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# The theory of heavy-fermion compounds from low temperatures to the classical regime

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**Abstract.** The solution of the mean field equations of the periodic Anderson model are studied in detail in order to compute the temperature dependence of the thermodynamic quantities for heavy-fermion compounds.

The mean field solution is valid only for temperatures  $T < T^*$ . In the impurity case  $T^* \sim T_K$  but for the lattice we find  $T^* \gg T_K$  because of the shift of the chemical potential which occurs as  $n_f$  is changed. We show that it is useful to introduce a further characteristic temperature,  $\tau$ , such that  $k_B \tau \simeq \langle V^2 \rangle^2 / W^3$  where  $\langle V^2 \rangle^{1/2}$  is the average hybridization over the Fermi surface and  $W$  is the band width.

We show that a linear approximation may be used for the full Fermi function which allows mean field theory to be evaluated easily. The susceptibility is evaluated in full mean field theory and using the linear approximation. The agreement is good.

At high temperatures  $T > T_K$  the mean field predicts quasi-classical behaviour  $\chi = C/T + \theta$ . This arises from a non-interacting Fermi gas because the band energies are functions of temperature. This result can be readily understood using the analytic approach.

## 1. Introduction

At high temperatures, heavy-fermion compounds behave as if they contain free (classical) spins. The susceptibility follows a Curie–Weiss law. As the temperature is lowered the electron degrees of freedom become incorporated into the Fermi liquid giving rise to the enhanced specific heat and enhanced Pauli susceptibility. The thermodynamic behaviour of heavy-fermion compounds bears some resemblance to the behaviour of dilute Kondo impurities. The transport properties of the two systems are markedly different at low temperatures because of the coherence in the periodic Anderson lattice. For a review see [1].

In this paper we concentrate on the thermodynamic properties and evaluate these as a function of temperature. We use the slave-boson method which has been successfully used to describe heavy-fermion behaviour at zero or low temperature [2–5]. The lowest approximation to this is the mean field theory. At finite temperature the mean field theory breaks down for  $T \simeq T_K$  for impurity systems [2] and in lattices if the chemical potential is held constant [6]. Evans *et al* [7, 8] found numerically that allowing the chemical potential to change gave a negative feedback effect delaying the onset of integral valence and that the temperature  $T^*$  at which  $n_f = 1$  in mean field theory can be very much higher than

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the effective Kondo temperature,  $T_K$ , which characterizes the low-temperature behaviour of a lattice problem [9]. This paper explores this result in more detail. It is important to understand the temperature dependence of the mean field solutions before considering the interactions.

For the impurity problem the transition predicted by mean field theory is certainly spurious. It is not clear if there should be a transition in an Anderson lattice as a function of temperature. The results of this paper are valid in the regime where  $n_f < 1$  and mean field theory is sensible. The mean field approximation leads to single quasiparticle states satisfying Bloch's theorem—this is usually a fermi liquid except when the degeneracy of the  $f$  level is equal to the number of electrons when it may be an insulator. Indeed the properties of the Anderson lattice are mapped on to a non-interacting Fermi gas but with an unusual density of states with an unusual temperature dependence. We show in this paper that this Fermi gas state may exhibit thermodynamic behaviour reminiscent of classical spins. Thus the existence of a susceptibility varying as  $C/(T + \theta)$  is not to be taken as evidence that there has been a transition to a classical state.

The mean field solution predicts a hybridization gap which is observed at low temperatures [10]. At  $T^*$  the gap vanishes. Hence, a measurement of the existence of a gap in the density of states at a temperature where the susceptibility is Curie-Weiss-like would confirm the prediction that the mean field theory does account for the 'classical regime' satisfactorily.

In this paper we obtain the numerical solutions of the mean field equations. We also set up a linear approximation [11] to the Fermi functions which allows us to obtain analytic solutions to the mean field equations and hence get a deeper understanding of the physics. We check the accuracy of this approximation in this paper by computing the thermodynamic quantities for both the full mean field theory and the linear approximation.

## 2. Mean field solution of the periodic Anderson model

In this section we derive the mean field solutions to the periodic Anderson lattice and investigate the conditions for them to be valid.

