n^f + b^+ b - 1)$$

(4)

where the last term is a Lagrange multiplier term enforcing the constraint (3). Here the Lagrange parameter λ is not a classical variable, but rather is a real, scalar quantum field, e.g. $\lambda = \frac{1}{\sqrt{2}}(\Lambda + \Lambda^+)$ where Λ is a Bose field. The constraint is enforced by requiring λ to be time-independent, i.e. $\frac{\partial}{\partial t}\lambda = 0$.

The mean field assumption now is to consider the Bose fields to be classical variables, which may be replaced by their (time-independent) expectation values $< b^+ >=< b >= b_o$ and $< \lambda >= \lambda_o$. This reduces the problem to diagonalization of a noninteracting system. Minimization of the free energy with respect to λ_o and b_o then gives the Euler-Lagrange equations

$$b_o^2 = 1 - < n^f >$$

(5a)

and

$$\tilde{V} N^{1/2} \sum_{\mathbf{k}} < f_\sigma^+ c_{\mathbf{k}\sigma} >= -\lambda_o b_o$$

(5b)

The f-particle Green's function is obtained as

$$G^f(\omega) = \frac{1}{\omega - \epsilon_f + i\Gamma}$$

(6a)

where

$$\epsilon_f = \epsilon_f^o - \lambda$$

(6b)

is the renormalized energy of the f-level and

$$\Gamma = \pi b_o^2 \frac{\tilde{V}^2}{N} \rho_c$$

(6c)

is its renormalized width (ρ_c is the DOS of the conduction band). The density of f-states is given by

$$\rho_f(\epsilon) = \frac{1}{\pi} \frac{\Gamma}{(\epsilon - \epsilon_f)^2 + \Gamma^2} \tag{7}$$

and the average number of f-particles is

$$n_f \equiv < \sum_\sigma f_\sigma^+ f_\sigma > = \frac{N}{\pi} tan^{-1}(\frac{\Gamma}{\epsilon_f}), \quad T = 0$$
$$\simeq \frac{N\Gamma}{\pi\epsilon_f} = b_o^2 \frac{\tilde{V}^2 \rho_c}{\epsilon_f} \tag{8}$$

In order to evaluate the second Euler-Lagrange equation (5b) one needs the local $f - c$ Green's function

$$G_{fc}(\omega) = b_o \tilde{V} N^{-1/2} G_c^o(\omega) G_f(\omega) \tag{9}$$

where

$$G_c^o(\omega) = \sum_k \frac{1}{\omega - \epsilon_k + i0} \tag{10}$$

Using

$$\sum_k < f_\sigma^+ c_{k\sigma} > = -\frac{1}{\pi} \int d\omega Im G_{fc}(\omega) \tag{11}$$

one finds from (9) the equation for the energy scale

$$\epsilon_f^o - \epsilon_f = \tilde{V}^2 \rho_f \ell n \left[\frac{(\epsilon_f^2 + \Gamma^2)^{1/2}}{D}\right] \tag{12}$$

which may be solved in the Kondo limit, i.e. for large negative ϵ_f^o, to give

$$(\epsilon_f^2 + \Gamma^2)^{1/2} \equiv T_K = D \exp(\frac{\epsilon_f^o}{\tilde{V}^2 \rho_c}) \tag{13}$$

Since we expect $n_f \to 1$ in the Kondo limit, we find from (8) that

$$\Gamma \simeq \frac{\pi\epsilon_f}{N} \tag{14}$$

and

$$b_o^2 = \frac{\epsilon_f}{\tilde{V}^2 p_c} \simeq \frac{T_k}{\tilde{V}^2 \rho_c} \tag{15}$$

The real f-electron propagator is defined in terms of the slave bosons b and pseudo fermions f as $G_\sigma^{f-el}(\tau) = - < T_\tau \left\{ b^+(\tau) f_\sigma(\tau) f_\sigma^+(0) b(0) \right\} >$. In the above MFA the Bose operators factorize, i.e. $G_\sigma^{f-el} = b_o^2 G_{f\sigma}$. Hence, the f-electron DOS is given by $\rho_{f-el}(\epsilon) = b_o^2 \rho_f(\epsilon)$, with $\rho_f(\epsilon)$ given by (7).

