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1993 J. Phys.: Condens. Matter 5 6277

(http://iopscience.iop.org/0953-8984/5/34/014)

J. Phys.: Condens. Matter 5 (1993) 6277–6288. Printed in the UK

Fermi liquid theory and magnetic impurity systems: I. Quasi-particle Hamiltonians and mean field theory

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Received 9 June 1993

Abstract. We give explicit quasi-particle Hamiltonians, including interactions, for several magnetic impurity models and show that the application of mean field theory to these gives asymptotically exact results as $T \to 0$ and $H \to 0$ corresponding to Fermi liquid theory. This approach provides a conceptual link between the intuitive phenomenological theory of Landau and Nozières, and the microscopic theory of Luttinger and Yamada.

1. Introduction

In this paper (I) we discuss the relation between the renormalization group approach [1] to the low-temperature behaviour of magnetic impurity models and the phenomenological Fermi liquid theory as formulated by Landau [2]. The link between these approaches was recognized by Nozières [3] soon after Wilson's original numerical renormalization group calculations on the s–d model. Nozières used arguments based on phenomenological Fermi liquid theory to give a simple derivation of Wilson's result for the 'χ/γ' ratio as well as a derivation of an exact expression for the T^2-term in the impurity contribution to the resistivity. Here we want to make that link rather more explicit by giving the effective Hamiltonian for the quasi-particle excitations and then show that the application of mean field theory to this model corresponds to the Landau-like Fermi liquid theory. In a subsequent paper (II) we develop these ideas further in the form of a renormalized perturbation expansion that can be used to extend the calculations beyond the Fermi liquid regime to all temperatures (for a preliminary account of this approach see [4]).

The Landau phenomenological Fermi liquid theory [2] is based on the assumption that the single- (quasi-)particle excitations at very low temperatures in an interacting Fermi system are in one-to-one correspondence with those of the non-interacting system. Using these one-electron states a total energy functional $E_{\rm tot}$ is then constructed of the form

$$E_{\rm tot} = \sum_{\alpha,\sigma} \tilde{\epsilon}^{(0)}_{\alpha,\sigma} \delta n_{\alpha,\sigma} + \frac{1}{2} \sum_{\alpha\alpha',\sigma\sigma'} f^{\sigma,\sigma'}_{\alpha,\alpha'} \delta n_{\alpha,\sigma} \delta n_{\alpha',\sigma'} + \cdots \tag{1}$$

where $\delta n_{\alpha,\sigma}$ is the deviation in occupation number of the single-particle state $|\alpha\rangle, \sigma$ with an excitation energy $\tilde{\epsilon}^{(0)}_{\alpha,\sigma}$ from its ground-state value, and $f^{\sigma,\sigma'}_{\alpha,\alpha'}$ is the leading term due to the quasi-particle interactions. A free-energy functional F is constructed from (1), retaining only the first two terms, together with the Fermi–Dirac form for the entropy of the quasi-particles. Minimization of F with respect to δn_α leads to asymptotically exact results for the thermodynamic behaviour as $T, H \to 0$ for systems in a normal paramagnetic ground

0953-8984/93/346277+12$07.50

state. The reason why the higher-order terms in (1) give negligible effects in this limit is because the expectation value of δn_α, $\langle \delta n_\alpha \rangle \to 0$ as $T \to 0$ and $H \to 0$. The effective quasi-particle energy $\tilde{\epsilon}_{\alpha,\sigma}$ in the presence of other excitations is given by

$$\tilde{\epsilon}_{\alpha,\sigma} = \tilde{\epsilon}^{(0)}_{\alpha,\sigma} + \sum_{\alpha\alpha',\sigma\sigma'} f^{\sigma,\sigma'}_{\alpha,\alpha'} \langle \delta n_{\alpha',\sigma'} \rangle. \tag{2}$$

Microscopic perturbation calculations verify the Landau results [5, 6] but, due to the mathematical complexity of the arguments used, some of the more intuitive ideas of Landau are lost. Here we show that the renormalization group, where one derives an explicit effective Hamiltonian for the low-energy excitations, provides a conceptual framework which can link the two approaches so retaining many of the intuitive aspects of the Landau theory.

We base our initial discussion on the Anderson model [7] for a 3d transition (or 4f rare earth) ion in a metallic host. In its simplest form the model has an impurity d level ϵ_d, taken to be non-degenerate, which is hybridized with the host conduction electrons via a matrix element V_k. When the interaction term U between the electrons in the local d state is included, the Hamiltonian has the form

$$H = \sum_\sigma \epsilon_{d,\sigma} c^\dagger_{d,\sigma} c_{d,\sigma} + U n_{d,\uparrow} n_{d,\downarrow} + \sum_{k,\sigma} (V_k c^\dagger_{d,\sigma} c_{k,\sigma} + V^*_k c^\dagger_{k,\sigma} c_{d,\sigma}) + \sum_{k,\sigma} \epsilon_{k,\sigma} c^\dagger_{k,\sigma} c_{k,\sigma} \tag{3}$$

where $\Delta(\omega) = \pi \sum_k |V_k|^2 \delta(\omega - \epsilon_k)$ is the function which controls the width of the virtual bound state resonance at ϵ_d in the non-interacting model ($U = 0$). In the limit of a wide conduction band with a flat density of states, $\Delta(\omega)$ becomes independent of ω and can be taken as a constant, Δ. For $\epsilon_d \ll \epsilon_F$, $\epsilon_d + U \gg \epsilon_F$, where ϵ_F is the Fermi level and $|\epsilon_d - \epsilon_F|, |\epsilon_d + U - \epsilon_F| \gg \Delta$, the model is equivalent to the s–d model with an antiferromagnetic interaction $J\rho_0 = (U\Delta/\pi)|\epsilon_d - \epsilon_F||\epsilon_d + U - \epsilon_F|$, where ρ_0 is the conduction electron density of states.