Our starting point is the Anderson lattice Hamiltonian in which we consider hybridization of the local  $N$ -fold degenerate  $f$ -electron states with  $N$  conduction bands in the usual way but also includes other conduction bands which do not hybridize with the  $f$  level. This is done in order to consider the change in the chemical potential for a concentrated lattice system and for when the rare-earth sites are diluted. (The extra  $s$  bands act as a reservoir for the electrons which move out of the localized  $f$  states).

The  $N$ -fold degeneracy for the  $f$  electrons is equal to  $2J + 1$ . The conduction electron states are expanded in spherical harmonics so the hybridization is diagonal in  $m$ . The angular momentum is not conserved as the conduction electrons propagate and hence the conduction electron energy has been approximated in the Hamiltonian which is given below by considering it to be also  $N$ -fold degenerate. This approximation is frequently used because it allows for an  $N^{-1}$  expansion. A more realistic model has the  $N$ -fold-degenerate  $f$  state hybridizing with a conduction band which is only doubly (spin) degenerate [12]. This leaves the structure of the theory unchanged [13] but gives rise to a direction-dependent hybridization potential  $V_k^m$  and a direction-dependent hybridization gap.

$$H = \sum_k \sum_{m=1}^N \varepsilon_{km} c_{km}^+ c_{km} + \sum_i \sum_{m=1}^N E_{0m} f_{im}^+ f_{im} - \sum_i \sum_k \sum_{m=1}^N V_{km} e^{ik \cdot R_i} c_{km}^+ f_{im} + \text{HC}$$

$$+ U \sum_i \sum_{m \neq m'}^N n_{im}^f n_{im'}^f + \sum_k \sum_{l=1}^s \varepsilon_{kl} d_{k,l}^+ d_{kl}. \quad (2.1)$$

Here  $\varepsilon_{km}$  are the band energies for the hybridizing conduction electrons,  $E_{0m}$  is the bare f-electron energy—it is assumed to be independent of  $m$  except when a magnetic field is acting,  $V_{km}$  is the hybridization term,  $U$  is the on-site Coulomb repulsion and the energies of the non-hybridizing bands are  $\varepsilon_{k,l}$ .

The large local Coulomb repulsion can be eliminated by introducing the slave-boson technique in which the f-electron occupation is restricted to be less than or equal to one by including the following constraint in the Lagrangian:

$$n_{if} + b_i^+ b_i = 1. \quad (2.2)$$

The mean field approximation consists in assuming that

$$\langle b_i^+ \rangle = \langle b_i \rangle = \sqrt{1 - n_f} \quad (\text{all } i), \quad (2.3)$$

This results in the following mean field Hamiltonian:

$$\begin{aligned} H_{mf} = & \sum_k \sum_{m=1}^N \varepsilon_k c_{km}^+ c_{km} + \sum_i \sum_{m=1}^N \varepsilon_{fm} f_{im}^+ f_{im} + \sum_k \sum_{m=1}^N (\tilde{V}_{k,m} c_{km}^+ f_{km} + \text{HC}) \\ & + \sum_k \sum_{l=1}^s \varepsilon_{kl} d_{kl}^+ d_{kl} + \text{constant}. \end{aligned} \quad (2.4)$$

Here  $\varepsilon_{fm}$  is the renormalized f energy and  $\tilde{V}_{km} = V_{km} \sqrt{1 - n_f}$  is the renormalized hybridization. This may be diagonalized to give hybridized bands with energies

$$E_{m\pm}(k) = \frac{1}{2} \left( \varepsilon_k + \varepsilon_{fm} \pm \sqrt{(\varepsilon_k - \varepsilon_{fm})^2 + 4 \tilde{V}_{km}^2} \right). \quad (2.5)$$