In the Kondo limit and for N large the density of states $\rho_{f-el}(\epsilon)$ shows a resonance of width $\Gamma \propto \frac{1}{N}$ located at energy T_K above the Fermi energy (see Fig. 1). A more refined calculation shows that there remains a broad maximum at ϵ_f^o, the position of the atomic level.
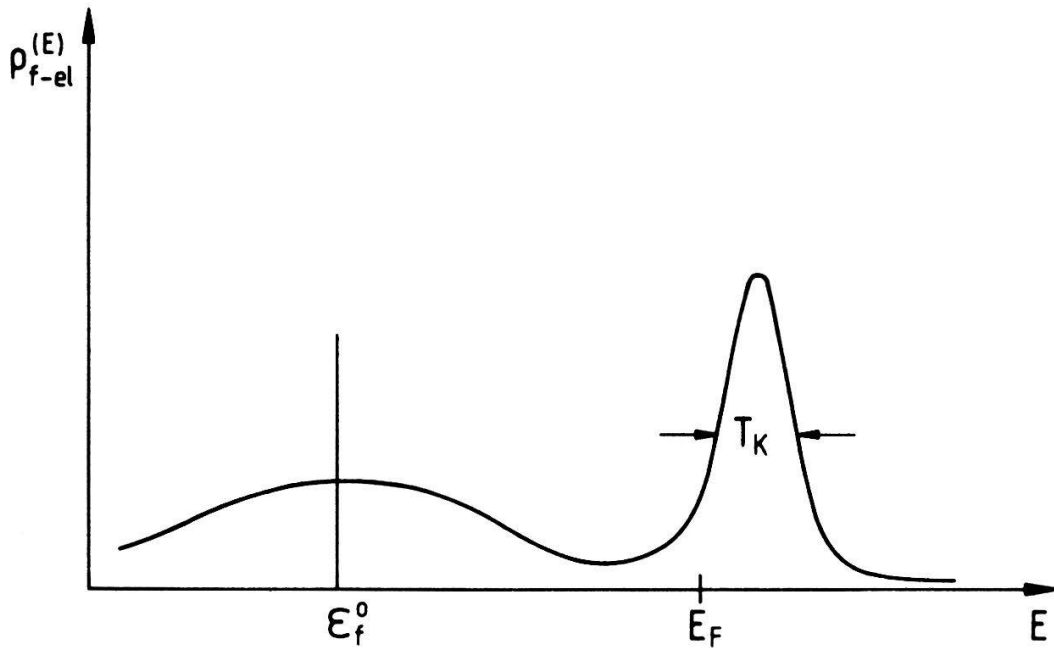

Fig. 1: Density of states of f-electrons in the Kondo problem.

The thermodynamic properties at low temperature may now easily be calculated (Read and Newns 1983). One finds a linear specific heat $c_v = \gamma T$, with

$$\gamma \simeq \frac{1}{3} k_B^2 n_f / \epsilon_f \tag{16}$$

and a T-independent magnetic susceptibility

$$\chi \simeq \mu_{eff}^2 n_f / \epsilon_f \tag{17}$$

as appropriate for a Fermi liquid at low temperature. A critical quantity in this problem is the so-called Wilson ratio

$$R = \left(\frac{\pi^2 k_B^2}{\mu_{eff}^2} \right) \frac{\chi}{\gamma} \tag{18}$$

found to be $R = 1$ in mean field theory. Deviations from $R = 1$ are a measure of the local Fermi liquid interaction induced by the Kondo impurity (Nozieres 1974).

The above results should be compared with the exact solution of the large N model, obtained using the Bethe ansatz method, which is given by (Andrei et al. 1983; Tsvelick and Wiegmann 1983)

$$R = 1 + \frac{1}{N - 1} \tag{19}$$

For $N = 2$, this is equal to $R = 2$, the value first obtained by Wilson. In the limit $N \to \infty$ the mean field result (16, 17) is seen to agree with (19), but one should also note that this limit is trivial in the sense that many body renormalization is absent from R.

Corrections to the mean field result may be calculated in a systematic way by expanding in $\frac{1}{N}$. The leading correction is obtained by summing the diagrams with

the maximum number of fermion loops in each order (this is similar to the usual RPA approximation for the electron gas, which is the first correction term in the limit of high electron density). Alternatively, the $\frac{1}{N}$-correction is obtained from a calculation of the Gaussian fluctuations about the mean field in a functional integral representation. The results (Rasul and Hewson 1984) obtained to $O(\frac{1}{N})$ for n^f, γ and χ are in agreement with exact Bethe ansatz results (Ogievetskii et al 1983, Schlottmann 1982), if the cutoff energy in the latter is suitably chosen.

3. Anderson Lattice

The preceding mean field theory may immediately be carried over to the Anderson lattice model (Read and Newns 1983; Auerbach and Levin 1986; Millis and Lee 1987), defined in slave boson representation by

$$
\begin{aligned}
H = H_c + \epsilon_f^o \sum_{i\sigma} n_{i\sigma}^f + \tilde{V} N^{-1/2} \sum_{i\sigma} \left[c_{i\sigma}^+ b_i^+ f_{i\sigma} + h.c. \right] \\
+ \sum_i \lambda_i \big(b_i^+ b_i + \sum_\sigma f_{i\sigma}^+ f_{i\sigma} - 1 \big)
\end{aligned}
\tag{20}
$$

Introducing the mean field values b_o and λ of b_i and λ_i one finds the effective Hamiltonian

$$
\begin{aligned}
H_{MF} = H_c + (\epsilon_f^o + \lambda) \sum_{k\sigma} f_{k\sigma}^+ f_{k\sigma} + b_o \tilde{V} N^{-1/2} \sum_{k\sigma} (c_{k\sigma}^+ f_{k\sigma} + h.c.) \\
+ \lambda (b_o^2 - 1).
\end{aligned}
\tag{21}
$$