The non-degenerate Anderson model is now very well understood as a result of numerical renormalization group[1] and exact Bethe *ansatz* calculations [8]. There are also exact relations for the model, such as the Friedel sum rule [9] and Ward identities [10], which have been established within the framework of microscopic perturbation theory. Our aim here is to attempt to gain insight into these solutions which might be of help in considering the problems posed by other strongly correlated fermion systems, such as heavy fermions and high-T_c superconductors, which at present are not well understood.

2. The non-degenerate Anderson model

In the numerical renormalization group approach devised by Wilson [1] and applied to the s–d and Anderson models wave packets for the conduction electrons about the impurity site were used so that the Hamiltonian could be cast in the form of an effective linear chain with the impurity at one end. The energy states over a decreasing energy scale were then calculated by the iterative diagonalization of chains of increasing length, retaining only the lower-energy states of the chain at each iteration. This calculation confirmed that the behaviour at low temperatures and low fields is governed by the strong coupling fixed point of the renormalization group transformation in the Kondo regime ($J \to \infty$, for the antiferromagnetic s–d model). Wilson derived the effective Hamiltonian for the low-lying energy states about this fixed point, which can be re-expressed in a form equivalent to the original Anderson model (3) with renormalized parameters [11], $\tilde{\Delta} = \pi \sum_k |\tilde{V}_k|^2 \delta(\epsilon - \epsilon_k)$,

$\tilde{U}$, and $\tilde{\epsilon}_{\rm d}$, corresponding to the effective Hamiltonian

$$H_{\rm eff} = \sum_{k,\sigma} \epsilon_{k,\sigma} c^{\dagger}_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} (\tilde{V}_k \tilde{c}^{\dagger}_{{\rm d},\sigma} c_{k,\sigma} + \tilde{V}^{*}_k c^{\dagger}_{k,\sigma} \tilde{c}_{{\rm d},\sigma}) + \sum_{\sigma} \tilde{\epsilon}_{{\rm d},\sigma} \tilde{c}^{\dagger}_{{\rm d},\sigma} \tilde{c}_{{\rm d},\sigma} + \tilde{U} \tilde{n}_{{\rm d},\uparrow} \tilde{n}_{{\rm d},\downarrow} \quad (4)$$

where the energy level $\tilde{\epsilon}_{{\rm d},\sigma}$ is measured with respect to the Fermi level.

In the first-principles calculation of Wilson for the s–d model, the renormalized parameters were determined by fitting the levels to those calculated by the iterative diagonalization scheme. In the s–d or local moment regime of the model there is only one energy scale involved which is the Kondo temperature $T_{\rm K}$. The important point which makes the renormalized effective Hamiltonian (4) tractable at low temperatures is that it describes excitations from the exact ground state so that the interaction term $\tilde{U}$ between excitations only comes into play when there is more than one excitation from the ground state. If a single-particle excitation or single-hole excitation is created this interaction term can be ignored and the one-electron Hamiltonian remaining can be diagonalized and written in the form

$$H_{\rm eff}(\tilde{U} = 0) = \sum_{l,\sigma} \tilde{\epsilon}^{(0)}_{l,\sigma} c^{\dagger}_{l,\sigma} c_{l,\sigma} \quad (5)$$

where $\tilde{\epsilon}^{(0)}_{l,\sigma}$ are the one-electron energies, and $c^{\dagger}_{l,\sigma}$ and $c_{l,\sigma}$ the corresponding creation and annihilation operators. The excitation energy $\tilde{\epsilon}^{(0)}_{l,\sigma}$ can be identified with that in the Landau free energy functional (1). We do not need to diagonalize (4) explicitly because we find later that we only need the result of the impurity quasi-particle density of states $\tilde{\rho}_{\rm imp}(\omega)$ which can be straightforwardly derived from the Hamiltonian for $\tilde{U} = 0$ using the equations of motion of the one-particle Green functions. This gives

$$\tilde{\rho}_{\rm imp}(\omega) = (1/\pi)\tilde{\Delta}/[(\omega - \tilde{\epsilon}_{\rm d})^2 + \tilde{\Delta}^2] \quad (6)$$

corresponding to a Lorentzian resonance.

For $\tilde{U} \neq 0$ (4) can be written using the single-particle eigenstates of (5) as a basis

$$H_{\rm eff} = \sum_{l,\sigma} \epsilon_{l,\sigma} c^{\dagger}_{l,\sigma} c_{l,\sigma} + \tilde{U} \sum_{l,l'} \sum_{l'',l'''} \alpha^{*}_{l} \alpha_{l'} \alpha^{*}_{l''} \alpha_{l'''} c^{\dagger}_{l,\uparrow} c_{l',\uparrow} c^{\dagger}_{l'',\downarrow} c_{l''',\downarrow} \quad (7)$$

where

$$\tilde{c}^{\dagger}_{{\rm d},\sigma} = \sum_{l} \alpha^{*}_{l,\sigma} c^{\dagger}_{l,\sigma}. \quad (8)$$