In the absence of a magnetic field  $\varepsilon_{fm}$  is independent of  $m$  and we can define an effective hybridization

$$V^2 = \frac{1}{N} \sum_{m=1}^N \langle V_{km}^2 \rangle$$

where the average is taken over the Fermi surface. The values of  $\varepsilon_f$ ,  $n_f$  and the chemical potential,  $\mu$ , are given by the following equations (the conduction electron density of states has been taken as a constant  $\rho_0$  ( $\rho_0 = 1/NW$ ), and  $W$  is an effective conduction electron band width):

$$n_f = N\rho_0 \int_{-W}^{(N-1)W} (A_+(k) f(E_-(k) - \mu) + A_-(k) f(E_+(k) - \mu)) d\varepsilon_k \quad (2.6)$$

$$\varepsilon_f = E_0 + N\rho V^2 P_0 \int_{-W}^{(N-1)W} \frac{f(E_-(k) - \mu) - f(E_+(k) - \mu)}{E_+(k) - E_-(k)} d\varepsilon_k \quad (2.7)$$

$$n_f + n_c = N\rho_0 \int_{-W}^{(N-1)W} (f(E_-(k) - \mu) + f(E_+(k) - \mu)) d\varepsilon_k + s = 2 + s. \quad (2.8)$$

P stands for the principal part of the integral in equation (2.7),  $f(E - \mu)$  is the Fermi function and  $A_{\pm}$  are the conduction electron weights in the two hybridized bands:

$$A_{\pm} = \frac{1}{2} \left[ 1 \pm \frac{\varepsilon_k - \varepsilon_f}{\sqrt{[(\varepsilon_k - \varepsilon_f)^2 + 4\tilde{V}^2]}} \right] = \frac{\partial E_{\pm}(k)}{\partial \varepsilon_k}. \quad (2.9)$$

Equations (2.6)–(2.8) are three coupled integral equations for  $n_f$ ,  $\varepsilon_f$  and  $\mu$ . Using the relations  $A_{\pm} = \partial E_{\pm}(k)/\partial \varepsilon_k$  and  $A_+(k) + A_-(k) = 1$  equation (2.6) and equation (2.8) may be integrated exactly to obtain an equation for  $\mu$  which is valid for all temperature such that  $n_f \leq 1$ :

$$2 - n_f + s = \beta^{-1} N \rho_0 \times \ln \left[ \frac{[1 + \exp(-\beta(E_-(-W) - \mu))][1 + \exp(-\beta(E_+(-W) - \mu))]}{[1 + \exp(-\beta(E_-(N-1)W - \mu))][1 + \exp(-\beta(E_+(N-1)W - \mu))]} \right] + N \rho_0 s \beta^{-1} \ln \left[ \frac{1 + \exp(\beta(W + \mu))}{1 + \exp(-\beta(N-1)W - \mu)} \right] \quad (2.10)$$

where

$$E_{\pm}(X) = \frac{1}{2}(\varepsilon_f + X \mp \sqrt{(X - \varepsilon_f)^2 + 4\tilde{V}^2})$$

and  $\beta = 1/T$  (we work in energy units so that  $k_B = 1$ ).

The band width  $W$  is very large, so terms of order  $e^{-W/T}$  are negligible. This allows us to simplify the logarithm in equation (2.8) to obtain

$$\mu(T) = \frac{W}{1+s} (1 - n_f(T)). \quad (2.11)$$

The constraint (2.2) requires  $1 - n_f > 0$  but the mean field equations have solutions which may be analytically continued to  $n_f > 1$ —these are physically meaningless. We now derive a temperature  $T^*$  which is at the limit of validity of the theory  $T \leq T^*$  for  $n_f \leq 1$ . The mean field equations are solved for  $n_f \rightarrow 1$ . It is important to note that this implies  $\tilde{V} = V\sqrt{1 - n_f} \rightarrow 0$  but this is not the unhybridized system for which  $V = 0$ . Since  $\mu = 0$  at  $n_f = 1$  this condition is in agreement with Harigaya [5] who assumed  $\mu = 0$  at all temperatures as is valid for the impurity problem.

Equation (2.8) can be evaluated immediately to give

$$Nf(\varepsilon_f^*) = \frac{N}{1 + \exp(\varepsilon_f^*/T^*)} = 1. \quad (2.12)$$

This is as one would expect for  $n_f = 1$  in an  $N$ -fold-degenerate level at  $\varepsilon_f^*$ .