Diagonalization yields renormalized quasiparticle bands with energy

$$
E_{\mathbf{k}}^{\pm} = \frac{1}{2} \left\{ \epsilon_f + \epsilon_{\mathbf{k}} \pm \sqrt{(\epsilon_f - \epsilon_{\mathbf{k}})^2 + 4 b_o^2 \tilde{V}^2 / N} \right\}
\tag{22}
$$

where the renormalized f- level energy is given by $\epsilon_f = \epsilon_f^o + \lambda$ (see Fig. 2). Minimization of the free energy yields the same Euler-Lagrange equations (14,15) for b_o

and λ as for the single impurity problem. In addition, the chemical potential μ needs to be determined by fixing the total number of particles

$$n = n^f + n^c = n^f + N(\mu - \epsilon_a)/2D \tag{23}$$

Here ϵ_a is the lower band edge of the lower quasiparticle band and a constant bare density of states $\rho_c = \frac{1}{2D}$ has been assumed. The characteristic energy scale is set by the renormalized f-energy:

$$T_A \equiv \epsilon_f - \mu \tag{24}$$

determined by the equation

$$T_A - (\epsilon_f^o - \mu) = -N\tilde{V}^2\rho_c^o \; \ell n(\frac{T_A}{D + \mu}) \tag{25}$$
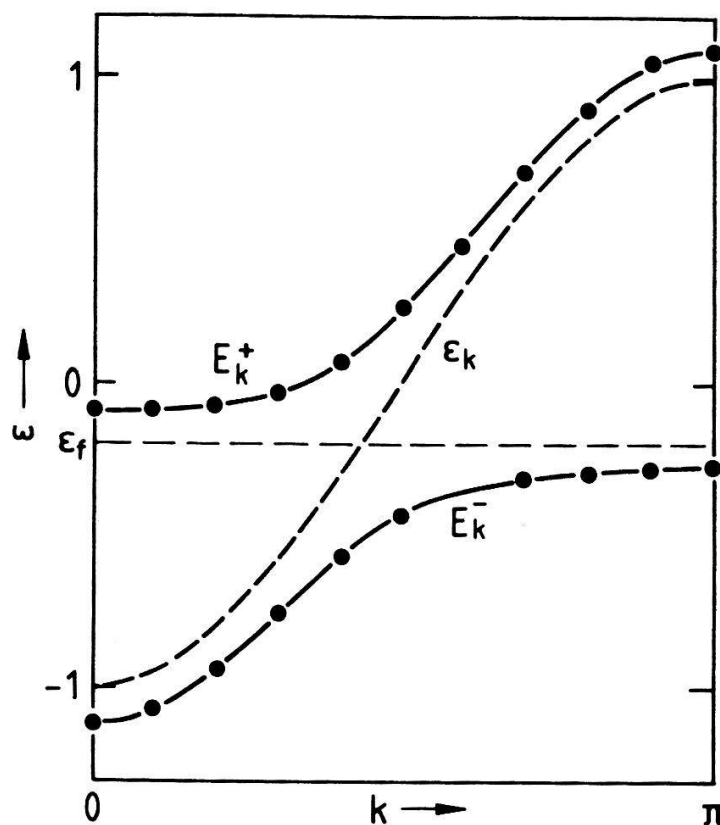
Fig. 2: Quasiparticle bands in a slave boson mean field theory of the Anderson lattice.

The specific heat coefficient γ and the magnetic susceptibility are given by the single impurity result (16,17) plus the conduction electron contribution

$$\gamma = \frac{\pi^2 k_B^2}{3}\left(\frac{n_f}{T_A} + \frac{N}{2D}\right) \tag{26a}$$

$$\chi = \frac{\mu_{eff}^2}{3}\left(\frac{n_f}{T_A} + \frac{N}{2D}\right) \tag{26b}$$

and the Wilson ratio $R = 1$ in MFA.

These results provide a first qualitative explanation of heavy fermion systems: for large negative $(\epsilon_f^o - \mu)$ and small hybridization $\bar{V}$ the characteristic temperature $T_A << T_F$, the Fermi temperature. Consequently, γ and χ are strongly enhanced by an effective mass factor $\frac{m^*}{m} \approx \frac{T_F}{T_A}$. The charge susceptibility χ_c, on the other hand, is found to be essentially unrenormalized.

The interpretation of this ground state is that of Kondo screened spins, where however the screening is a collective effect. This is seen by analyzing the conduction electron Green's function, which in MFA takes the form

$$G^c(k,\omega) = \frac{1}{\omega + \mu - \epsilon_k - \frac{V^2 b_o^2}{\omega + \mu - \epsilon_f}} \tag{27a}$$

At low frequencies, G^c reduces to the quasiparticle form

$$G^c(k,\omega) = \frac{z}{\omega - v_F^* \mid k - k_F \mid} \quad , \omega << \mid \epsilon_f - \mu \mid \tag{27b}$$

where $v_F^* = \frac{m}{m^*} v_F$ and $z = \frac{m}{m^*}$ is the quasiparticle weight factor. As seen from (27a), $G^c(k,\omega)$ approaches its noninteracting form $G^{c\,o} = (\omega - \epsilon_k)^{-1}$ only at much higher energies $\omega >> \mid V b_o \mid$, i.e. energy states in a shell of width $\sim \mid V b_o \mid$ about the Fermi surface participate in the formation of the Fermi liquid.