Since it is the excitations of the interacting system from its ground state which are described by the effective Hamiltonian (4), it is appropriate to transform this Hamiltonian to operators which describe the single-particle excitations

$$c^{\dagger}_{l,\sigma} = p^{\dagger}_{l,\sigma} \qquad c_{l,\sigma} = p_{l,\sigma} \qquad \epsilon_{l,\sigma} > \epsilon_{\rm F} \quad (9)$$

$$c^{\dagger}_{l,\sigma} = h_{l,\sigma} \qquad c_{l,\sigma} = h^{\dagger}_{l,\sigma} \qquad \epsilon_{l,\sigma} < \epsilon_{\rm F} \quad (10)$$

where the ground state is such that $p_{l,\sigma}|0\rangle = 0$ and $h_{l,\sigma}|0\rangle = 0$. The interaction term has to be normal ordered in terms of these operators so that $H_{\rm eff}|0\rangle = 0$, and the Hamiltonian describes interactions only between excitations from the ground state. In the mean field approximation the expectation value of operators in the interaction terms such as $p^{\dagger}_{l,\uparrow} p_{l',\uparrow} p^{\dagger}_{l'',\downarrow} p_{l''',\downarrow}$ are approximated by

$$\langle p^{\dagger}_{l,\uparrow} p_{l',\uparrow} p^{\dagger}_{l'',\downarrow} p_{l''',\downarrow} \rangle = \langle p^{\dagger}_{l,\uparrow} p_{l,\uparrow} \rangle \langle p^{\dagger}_{l'',\downarrow} p_{l'',\downarrow} \rangle \delta_{l,l'} \delta_{l'',l'''}. \quad (11)$$

The quasi-particle energy of the Landau theory in the presence of other excitations can be identified as the effective one-particle energy in this approximation

$$\tilde{\epsilon}_{l,\sigma} = \tilde{\epsilon}^{(0)}_{l,\sigma} + \tilde{U}|\alpha_l|^2 \sum_{l'} |\alpha_{l'}|^2 \langle \delta n_{l',-\sigma} \rangle \tag{12}$$

where $\langle \delta n_{l',\sigma} \rangle = \langle p^\dagger_{l',\sigma} p_{l',\sigma} \rangle$ for $\epsilon_{l'} > \epsilon_F$ and $\delta n_{l',\sigma} = -\langle h^\dagger_{l',\sigma} h_{l',\sigma} \rangle$ for $\epsilon_{l'} < \epsilon_F$. As $|\alpha_l|^2$ is proportional to $1/N_s$ (where N_s is the number of sites) because the scattering potential is due to a single impurity, the energy shift in (12) is of the order of $1/N_s$.

As $\langle p^\dagger_{l,\sigma} p_{l,\sigma} \rangle \to 0$ as $T \to 0$, the quasi-particle interaction does not contribute to the linear term in the specific heat which can be calculated from the non-interacting quasi-particle Hamiltonian (5). Using the Sommerfeld expansion we find for the total specific heat coefficient γ

$$\gamma = \frac{2\pi^2 k_B^2}{3} \sum_l \delta(\epsilon_F - \tilde{\epsilon}^{(0)}_l) = \frac{2\pi^2 k_B^2}{3} (\rho_0(\epsilon_F) + \tilde{\rho}_{imp}(\epsilon_F)), \tag{13}$$

where $\rho_0(\omega)$ is the density of states of the conduction electrons alone, $\tilde{\rho}_{imp}(\omega)$ is the extra impurity contribution, and ϵ_F is the Fermi energy. In calculating the susceptibility the quasi-particle interaction has to be taken into account. Using the mean field approximation for this interaction we obtain for the total susceptibility in zero field

$$\chi = \frac{(g\mu_B)^2}{2} \sum_l \delta(\epsilon_F - \tilde{\epsilon}_l)(1 + |\alpha_l|^2 \tilde{U} \partial \langle \delta n_{d,-\sigma} \rangle / \partial h) \tag{14}$$

where $\langle \delta n_{d,-\sigma} \rangle = \sum_l |\alpha_l|^2 \langle \delta n_{l,-\sigma} \rangle$, and $h = g\mu_B H/2$.

We can forget about the quasi-particle interaction term in calculating $\partial \langle \delta n_{d,-\sigma} \rangle / \partial H$ on the right-hand side of (14) as it will gives terms of the order of $1/N_s^2$ which can be ignored, where N_s is the total number of sites in the lattice. Working to order $1/N_s$ we find

$$\partial \langle \delta n_{d,-\sigma} \rangle / \partial h = \tilde{\rho}_d(\epsilon_F) \tag{15}$$

where $\tilde{\rho}_d(\omega) = \sum_l |\alpha_l|^2 \delta(\omega - \tilde{\epsilon}^{(0)}_l)$. We also have in zero field

$$\sum_l \delta(\omega - \tilde{\epsilon}_l) = \rho_0(\omega) + \tilde{\rho}_{imp}(\omega). \tag{16}$$

Hence, to leading order $1/N_s$, the impurity susceptibility is given by

$$\chi_{imp} = \tfrac{1}{2}(g\mu_B)^2 (\tilde{\rho}_{imp}(\epsilon_F) + \tilde{U}\tilde{\rho}_d^2(\epsilon_F)). \tag{17}$$

The total charge susceptibility at $T = 0$, $\chi_c = dN_0/d\epsilon_F$, where N_0 is the expectation value of the total number operator for the electrons, can be calculated following precisely the same argument. The result for the impurity contribution is

$$\chi_{c,imp} = 2(\tilde{\rho}_{imp}(\epsilon_F) - \tilde{U}\tilde{\rho}_d^2(\epsilon_F)). \tag{18}$$

Eliminating the term in $\tilde{U}$ between (17) and (18), and the term in $\tilde{\rho}_{imp}(\epsilon_F)$ using (13), gives the well known Fermi liquid relation

$$4\chi_{imp}/(g\mu_B)^2 + \chi_{c,imp} = 6\gamma_{imp}/\pi^2 k_B^2. \tag{19}$$

In the Kondo limit $\chi_{c,imp} = 0$ as the occupation of the impurity state is always unity. This constraint is achieved in the quasi-particle picture by the interaction term $\tilde{U}$, the interaction

term self-consistently maintains the many-body resonance at the Fermi level so that the impurity occupation is not changed as was first pointed out by Nozières [3]. This condition can be used to deduce $\tilde{U}$. For a flat conduction band it is straightforward to show that $\tilde{\rho}_d(\omega) = \tilde{\rho}_{imp}(\omega)$, and for particle–hole symmetry $\tilde{\epsilon}_d = 0$ so that the resonance in the quasi-particle density of states (6) is peaked at the Fermi level and $\tilde{\rho}_{imp}(\epsilon_F) = 1/\pi\tilde{\Delta}$. We then find on substituting into equations (17) and (18)

$$\tilde{U} = \pi\tilde{\Delta} = 4k_B T_K \tag{20}$$

where the Kondo temperature is defined by $\chi_{imp} = (g\mu_B)^2/4k_B T_K$.