Another relation between  $\varepsilon_f^*$  and  $T^*$  is found from equation (2.7):

$$\varepsilon_f^* = E_0 + N \rho_0 V^2 P \int_{-W}^{(N-1)W} \frac{d\varepsilon}{\varepsilon - \varepsilon_f^*} [f(\varepsilon_f^*) - f(\varepsilon)]. \quad (2.13)$$

This leads to the following equation for  $T^*$  in terms of the bare Anderson lattice parameters ( $N$ ,  $WE_0$  and  $V$ ) and  $\varepsilon_f^*$ , which is found from equation (2.12) to be  $\varepsilon_f^* = T^* \ln(N-1)$ , as found by Harigaya [6]:

$$T^* = \frac{2j(N)}{\pi W} \sqrt{[(N-1)W - \varepsilon_f^*](W + \varepsilon_f^*)} \left| \frac{W + \varepsilon_f^*}{(N-1)W - \varepsilon_f^*} \right|^{(N-1)/2N} \times T_0 \exp \left( \frac{T^* W \ln(N-1)}{V^2} \right) \quad (2.14)$$

where  $j(N)$  is defined by

$$\ln \frac{\pi}{4j(N)} = \frac{1}{2} \int_{-\infty}^{\infty} dx \ln |x| \operatorname{sech}^2 [x + \frac{1}{2} \ln(N-1)]$$

and

$$T_0 = W \exp(E_0 W / V^2) \quad (2.15)$$

is the characteristic energy scale; all the temperatures we shall derive will be expressed in terms of  $T_0$ .

We are interested in the wide-band limit in which  $W$  is the largest energy in the problem, so  $\varepsilon_f / W \ll 1$ , and equation (2.10) simplifies to:

$$T^* = T_0 \frac{2j(N)(N-1)^{1/N}}{\pi} \exp \left[ -\frac{T^* W \ln(N-1)}{V^2} \right]. \quad (2.16)$$

The numerical factors are of the order of unity. In the Kondo regime  $T^* W \ln(N-1) / V^2$  is small and the exponential factor in (2.16) may be put equal to unity.

For  $N = 2$  we confirm Harigaya's result:

$$T^* = 1.134 T_0. \quad (2.17)$$

For larger  $N$  the integral for  $j(N)$  cannot be done analytically and numerical calculations show that  $T^*$  is a decreasing function of  $N$ .

Thus we find that for  $T < T^*$  the mean field solution is well behaved. The value of  $T^*$  is similar to  $T_0$ —the Kondo temperature for an impurity with the bare energy  $E_0$ .

The entropy can also be obtained for  $T = T^*$ :

$$S(T^*) = \ln N + (N-1) \ln \left( \frac{N}{N-1} \right). \quad (2.18)$$

This is the entropy of a system of  $N$  independent Fermion states [2, 5, 7] each with probability of occupation of  $1/N$ . The entropy of a single occupied localized state of degeneracy  $N$  is the classical value  $S_{\text{classical}} = \ln N$ . The entropy given by (2.18) is higher than the classical value because of the additional fluctuation in the values of  $n_f$  allowed by the mean field theory [5]. However, (2.18) does approach the classical value  $\ln N$  for large  $N$ , as expected.

### 3. Solution at low temperatures

We investigate the lattice problem at low temperatures in order to calculate the appropriate low-temperature energy scale,  $T_K$ , for the lattice. This will be compared with the Kondo temperature for an impurity  $T_K^i$ , and the limiting temperature  $T^*$ .

At  $T = 0$  equations (2.6) and (2.7) simplify because the Fermi functions are unity for  $E_-(\varepsilon_k) < \mu$  and zero for  $E_-(\varepsilon_k) > \mu$  and all  $E_+(\varepsilon_k)$ . This leads to the following equations:

$$n_f^0 = \left[ 1 + \frac{W(\varepsilon_f^0 - \mu)}{V^2} \right]^{-1} \quad (3.1)$$

and

$$T_K = \varepsilon_f^0 - \mu = T_0 e^{-\varepsilon_f^0 W/V^2}. \quad (3.2)$$

The Kondo temperature for the impurity  $T_K^i$ , for which  $\mu = 0$  is very close to  $T_0$  (equation (2.15)) because  $T_0 W/V^2 \ll 1$

$$T_K^i = T_0 e^{-T_K^i W/V^2}. \quad (3.3)$$

However, for the lattice problem, equations (3.1) and (3.2) must be solved together with equation (2.11); this leads to

$$T_K = T_0 \exp \left[ -T_K \frac{W}{V^2} \left( 1 + \frac{W^2}{(1+s)V^2} \right) \right]. \quad (3.4)$$