Furthermore, the spin polarization cloud around a given f spin may be shown to contain only $\Gamma/D << 1$ electrons, in contrast to the impurity case, where exactly one conduction electron is needed to screen a local spin$\frac{1}{2}$ (Millis and Lee 1987). Nozieres (1985) has pointed out that the screening of magnetic moments in an Anderson lattice can not easily take place locally at each site in an independent fashion. Given the extension of a screening cloud by $\xi = \hbar v_F/T_K$, for $T_K << T_F$ the screening clouds overlap substantially. If the characteristic velocity is replaced by $v_F^* = \frac{m}{m^*}v_F$, ξ turns out to be of the order of one lattice spacing, which would be acceptable. On the other hand, only a fraction T_K/T_F of the conduction electrons takes part in the screening of a single local spin, whereas the total number of conduction electrons would be necessary in the lattice case, i.e. all states in the energy band. This is clearly not the case, and as explained above only a fraction Γ/T_F of the electrons participate in the correlation effect, in contrast to the simple independent Kondo ion picture. Similar results have been obtained by variational methods using an adaptation of the Gutzwiller approach to the Hubbard model for the Anderson lattice (Rice and Ueda 1986), with one important difference: the Wilson ratio R, found in slave boson theories as given by (19), is found in the variational theory to depend crucially on the ratio $\alpha = [(\epsilon_f^o - \mu)/(\frac{1}{2}N\bar{V}^2)]$, as $R \propto -\ln^{-1}\alpha$. For $\alpha < 1$ the spin susceptibility is found to be negative, signalling a ferromagnetic phase transition. In other words, the normal Fermi liquid state is stable only for sufficiently large degeneracy N. It is unclear whether the variational result (presumably valid for all N) or the slave boson result for R (up to order $1/N$) are more reliable.

While the above mean field results appear reasonable, an extension of the theory to higher temperatures, to dynamical properties and to the calculation of the

quasiparticle interaction has proved to be difficult. A straightforward evaluation of the mean field theory at finite temperatures gives poor results. Here the main problem is that the mean field assumption $< b >= b_o$ corresponds to introducing a Bose condensed ground state. With increasing temperature the condensate will be depleted until at the critical temperature T_c^B a thermodynamic phase transition into the normal state takes place. The latter is an artefact of the meanfield assumption. In fact Bose condensation of slave bosons is impossible because the bosons at each lattice site are separately constrained by (3). As a consequence the model has a local gauge symmetry with respect to simultaneous gauge transformations $f_{i\sigma} \rightarrow e^{i\phi_i} f_{i\sigma}$ and $b_i \rightarrow e^{i\phi_i} b_i$, which eliminates the possibility of spontaneous symmetry breaking as implied by a finite expectation value $< b_i >$ (Elitzur 1975). Indeed, the calculation of $< b_i b_j^+ >$ to order $\frac{1}{N}$ shows that long range order, present in mean field theory, where $< b >\neq 0$, is destroyed by the phase fluctuations and only power law behavior $< b_i b_j^+ >\propto (R_{ij})^{-1/N}$ remains at $T = 0$ (Read 1985). At finite temperatures the spatial decay of $< b_i b_j^+ >$ is exponential. The effect of fluctuations can be expected to be largest in the transition regime and $T \simeq T_A$ or $\omega \simeq T_A$. A meaningful treatment of fluctuations clearly requires a nonlinear theory.

In a certain sense, such a theory already exists in the form of a self-consistent theory for the pseudo fermion and slave boson propagators: the non-crossing approximation or NCA (Kuramoto 1983). Originally derived diagrammatically using a particular form of perturbation theory in V (Keiter and Kimball 1971), the NCA is a kind of self-consistent one-loop approximation for the fermion and boson self-energies Σ_σ^f and Σ^b. The NCA may also be motivated using the slave boson method. For the

impurity problem, the selfenergies are found to satisfy the coupled equations

$$\Sigma_\sigma^f(\omega) = V^2 \sum_{\mathbf{k}}(1 - f_{\mathbf{k}}) \frac{1}{\omega - \epsilon_k - \sum^b(\omega - \epsilon_k)} \tag{28a}$$

$$\Sigma^b(\omega) = NV^2 \sum_{\mathbf{k}} f_{\mathbf{k}} \frac{1}{\omega + \epsilon_k - \epsilon_f^o - \sum_\sigma^f(\omega + \epsilon_k)} \tag{28b}$$

In general these equations have to be solved numerically.

Comparing the NCA results at not too low temperatures with exact results for the static properties one finds remarkably good agreement. Unfortunately the violation of exchange symmetry inherent in the NCA leads to spurious singularities in the NCA solutions in the limit of zero frequency and temperature, such that all Fermi liquid relations are badly violated for finite N. However, the energy scale below which the singular behavior develops is given by $T_{NCA} = T_K^2/\Gamma$, which in the Kondo limit is well below T_K itself, so that the NCA describes the crossover from low temperatures Fermi liquid behavior to high temperature local moment behavior correctly (Bickers 1987). An extension of the NCA has been applied to the lattice case (Grewe 1987).