These parameters give for the 'χ/γ' or Wilson ratio R

$$R = \frac{4\pi^2 k_B^2 \chi_{imp}}{3(g\mu_B)^2\gamma_{imp}} = \frac{\chi_{imp}/\chi_0}{\gamma_{imp}/\gamma_0} = 2 \tag{21}$$

where χ_0 and γ_0 are the susceptibilities and specific heat coefficients for the conduction electrons alone. The argument leading to this result is essentially a reformulation of the one originally given by Nozières [3].

The result (20) for the renormalized parameters can be related to the microscopic perturbation theory of Yamada and Yosida [10] for the symmetric model [11]. If we define $\tilde{\Delta}$ and $\tilde{U}$ via

$$\tilde{\Delta} = z\Delta \qquad \tilde{U} = z^2\Gamma^{\uparrow\downarrow}_{\uparrow\downarrow}(0,0:0,0) \tag{22}$$

where z is the wave function renormalization factor defined in terms of the self-energy $\Sigma_\sigma(\omega)$ of the d electron Green function by

$$z = 1/[1 - \Sigma'_\sigma(0)] \tag{23}$$

and $\Gamma^{\sigma\sigma'}_{\sigma''\sigma'''}(\omega,\omega' : \omega'',\omega''')$ is the four-point irreducible vertex function evaluated at the Fermi level, then the same result (20) in the Kondo limit can be deduced from the Ward identities given by Yamada. This result will be exploited in the renormalized perturbation expansion developed in the forthcoming paper II.

We can conjecture that the form of the effective Hamiltonian derived by Wilson for the s–d model is a valid description of the Fermi liquid fixed point for all parameter regimes of the Anderson model (we will also justify this conjecture in II). In the other regimes the parameters do not merge into a single energy scale. They can be deduced from some of the other techniques which have been applied to the Anderson model. For example for the particle–hole symmetric model, $\epsilon_d - \epsilon_F = -U/2$, it is possible to calculate the renormalized parameters in powers of $U/\pi\Delta$ using the perturbation theory results for $\chi_{c,imp}$ and γ_{imp} of Yosida and Yamada [10]. For the particle–hole symmetric model to third order they are given by

$$\tilde{\Delta} = \Delta\left(1 - (12 - \pi^2)/4\,(U/\pi\Delta)^2 + O\left((U/\pi\Delta)^4\right)\right) \tag{24}$$

and

$$\tilde{U} = U\left(1 - (\pi^2 - 9)\,(U/\pi\Delta)^2 + O\left((U/\pi\Delta)^4\right)\right) \tag{25}$$

which are valid for $U \ll \pi\Delta$. So in the weak-coupling regime we find $\tilde{U} \sim U$ as one would expect. More generally we can deduce $\tilde{U}$ and $\tilde{\Delta}$ for the symmetric model in a similar way from the exact Bethe *ansatz* results which have been expressed in a power series in $U/\pi\Delta$ [8]. The results for these are shown in figure 1 plotted as a function of $U/\pi\Delta$.

The asymptotic results at weak coupling correspond to (24) and (25), and those at strong coupling $U/\pi\Delta > 2$ merge into a single energy scale corresponding to equation (20) with T_K given by

$$k_B T_K = U\,(\Delta/2U)^{1/2}\exp(-\pi U/8\Delta + \pi\Delta/2U). \tag{26}$$

Without the term $\pi\Delta/2U$ in the exponential (which is often the form used for T_K for this model) the asymptotic agreement with $4T_K$ for $U \gg \pi\Delta$ is not so good until U is in excess of $5\pi\Delta$.

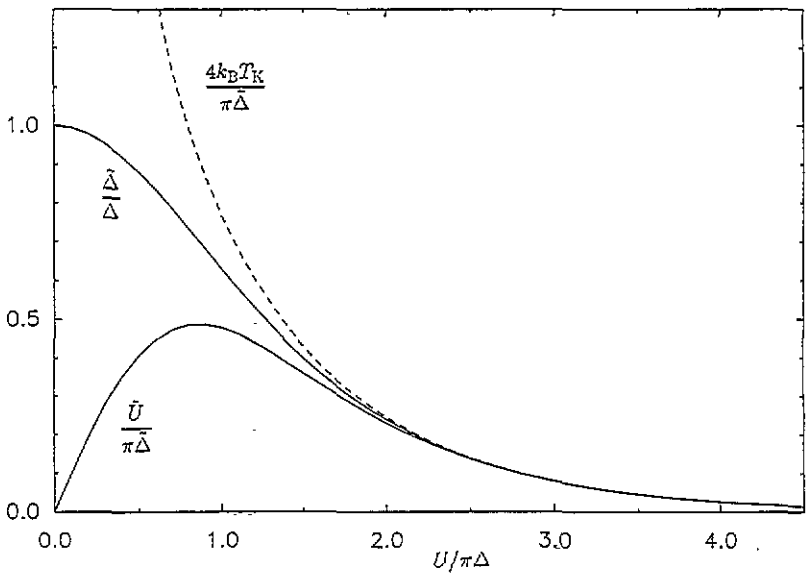

Figure 1. A plot of the renormalized parameters $\tilde{U}$ and $\tilde{\Delta}$ for the symmetric Anderson model in terms of the bare parameters U and Δ. For the comparison of these parameters with $4k_BT_K$ for $U \gg \pi\Delta$, the value for T_K is given by (26).