The coefficient in the exponential in equation (3.4) is much larger than the one in equation (3.3). We define a temperature  $\tau$

$$\frac{1}{\tau} = \frac{W}{V^2} \left( 1 + \frac{W^2}{(1+s)V^2} \right) \cong \frac{W^3}{(1+s)V^4} \quad \text{lattice} \quad (3.5)$$

$$\frac{1}{\tau} = \frac{W}{V^2} \left( 1 + \frac{W^2}{(1+s)V^2} \right) = 1/NV^2 \rho_0 = W/V^2 \quad \text{impurity}. \quad (3.6)$$

Hence equation (3.4) becomes

$$T_K = T_0 e^{-T_K/\tau}. \quad (3.7)$$

The lattice effective Kondo temperature,  $T_K$ , is reduced strongly if  $\tau \ll T_0$ . In heavy-fermion compounds we usually have  $W \simeq 10$  eV and  $V \simeq 1$  eV which leads to values of  $\tau \simeq 11$  K for the lattice ( $s = 0$ ) and  $\tau \simeq 1100$  K for an impurity. In figure 1 we show a plot of  $T_K/T_0$  as a function of  $T_0/\tau$ . For example the parameters taken by Evans *et al* [7] correspond to  $s = 0$ ,  $T_0 \cong 782$  K,  $\tau = 11$  K and  $T_K \cong 38$  K. It is straightforward to show that equation (3.7) implies that  $\tau < T_K < T_0$  if  $\tau < T_0$ .

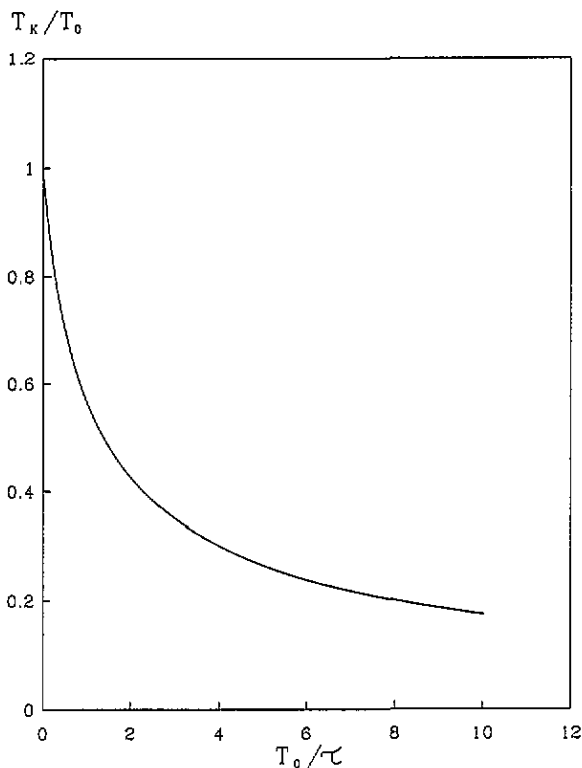
For the lattice  $\tau < T_0$  leading to  $T_K \ll T_0$  whereas for the impurity case  $\tau \gg T_0$  leading to  $T_K \cong T_0$  (as given in equation (3.3)). The reduction of  $\tau$  arises because of the shift of the chemical potential for the lattice problem.

It has recently been found [11] that the characteristic temperature  $\tau$  is also important in determining the shape of the magnetic susceptibility.

We note that in section 2 we found that  $T^* \cong T_0$  thus we find that for  $T_0/\tau \ll 1$  that  $T_K \sim T_0 \sim T^*$  but that for the lattice problem for which  $T_0/\tau \geq 1$  then  $T_K \ll T^*$ . This means that the mean field equations are valid for temperatures considerably greater than  $T_K$  (the low-temperature Kondo scale).