More recently Jin and Kuroda (1988) have reported a diagrammatic $1/N$ expansion for both the impurity and the lattice Anderson model, which reproduces the limiting behavior at low temperatures and at high temperatures correctly and is free of spurious singularities. Starting point is the Hamiltonian (20), for which a perturbation theory in V is considered. The three propagators for the pseudo fermions, $G_\sigma^f(i\omega_n)$, the conduction electrons $G_{\mathbf{k}\sigma}^c(i\omega_n)$ and the slave bosons, $D(i\nu_n)$, are given in the lowest order by

$$G_\sigma^{f\,(0)}(i\omega_n) = (i\omega_n - \lambda - \epsilon_f^o)^{-1} \tag{29a}$$

$$Gk\sigma^{c\,(0)}(i\omega_n) = (i\omega_n - \epsilon_k)^{-1} \tag{29b}$$

$$D^{(0)}(i\nu_n) = (i\nu - \lambda)^{-1} \qquad (29c)$$

At this level one is working with a grand canonical ensemble with respect to the particle numbers Q_i. The physical subspace $(Q_i = 1)$ may be projected out of any correlation function or expectation value by considering the limit $\lambda \to \infty$ as defined by (Coleman 1984)

$$< \hat{O} >= \lim_{\lambda \to \infty} \Big[< \hat{O}\Pi_i Q_i >_\lambda / < \Pi_i Q_i >_\lambda \Big], \qquad (30)$$

where $< >_\lambda$ denotes the expectation value in the grand canonical ensemble. The limiting process (30) allows to pick out of the fugacity expansion of $< \hat{O} >_\lambda= \sum_{\{Q_i\}} < \hat{O} >_{\{Q_i\}} e^{-\beta \sum_i Q_i}$ the terms with $Q_i = 1$. For the free energy, a more convenient expression is (Coleman 1984)

$$\Delta F = -\frac{1}{\beta} \lim_{\lambda \to \infty} \Big[ln\{< \Pi_i Q_i >_\lambda \exp(-\beta \sum_i \lambda_i)\} \Big] \qquad (31)$$

$\mathsf{G_c}$: 〜〜〜

$\mathsf{G_f}$: ———

$\mathsf{G_b}$: - -►- -

$\mathsf{F} = $ [diagram] $+ \sigma$ [diagram] σ' $O(1)$

$+$ [diagram] $+ i,\sigma$ [diagram] j,σ $O\left(\frac{1}{N}\right)$

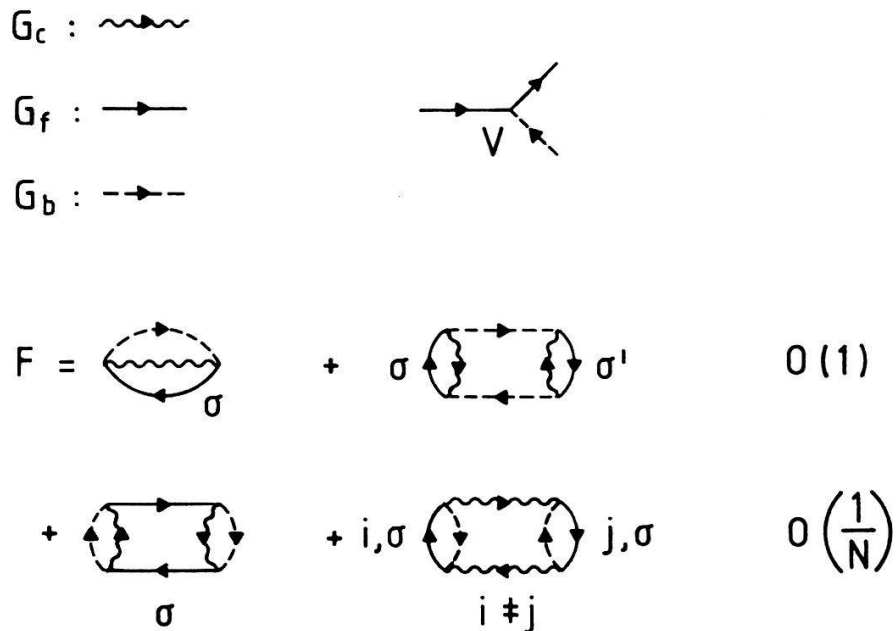σ $i \neq j$

Fig. 3: Diagrams for the free energy of the Anderson lattice.

The diagrams may now be selected according to the following rules: (i) only diagrams with exactly one loop of fermion-boson propagators need to be considered (ii) diagrams with n fermion loops (consisting of pseudo fermions and conduction electrons) and $2m$ hybridization vertices contribute in order N^{n-m} (see Fig. 3).

For the single impurity problem Jin and Juroda (1988) calculated the thermal properties free energy F, number of fermions n_f, spin and charge susceptibility, analytically to order $1/N$ in the three temperature regimes defined by $T << T_o$, $T_o \stackrel{\sim}{>} T << T_K$ and $T >> T_K$, where $T_o = T_K/\ell n N$, and T_K is the Kondo temperature. The results agree with those of previous $1/N$ calculations for $T << T_o$ and with standard perturbation theory at $T >> T_K$. These authors also discuss the relaxation time of a conduction electron due to scattering off the impurity, and find

$$\frac{1}{2\tau} = \begin{cases} \frac{\pi c}{\rho_c} \frac{1}{N^2} [1 - \frac{2}{3}\pi^2 (\frac{T}{T_K})^2] \ , & T << T_o \\ \frac{\pi c}{\rho_c} \frac{1}{N} \frac{1}{[\ell n \frac{T_K}{2\pi T} - 4(\frac{1}{2})]^2 + (\frac{\pi}{2})^2} \ , & T \stackrel{\sim}{>} T_K \end{cases} \qquad (32)$$

in agreement with a $\frac{1}{N}$ expansion at $T << T_o$ (Houghton, Read and Won 1987) and the high T limiting behavior (here c is the impurity concentration). It may be shown that the Friedel sum rule

$$\frac{1}{2\tau} = \frac{c}{\pi \rho_c} \sin^2(\frac{\tau n_f}{N}) \ , \quad T = 0 \qquad (33)$$

is satisfied up to and including $O(\frac{1}{N^3})$ terms.