3. N-fold degenerate Anderson model

This approach to Fermi liquid theory can be extended to other magnetic impurity models. For example, it can be generalized easily to the N-fold degenerate Anderson model which has been used widely to describe Ce and Yb impurities in simple metallic hosts, where the local states now correspond to 4f electrons or holes [12]. This model takes the form

$$H = \sum_{k,m}\epsilon_{k,m}c^\dagger_{k,m}c_{k,m} + \sum_{k,m}(V_k c^\dagger_{f,m}c_{k,m} + V_k^* c^\dagger_{k,m}c_{f,m}) + \sum_m \epsilon_{f,m}c^\dagger_{f,m}c_{f,m} + \sum_{m<m'} U n_{f,m}n_{f,m'} \tag{27}$$

where the quantum number m corresponds to the z-component of the total angular momentum j. m takes on $2j + 1 = N$ values, and plays a role similar to σ in the non-degenerate model, which corresponds to $N = 2$. There have been no first-principles numerical renormalization group calculations for this model giving the form of the effective Hamiltonian for the low-energy excitations. However, we can conjecture by analogy with

the non-degenerate case that this is given by

$$H_{\text{eff}} = \sum_{k,m} \epsilon_{k,m} c^{\dagger}_{k,m} c_{k,m} + \sum_{k,m} (\tilde{V}_k \tilde{c}^{\dagger}_{\text{f},m} c_{k,m} + \tilde{V}^{*}_k c^{\dagger}_{k,m} \tilde{c}_{\text{f},m}) + \sum_{m} \tilde{\epsilon}_{\text{f},m} \tilde{c}^{\dagger}_{\text{f},m} \tilde{c}_{\text{f},m} + \sum_{m<m'} \tilde{U} \tilde{n}_{\text{f},m} \tilde{n}_{\text{f},m'} \tag{28}$$

where all the quantities in the original model are renormalized. This form will be justified in paper II. We can now proceed to calculate χ_{imp}, $\chi_{\text{c,imp}}$ and γ_{imp} at $T = 0$ with our mean field approximation as we did earlier. The quasi-particle density of states $\tilde{\rho}_{\text{imp}}(\omega)$ is again a resonance but due to the lack of particle–hole symmetry $\tilde{\epsilon}_{\text{f}} \neq 0$ so that the peak of the resonance in general is displaced from the Fermi level. The results for χ_{imp}, $\chi_{\text{c,imp}}$ and γ_{imp} are

$$\chi_{\text{imp}} = \tfrac{1}{3}(g\mu_{\text{B}})^2 j(j+1) N \tilde{\rho}_{\text{imp}}(\epsilon_{\text{F}})(1 + \tilde{U}\tilde{\rho}_{\text{imp}}(\epsilon_{\text{F}})) \tag{29}$$

$$\chi_{\text{c,imp}} = N \tilde{\rho}_{\text{imp}}(\epsilon_{\text{F}})(1 - (N-1)\tilde{U}\tilde{\rho}_{\text{imp}}(\epsilon_{\text{F}})) \tag{30}$$

and (31)

$$\gamma_{\text{imp}} = \tfrac{1}{3}\pi^2 k_{\text{B}}^2 N \tilde{\rho}_{\text{imp}}(\epsilon_{\text{F}}) \tag{32}$$

where $\tilde{\rho}_{\text{imp}}(\omega)$ is the quasi-particle density of states (we have assumed a flat band so $\tilde{\rho}_{\text{f}}(\omega)$ is the same as $\tilde{\rho}_{\text{imp}}(\omega)$). Eliminating the density of states gives the relation

$$\frac{3(N-1)\chi_{\text{imp}}}{j(j+1)(g\mu_{\text{B}})^2} + \chi_{\text{c,imp}} = \frac{3N\gamma_{\text{imp}}}{\pi^2 k_{\text{B}}^2} \tag{33}$$

which is a generalization of (19). In the local moment limit $\chi_{\text{c,imp}} \to 0$, we can obtain from this result for the Wilson ratio R for general N which is $N/(N-1)$ [13, 14].

If we assume that the Friedel sum rule is applicable to the quasi-particles, then the occupation number of the impurity level n_{f} is given by

$$n_{\text{f}} = (N/\pi)\tan^{-1}\left(\tilde{\Delta}/\tilde{\epsilon}_{\text{f}}\right). \tag{34}$$

This relation can be verified within perturbation theory in U from the results of Yoshimori [15] if we identify the renormalized f level as $\tilde{\epsilon}_{\text{f}} = z(\epsilon_{\text{f}} - \epsilon_{\text{F}} + \Sigma(\epsilon_{\text{F}}))$. If we assume n_{f} as given, we can write (34) as a relation between $\tilde{\epsilon}_{\text{f}}$ and $\tilde{\Delta}$

$$\tilde{\epsilon}_{\text{f}} = \tilde{\Delta}\cot(\pi n_{\text{f}}/N) \tag{35}$$

and express the quasi-particle density of states evaluated at the Fermi level in the form

$$\tilde{\rho}_{\text{imp}}(\epsilon_{\text{F}}) = \sin^2(\pi n_{\text{f}}/N)/\pi\tilde{\Delta}. \tag{36}$$