#### 4. The linear approximation method

While the mean field (MF) equations can be solved analytically at zero temperature, it is difficult to obtain temperature dependences at finite temperatures. One can find low-temperature behaviour of the mean field equations using the Sommerfield expansion for the



**Figure 1.** A plot of the solution of equation (3.7). The lattice Kondo temperature  $T_K$  as divided by  $T_0$  (the impurity Kondo temperature) as function of  $T_0/\tau$  where  $\tau$  is defined by equation (3.5).

Fermi function, which gives typical Fermi liquid  $T^2$  behaviour near zero temperature. By solving the MF equations numerically, Evans *et al* [7] showed that the MF gives a good description for the specific heat and magnetic susceptibility over the whole temperature regime  $0 < T < T^*$ . It is desirable to find how this agreement arises analytically. We are able to get analytic expressions for MF equations by employing a simple approximation for the Fermi function. Our strategy is to replace the smeared part of the Fermi function by a straight line which enables us to carry out all integrals involved exactly over the whole temperature regime. We shall see this approximation preserves the essential physics of the system and leads to the correct qualitative behaviour over the temperature where the MF approximation is valid.

We adopt the simplest linear approximation to the Fermi function  $f(\varepsilon)$ :

$$f_L(\varepsilon) = \begin{cases} 1 & \text{for } \varepsilon - \mu \leq -\Delta \\ [\Delta - (\varepsilon - \mu)]/2\Delta & \text{for } -\Delta \leq \varepsilon - \mu \leq \Delta \\ 0 & \text{for } \varepsilon - \mu > \Delta. \end{cases} \quad (4.1)$$

Here  $\Delta = 4T \ln 2$  is a measure of the temperature and is determined by the condition that the number of excited quasiparticles is the same for the linear and full Fermi functions

$$\int_{\mu}^{\infty} f(\varepsilon) d\varepsilon = \int_{\mu}^{\infty} f_L(\varepsilon) d\varepsilon. \quad (4.2)$$



Depending on the size of  $\Delta$ , we have to consider three different regimes which are indicated schematically in figure 2. In regime I,  $\mu + \Delta$  lies in the lower band. This corresponds to the low-temperature regime in which only part of the lower band contributes. Regime II is the intermediate-temperature case in which  $\mu + \Delta$  lies in the gap. In this case the whole of the lower band contributes. Finally when  $\mu + \Delta$  is big enough to cross into the upper band (regime III), we have contributions from the upper band as well as the lower band. We evaluate the MF solutions within this approximation and assume that  $W$  is large.

$$\text{Regime I} \quad \Delta < \tilde{\varepsilon}_f - \frac{\tilde{V}^2}{(N-1)W}$$

$$n_f = N\rho_0 \frac{\tilde{V}^2}{2\Delta} \ln \left[ \frac{\varepsilon_f + \Delta}{\tilde{\varepsilon}_f - \Delta} \right] \quad (4.3)$$

$$\varepsilon_f - E_0 = N\rho_0 V^2 \left\{ 1 + \ln \left[ \frac{W}{\tilde{\varepsilon}_f + \Delta} \right] + \frac{\Delta - \tilde{\varepsilon}_f}{2\Delta} \ln \left[ \frac{\tilde{\varepsilon}_f + \Delta}{\tilde{\varepsilon}_f - \Delta} \right] \right\}$$

$$\mu = \frac{W}{1+s} (1 - n_f) \quad (4.4)$$

Here  $\tilde{\varepsilon}_f = \varepsilon_f - \mu$  is the Kondo energy.

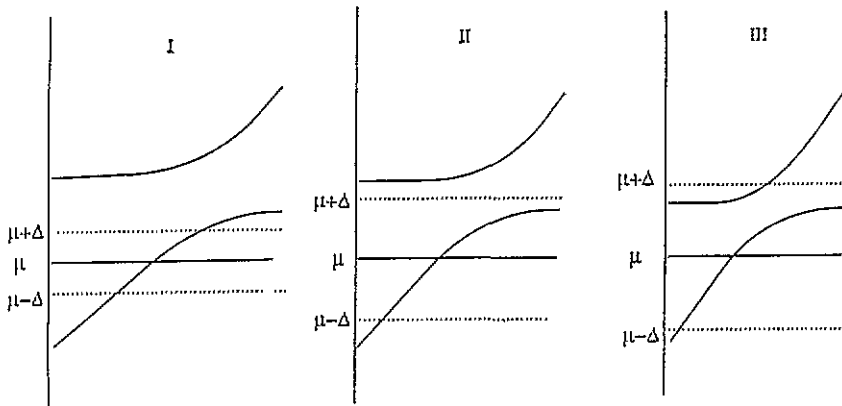


Figure 2. A diagram illustrating the values of  $\Delta$  for regions I, II, III.