The transport properties of the lattice may also be calculated using this method. Defining the T matrix in the grand canonical ensemble by

$$T_{ij}(i\omega_n) \equiv -V^2 \int_o^\beta e^{i\omega_n \tau} < T_\tau[f_{i\sigma}(\tau)b^+(\tau)b_j(0)f_{j\sigma}^+(0)]\Pi_i Q_i >_\lambda \qquad (34)$$

the quasiparticle relaxation rate is given by

$$\frac{1}{2\tau_k} = -Im\left\{ \lim_{\lambda\to\infty} \left[\sum_j e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} T_{ij}(\epsilon_k + i0)/ < \pi Q >\right]\right\} \tag{35}$$

It turns out that the dominant term at low T appears only in order $\frac{1}{N^3}$, such that (Jin and Kuroda 1988)

$$\frac{1}{2\tau_k} \simeq \frac{\pi^2}{18} \frac{1}{N^3} \frac{\epsilon_F}{T_K^2}[(\pi T)^2 + \epsilon_\mathbf{k}^2], \qquad T \ll T_0 \tag{36}$$

in agreement with Fermi liquid theory. The numerical coefficient in (36) has not been confirmed yet by an independent, e.g. functional integral, calculation.

The above results are encouraging and raise the hope that a controlled theory of the Anderson lattice model may be within reach. There remains the question of how rapidly the $1/N$ expansion converges. Is it sufficient to calculate quantities to order $1/N^3$, if one is actually interested in $N = 2$, or does one need to sum up an infinite class of contributions of the $1/N$ expansion? The answer to this is not known at present, but it is more likely that the latter alternative applies. In this case it is advisable to look for a self-consistent approach in which large classes of diagrams are summed, while at the same time certain exact relations are conserved in the approximation. One possible approach would be to work within the grand canonical ensemble (with respect to Q_i) and to attempt to recover the exact constraint by including suitable vertex corrections (Hirschfeld, Muttalib and Wölfle 1989). The vertex functions $\Lambda_{f,b}$ defined by

$$\Lambda^f(t_1, t_2, t_3) \equiv -\langle T\{Q(t_1)f_\sigma(t_2)f_\sigma^+(t_3)\}\rangle$$

$$\Lambda^b(t_1, t_2, t_3) \equiv -\langle T\{Q(t_1)b(t_2)b^+(t_3)\}\rangle \tag{37}$$

obey the Ward identities (in frequency space)

$$\Omega\Lambda^a(\omega + \Omega, \omega) = G^a(\omega + \Omega) - G^a(\omega), \qquad a = f,b \tag{38}$$

which are crucial for the preservation of the constraint (3). In fact from (38) it follows that the constraint correlation function $\langle Q(t)Q(0)\rangle$ is identically zero at all times, provided the Λ's are smoothly varying functions.

Conserving approximations are introduced for the fermion and boson self-energies Σ_σ^f and Σ^b, defined as usual by

$$G_\sigma^f(\omega_n) = \frac{1}{\omega_n - \epsilon_f^o - \lambda - \Sigma_\sigma^f(\omega_n)} \qquad (39a)$$

and

$$G^b(\nu_n) = \frac{1}{\nu_n - \lambda - \Sigma^b(\nu_n)} \qquad (39b)$$

Bose condensation is not allowed to occur and the average constraint is used to determine λ. This requires a particular shape of the Bose spectral function $A^b(\omega) = \frac{1}{\pi}\text{Im}G^b(\omega)$ in order to allow for a finite number of bosons at $T = 0$. Since $\omega A^b(\omega) \geq 0$ on general grounds, one must have a finite negative portion of $A^b(\omega)$ for $\omega < 0$, such that at $T = 0$ the number of bosons is given by

$$n_b = -\int_{-\infty}^0 d\omega A^b(\omega). \qquad (40)$$

A finite negative frequency part of A^b can only appear through a frequency dependent self-energy. Since we are interested in the Kondo limit, the number of Bosons n_b may be assumed to be small. In this case the ladder diagrams give the dominant contribution (see Fig. 4) and Σ^f and Σ^b may be approximated by

$$\Sigma^f(\omega_n) = -V^2 T \sum_{\omega_n'} G^b(\omega_n - \omega_n')\tilde{G}^c(\omega_n') \qquad (41a)$$

$$\Sigma^b(\nu_n) = (2S+1)V^2 T \sum_{\omega_n'} G^f(\omega_n' + \nu_n')\tilde{G}^c(\omega_n') \qquad (41b)$$