In the localized or Kondo limit $n_{\text{f}} \to 1$, $\chi_{\text{c,imp}} \to 0$ we can again derive expressions for $\tilde{\Delta}$, $\tilde{\epsilon}_{\text{f}}$ and $\tilde{U}$ in terms of a single energy scale, the Kondo temperature, using $\chi_{\text{imp}} = (g\mu_{\text{B}})^2 j(j+1)/3k_{\text{B}}T_{\text{K}}$ as a more general definition of the Kondo temperature. The result for $\tilde{\Delta}$ is

$$\tilde{\Delta} = k_{\text{B}}T_{\text{K}}[N^2\sin^2(\pi/N)/\pi(N-1)] \tag{37}$$

and for $\tilde{\epsilon}_{\text{f}}$ from (35)

$$\tilde{\epsilon}_{\text{f}} = k_{\text{B}}T_{\text{K}}[N^2\sin(\pi/N)\cos(\pi/N)/\pi(N-1)]. \tag{38}$$

Using $\chi_{c,imp} = 0$, $\tilde{U}$ can be deduced from (30)

$$\tilde{U} = (N/(N-1))^2 k_B T_K. \tag{39}$$

From these results we can see the change in form of the quasi-particle density of states from the case $N = 2$ to the large N limit. These are shown in figure 2 with results ranging from $N = 2$ to $N = 8$. With increasing N, the peak shifts above the Fermi level to satisfy the Friedel sum rule. At the same time the resonance narrows and the width scales as $\tilde{\Delta} \sim 1/N$ for large N. As $N \to \infty$, $\tilde{\epsilon}_f \to k_B T_K$ and the Kondo resonance becomes a delta function at $k_B T_K$, a result which is well known from $1/N$ and slave boson calculations [12]. It is interesting to note that $\tilde{U}$ does not tend to zero in the large N limit. Quasi-particle scattering diagrams, however, are negligible due to the fact that the quasi-particle density of states in the vicinity of the Fermi level falls off at $1/N$ for large N in this limit as can be seen from (36). As a consequence, only the mean field diagram survives in this limit; higher-order diagrams have additional $1/N$ factors from the integrals over the quasi-particle density of states.

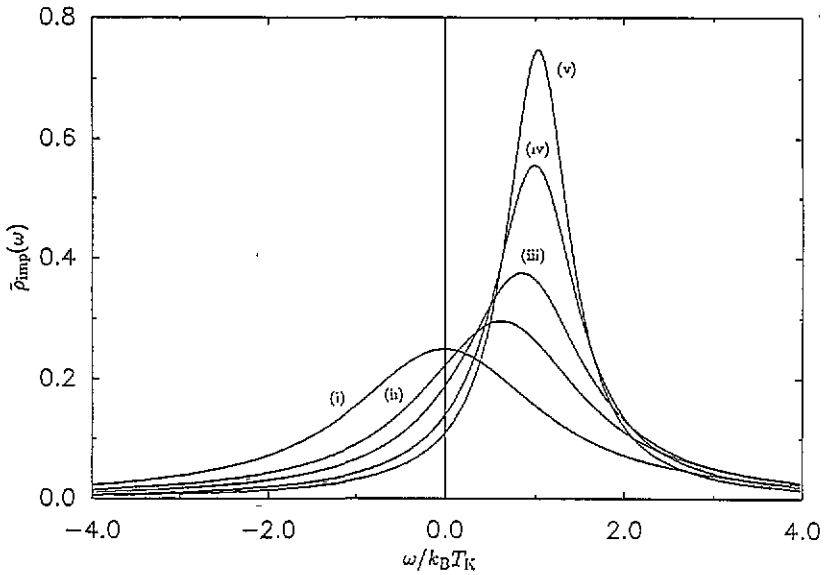

Figure 2. The quasi-particle density of states $\tilde{\rho}_{imp}(\omega)$ for the N-fold degenerate model in the Kondo limit as a function of $\omega/k_B T_K$ for: (i) $N = 2$, (ii) $N = 3$, (iii) $N = 4$, (iv) $N = 6$, and (v) $N = 8$.

We can also look at the large N limit quite apart from the localized limit $n_f = 1$. We take $\chi_{imp} = (g\mu_B)^2 j(j+1) n_f / 3k_B T_A$, which defines an energy scale $k_B T_A$; the n_f is included so $\chi_{imp} \to 0$ as $n_f \to 0$ in the non-magnetic limit. The Friedel sum rule (34) and the quasi-particle density of states in this limit become

$$n_f = N\tilde{\Delta}/\pi\tilde{\epsilon}_f \qquad \tilde{\rho}_{imp}(0) = \tilde{\Delta}/\pi\tilde{\epsilon}_f^2 = n_f/N\tilde{\epsilon}_f \tag{40}$$

as $\tilde{\Delta} \to 0$ as $N \to \infty$. Substituting $N\tilde{\rho}_{imp}(0)$ from (40) into (29) and (35) gives

$$\tilde{\epsilon}_f = k_B T_A \qquad \tilde{\Delta} = \pi n_f k_B T_A / N \tag{41}$$

and from (6) for large N

$$\tilde{\rho}_{\rm imp}(\omega) = \frac{(n_{\rm f} k_{\rm B} T_{\rm A}/N)}{(\omega - k_{\rm B}T_{\rm A})^2 + (n_{\rm f}\pi k_{\rm B} T_{\rm A}/N)^2}. \tag{42}$$

Hence we find more generally a delta-function form for the density of quasi-particle states in the large N limit. In this case, however, we cannot deduce $\tilde{U}$ without having more information about the charge susceptibility $\chi_{\rm c,imp}$, which we only know in the localized limit.