Here $\tilde{G}^c$ is a "screened" conduction electron propagator, given by

$$\tilde{G}^c(\omega_n) = G^c(\omega_n)[1 + L(\omega_n)G^c(\omega_n)], \qquad (42)$$

where G^c is the bare local conduction electron Green's function and $L(\omega_n)$ is the sum of the f-b ladder diagrams,

$$L_{bf} = [(L_{bf}^0)^{-1} - V^2 G^c(\omega_n)]^{-1} \qquad (43)$$

with

$$L_{bf}^0(\omega_n) = -T \sum_{\omega_\ell} G^f(\omega_\ell) G^b(\omega_\ell - \omega_n). \qquad (44)$$
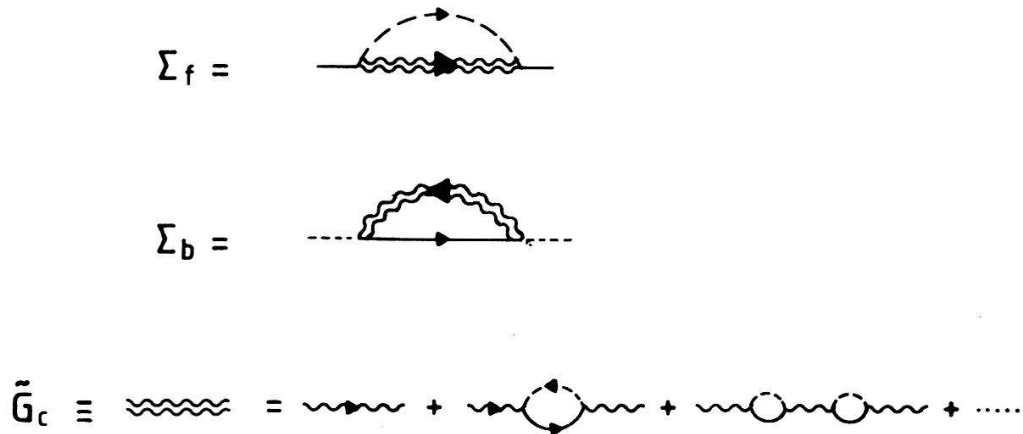

Fig. 4: Fermion and boson self-energies in a self-consist ent theory of the Anderson lattice.

It may be shown that the above approximation is conserving in the sense that the Ward identities (38) are satisfied, provided the irreducible vertex function is chosen to be equal to $\tilde{G}^c$.

One may also show that the Fermi liquid relations, e.g. the Friedel sum rule (33), are satisfied in the above scheme. The evaluation of the self-consistent equations for Σ^f and Σ^b requires a substantial numerical effort and has not been completed yet.

Finally there remains the important problem of magnetic interactions between localized spins in the Anderson lattice. Crudely speaking, one expects a magnetically ordered state for sufficiently small exchange interaction $J = \frac{V^2}{\epsilon_f^0 - \mu}$ of localized spins and conduction electron spins. The effective spin–spin interaction is in lowest order given by the RKKY expression

$$H_{RKKY} = \Sigma_{i,j} I_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{45}$$

with

$$I_{ij} = (J\rho_c)^2 \epsilon_F F(2k_F R_{ij}) \tag{46a}$$

and

$$F(x) = (x\cos x - \sin x)/x^4. \tag{46b}$$

A simple, and possibly too naive estimate of the region of stability of the magnetically ordered state is obtained by comparing the energy gain of a pair of localized spins at distance R in the Kondo effect, $2(\epsilon_f^0 - \epsilon_f)$, to the energy gain by magnetic ordering, $2\epsilon_f^0 - \langle H_{RKKY} \rangle$. For nearest neighbor distances R satisfying the condition

$$(k_F R)^3 \lesssim \frac{1}{N^2} (N J \rho_c)^2 \frac{D}{T_K} \tag{47}$$

one expects magnetic ordering to play an important role. The latter is clearly suppressed at large N and for not too small exchange coupling J (recall $T_K \sim \exp(-\frac{1}{N J \rho_c})$).

The above simple estimate is contradicted by a numerical study of the two impurity problem using Wilson's renormalization group transformation. (Jones and Varma 1987; Jones, Varma and Wilkins 1988). There one finds that a Kondo quenched-moment state is formed for all values of ferromagnetic (i.e. negative) RKKY coupling, and for antiferromagnetic coupling such that $I < 2T_K$. The actual screening process may take place in several stages, depending on whether the two impurity spins form a singlet or a triplet state first or do not bind at all, before the spins are quenched at lower temperature. An unstable fixed point of the RG procedure is found at the relatively large antiferromagnetic value $I \simeq -2T_K$. At this point the staggered magnetic susceptibility and the specific heat coefficient γ are found to diverge whereas the uniform susceptibility remains finite. Beyond this point, i.e. in the limit of large AF local-moment coupling the local moments are not screened anymore and a total singlet state is formed. Apparently the AF correlations between the two conduction electron spin clouds screening the local moments become so strong as to render a complete screening impossible.

There does not exist a theoretical formulation which would allow to reproduce the above findings in a simple qualitative way. The problem seems to be that in the conventional slave boson formulations discussed before the RKKY interaction comes in only at order $1/N^2$, which implies that any interference effects between RKKY and Kondo interaction would have to be looked for in even higher order of $1/N$. The fact that the slave bosons do not carry spin introduces an assymmetry in the treatment of charge and spin fluctuations, which is an unpleasant feature of this approach. There are, however, alternative slave boson representations of the Anderson model, such as the "labelling of states" approach introduced by Kotliar and Ruckenstein (KR) (1986)

mainly for the Hubbard model. There one defines slave bosons for each atomic state at the lattice site i, the empty state $|i0\rangle$, the singly occupied ones $|i\uparrow\rangle$, $|i\downarrow\rangle$ and, if necessary, also the doubly occupied one $|i\uparrow\downarrow\rangle$, so that

$$|i0\rangle = e_i^+|vac\rangle \tag{48a}$$

$$|i\sigma\rangle = (f_i^+ p_i)_\sigma|vac\rangle \qquad \sigma = \uparrow,\downarrow \tag{48b}$$

$$|i\uparrow\downarrow\rangle = d_i^+ f_{i\uparrow}^+ f_{i\downarrow}^+|vac\rangle, \tag{48c}$$

where f, f^+ are the fermion operators of the localized electrons. In the original formulation of KR only two bosons $p_\uparrow$, $p_\downarrow$ for the singly occupied state were introduced, leading to a violation of spin rotation invariance. A manifestly spin rotation invariant formulation requires the introduction of four bosons, a scalar (spin 0) boson p_0, and a vector (spin 1) boson $\mathbf{p} = (p_1, p_2, p_3)$ (Li, Wölfle and Hirschfeld 1989).

The Anderson lattice Hamiltonian can be expressed as

$$H = H_c + H_f + V \sum_{i,\sigma,\sigma'} \left(c_{i\sigma}^+ e_i^+ f_{i\sigma'} p_{i\sigma'\sigma} + h.c. \right) \\ + (\text{constraint terms}), \tag{49}$$

where $p_{i\sigma\sigma'} = 1/\sqrt{2} \sum_\mu p_{i\mu}(\tau_\mu)_{\sigma\sigma'}$ and the τ_μ are the unit matrix τ_0 and the three Pauli matrices τ_j. There are now two types of constraints, the one expressing the fact that there is exactly one boson at each lattice site at any time, or

$$Q_i = e_i^+ e_i + p_{i\sigma}^+ p_{i\sigma} + \mathbf{p}_i^+ \cdot \mathbf{p}_i = 1 \tag{50}$$

and a further constraint guaranteeing the correspondence of fermions and bosons,

$$\text{tr}(\tau_\mu p_i^+ p_i) = \sum_{\sigma,\sigma'} f_{i\sigma}^+ (\tau_\mu)_{\sigma\sigma'} f_{i\sigma'}. \tag{51}$$

As pointed out by Kotliar and Ruckenstein, the straightforward introduction of the slave bosons into the mixing term as in (49) leads to problems in the weak coupling limit $U \to 0$. Therefore, they proposed to define a "normalized" projection operator in (49)

$$H_{mix} = \sum_{i,\sigma,\sigma'} \left(c_{i\sigma}^{+} f_{i\sigma'} z_{i\sigma'\sigma} + h.c. \right) \tag{52}$$

with z (generalized to the spin-rotation invariant formulation) given by

$$\underline{z}_i = \left[(1 - d_i^{+} d_i) \underline{\tau}_0 - \underline{p}_i^{+} \underline{p}_i \right]^{-1/2} \left(e_i^{+} \underline{p}_i + \underline{\tilde{p}}_i^{+} d_i \right) \left[(1 - e_i^{+} e_i) \underline{\tau}_0 - \underline{\tilde{p}}_i^{+} \underline{\tilde{p}}_i \right]^{-1/2} \tag{53}$$

In the weak coupling limit and for $n_f \to 1$, the expectation value of all the Bose fields tends to $1/2$ and hence $z \to 1$, as it should. The latter choice of H_{mix} leads in mean field theory to the same results as have been found within the Gutzwiller variational approximation (Rice and Ueda 1986). In particular, the characteristic temperature for Kondo screening is found to have an additional factor of $1/2$ in the exponent (this holds for degeneracy $N = 2$), as compared to the standard definition of the Kondo temperature. In the above formulation the same result would be obtained for the single impurity in contradiction to exact results. Therefore, in order to recover the known Kondo temperature T_K for the $N = 2$ Anderson impurity in the above formulation fluctuation corrections must be taken into account. A systematic investigation along these lines has not been performed yet. The above formulation does have the attractive feature of treating charge and spin degrees of freedom on the same level. It therefore should be better adapted to describing the competition between Kondo screening and RKKY interaction.

Even if all the above questions have been answered, the application of the Anderson lattice model to real systems still requires to take the lattice structure into

account. This problem has been addressed by Fulde et.al. (1988) in a model where the Kondo ions are described as atomic potentials scattering electrons resonantly (i.e. the scattering phase shift is $\pi/2$). In this way one hopes to take into account the many-body renormalizations of the band structure.

4. Conclusion

As discussed above, important progress has been made in recent years in understanding the physics of the Anderson lattice. The properties of the ground state and the weakly excited states are believed to be reasonably well described by the $1/N$ slave boson techniques, although even there discrepancies between different approaches (e.g. slave boson versus Gutzwiller approaches) still exist. The behavior at higher energies and/or temperatures is not well understood, especially regarding the crossover from the low temperature Fermi liquid regime to the high temperature local moment regime. The importance of the RKKY interaction for the interesting case of moderately small antiferromagnetic Kondo coupling is unclear. Possible approaches for solving these problems have been suggested here.

Acknowledgements

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