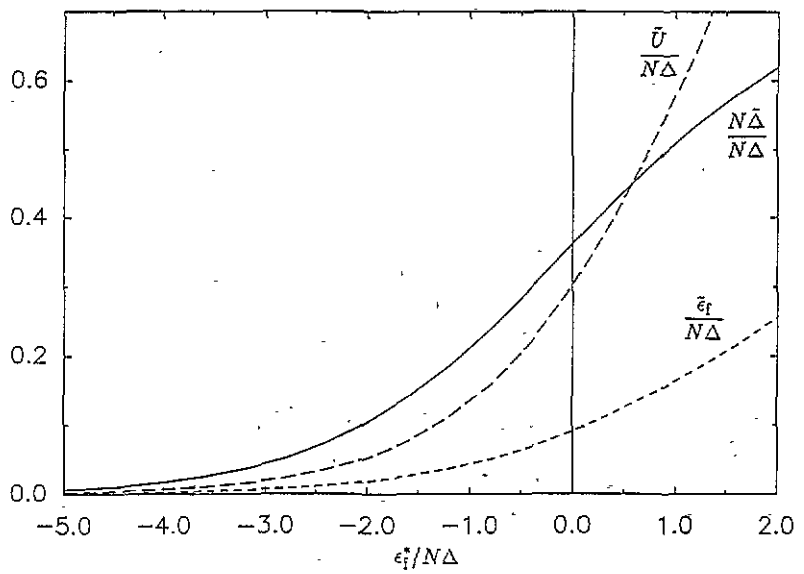

Figure 3. The behaviour of the quasi-particle parameters $\tilde{\Delta}$, $\tilde{\epsilon}_{\rm f}$ and $\tilde{U}$ for the N-fold degenerate model ($U = \infty$, $N = 8$) as a function of $\epsilon_{\rm f}^*/N\Delta$.

There are exact Bethe *ansatz* results [14] for the model for $U \to \infty$, however, which allow the quasi-particle parameters to be estimated as we did earlier for the non-degenerate model. The results are shown in figures 3 and 4 for $N = 8$ plotted as a function of the bare parameter ratio $\epsilon_{\rm f}^*/N\Delta$, where $\epsilon_{\rm f}^* = \epsilon_{\rm f} + \Delta(N-1)/\pi \ln(\pi D/N\Delta)$ and D is the half bandwidth. As the renormalized parameters in the localized regime all scale as $T_{\rm K}$, where $T_{\rm K} \sim \exp(\epsilon_{\rm f}^*/N\Delta)$, they are very small as can be seen in figure 3. In figure 4 where the ratios $\tilde{\epsilon}_{\rm f}/N\Delta$ and $\tilde{U}/N\Delta$ are plotted, it can be seen that the Kondo regime, where there is a single energy scale and the curves are flat, applies in the regime $\epsilon_{\rm f}^* < N\Delta$.

4. n-channel Kondo model for $n = 2S$

Finally we can develop a Fermi liquid theory along similar lines for the n-channel Kondo problem for $n = 2S$ which is appropriate for Mn impurities which have a half-filled d shell and no spin–orbit coupling. The model is of the same form as the s–d model with an exchange interaction between the impurity spin S and the conduction electrons but includes

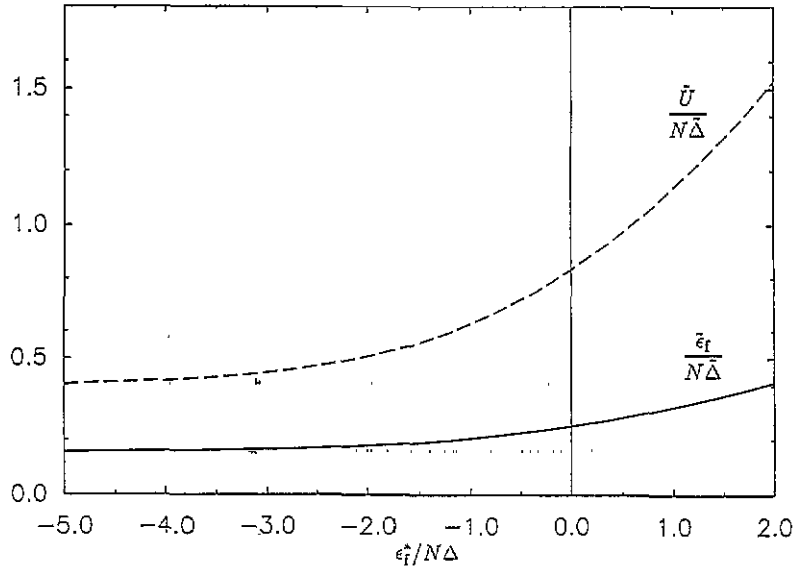

Figure 4. The ratio of the quasi-particle parameters, $\tilde{\epsilon}_f/\tilde{\Delta}$ and $\tilde{U}/\tilde{\Delta}$, for the N-fold degenerate model ($U = \infty$, $N = 8$) as a function of $\epsilon_f^*/N\Delta$. Only in the very localized regime $\epsilon_f^*/N\Delta < -3$ are the two curves flat corresponding to a single energy scale.

a sum over n individual conduction scattering channels

$$H_{\text{exc}} = 2J \sum_{k,k',m} \boldsymbol{S} \cdot c^{\dagger}_{k,m,\sigma}(\boldsymbol{s})_{\sigma\sigma'} c_{k',m,\sigma'} \tag{43}$$

where m is the channel index. For manganese ions the number of channels is $n = 2l + 1$ with $l = 2$, where l is the angular momentum quantum number corresponding to d wave scattering and $S = 5/2$ for a half-filled d shell. This model can be derived from the corresponding Anderson model

$$H_{\text{d}} = \sum_{m,\sigma} \epsilon_{\text{d}} c^{\dagger}_{\text{d},m,\sigma} c_{\text{d},m,\sigma} + \frac{(U + J_{\text{H}})}{2} \sum_{mm',\sigma\sigma'} c^{\dagger}_{\text{d},m,\sigma} c^{\dagger}_{\text{d},m',\sigma'} c_{\text{d},m',\sigma'} c_{\text{d},m,\sigma} + \sum_{k,m} \epsilon_k c^{\dagger}_{k,m} c_{k,m}$$
$$+ \sum_{k,m} (V_k c^{\dagger}_{k,m} c_{\text{d},m} + V_k^* c^{\dagger}_{\text{d},m} c_{k,m}) - \frac{J_{\text{H}}}{2} \sum_{mm',\sigma\sigma'} c^{\dagger}_{\text{d},m,\sigma} c^{\dagger}_{\text{d},m',\sigma'} c_{\text{d},m,\sigma'} c_{\text{d},m',\sigma} \tag{44}$$

which now includes a Hund's rule coupling term, J_{H}, which aligns the individual spins of the electrons in the impurity d shell. The $n = 2S$ Kondo Hamiltonian follows from a Schrieffer–Wolff transformation in the large Hund's rule limit $J_{\text{H}} \to \infty$, when the ground-state configuration corresponds to a half-full shell and virtual transitions to states with one more and one less electron in the d shell are taken into account. This is not the most general Hamiltonian of this type, it contains no off-diagonal interaction terms in the channel index m. The n-channel Kondo model is diagonal in the channel index so it should not be necessary to include non-diagonal terms for the physics of this model. We again conjecture that the appropriate form for the quasi-particle Hamiltonian describing the excitations near the Fermi liquid fixed point corresponds to a Hamiltonian of the same form but with renormalized

parameters. Performing a mean field calculation as earlier for γ_{imp}, χ_{imp} and $\chi_{c,imp}$

$$\gamma_{imp} = \tfrac{1}{3}\pi^2 k_B^2 2n\tilde{\rho}_{imp}(\epsilon_F)$$

$$\chi_{imp} = (g\mu_B)^2 2n\tilde{\rho}_{imp}(\epsilon_F)(1 + (\tilde{U} - \tilde{J}_H(n-1))\tilde{\rho}_{imp}(\epsilon_F)) \tag{45}$$

$$\chi_{c,imp} = (g\mu_B)^2 2n\tilde{\rho}_{imp}(\epsilon_F)[1 - (\tilde{U}(2n-1) + 3\tilde{J}_H(n-1))\tilde{\rho}_{imp}(\epsilon_F)] \tag{46}$$

where the renormalized parameters are indicated with a tilde. If non-diagonal interaction terms had been included in the Hamiltonian they would not have contributed to the mean field equations.

The Friedel sum rule still applies in the Kondo limit and implies $\tilde{\rho}_{imp}(\omega) = 1/\pi\tilde{\Delta}$. The condition $\chi_{c,imp} \to 0$ just gives one condition on the quasi-particle parameters. A further condition can be obtained, as pointed out by Nozières and Blandin [13], by using the fact that there should be no change in the occupation of the m-channel if the chemical potential changes in one of the other channels $m' \neq m$. The response in the m-channel to such a change is proportional to $(2\tilde{U} + 3\tilde{J}_H)\tilde{\rho}(\epsilon_F)$, which we equate to zero. These conditions give

$$\tilde{U} = -\tfrac{3}{2}\tilde{J}_H = \pi\tilde{\Delta} = 4k_B T_K \tag{47}$$

with the resonance at the Fermi level, and the Kondo temperature is defined for general n via $\gamma_{imp} = \pi^2 n k_B/6T_K$. These agree with the results for the s–d model (the Kondo limit of the non-degenerate Anderson model) for $n = 1$. With these values for the renormalized parameters the susceptibility is given by

$$\chi_{imp} = (g\mu_B)^2 n(n+2)/12k_B T_K \tag{48}$$

and the Wilson 'χ/γ' ratio

$$R = \frac{\chi_{imp}/\chi_0}{\gamma_{imp}/\gamma_0} = \frac{2(n+2)}{3} \tag{49}$$

which is as derived by Nozières and Blandin [13] and can also be deduced from the exact Bethe *ansatz* results [16] and microscopic Fermi liquid theory [17]. The model does not behave as a Fermi liquid in the underscreened case $n < 2S$ or the overscreened case $n > 2S$. It is not clear whether or not a simple effective Hamiltonians can be found to give the low-temperature behaviour in these more general models [16].

5. Conclusions

We have shown that it is possible to give explicit quasi-particle Hamiltonians for several magnetic impurity models which, within a Landau-like mean field approximation, give exact results in the Fermi liquid regime as $T \to 0$. The renormalized parameters, $\tilde{\epsilon}_d$, $\tilde{\Delta}$, $\tilde{U}$, and $\tilde{J}_H$, can be expressed in terms of the self-energy, its derivative, and the irreducible four-point vertices (which are local for all these impurity models) of the conventional diagrammatic perturbation theory, evaluated at the Fermi level. This approach to Fermi liquid theory combines the intuitive elements of the phenomenological theory of Landau with the concept of an effective Hamiltonian about the relevant fixed point in the renormalization group approach. We leave the calculation of transport properties to the sequel paper. There we will develop the approach further within the revised framework of a renormalized perturbation theory. The starting point will be the quasi-particle Hamiltonians used here but additional interactions have to be included to allow the extension of the calculations beyond the Fermi liquid regime.

Acknowledgments

I am grateful to N Andrei, Y Chen, D M Edwards and J Jefferson for helpful discussions and comments, and for their general encouragement.

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