For small  $\Delta$  it is easy to show that

$$n_f = n_f^0 \left[ 1 + \frac{1}{2} \left( \frac{\Delta}{\tilde{\varepsilon}_f^0} \right)^2 \right] \quad (4.5)$$

$$\varepsilon_f = \varepsilon_f^0 \left[ 1 - \frac{NV^2}{3\pi \varepsilon_f^0 W} \left( \frac{\Delta}{\tilde{\varepsilon}_f^0} \right)^2 \right] \quad (4.6)$$

$$\mu = \frac{W}{1+s} \left[ 1 - n_f^0 - \frac{n_f^0}{2} \left( \frac{\Delta}{\tilde{\varepsilon}_f^0} \right)^2 \right] \quad (4.7)$$

$$\tilde{\varepsilon}_f \equiv \varepsilon_f - \mu = \tilde{\varepsilon}_f^0 + \left( \frac{\Delta}{\tilde{\varepsilon}_f^0} \right)^2 \left[ \frac{W}{2(1+s)} - \frac{NV^2}{3\pi W} \right]. \quad (4.8)$$

Here  $n_f^0$ ,  $\varepsilon_f^0$  and  $\tilde{\varepsilon}_f^0$  are the zero-temperature solutions obtained in section 3. We see that although  $\varepsilon_f$  falls with increasing temperature the effective Kondo energy  $\tilde{\varepsilon}_f$  is rising.

We also evaluate  $n_f$  and  $\varepsilon_f$  for the other regimes:

$$\begin{aligned} \text{Regime II} \quad & \tilde{\varepsilon}_f - \frac{\tilde{V}^2}{(N-1)W} < \Delta < \tilde{\varepsilon}_f + \frac{\tilde{V}^2}{W} \\ n_f = N\rho_0 & \left\{ \frac{\Delta - \tilde{\varepsilon}_f}{2\Delta} (N-1)W + \frac{\tilde{V}^2}{2\Delta} \left( 1 - \ln \left[ \frac{\tilde{V}^2/(\tilde{\varepsilon}_f + \Delta)}{(N-1)W} \right] \right) \right\} \\ \varepsilon_f - E_0 = N\rho_0 V^2 & \left\{ \ln \left[ \frac{W}{\tilde{\varepsilon}_f + \Delta} \right] + \frac{\Delta - \tilde{\varepsilon}_f}{2\Delta} \ln \left[ \frac{(N-1)W}{\tilde{V}^2/(\tilde{\varepsilon}_f + \Delta)} \right] + \frac{\tilde{\varepsilon}_f + \Delta}{2\Delta} - \frac{\tilde{V}^2}{2\Delta} \frac{N}{(N-1)W} \right\} \end{aligned} \quad (4.9)$$

$$\begin{aligned} \text{Regime III} \quad & \Delta > \tilde{\varepsilon}_f + \tilde{V}^2/W \\ n_f = N\rho_0 & \left\{ \frac{\Delta - \tilde{\varepsilon}_f}{2\Delta} NW + \frac{\tilde{V}^2}{2\Delta} \ln \left[ (N-1) \frac{\tilde{\varepsilon}_f + \Delta}{\Delta - \tilde{\varepsilon}_f} \right] \right\} \\ \varepsilon_f - E_0 = N\rho_0 V^2 & \left\{ 1 + \ln \left[ \frac{W}{\tilde{\varepsilon}_f + \Delta} \right] + \frac{\Delta - \tilde{\varepsilon}_f}{2\Delta} \ln \left[ (N-1) \frac{\tilde{\varepsilon}_f + \Delta}{\Delta - \tilde{\varepsilon}_f} \right] - \frac{\tilde{V}^2}{2\Delta} \frac{N}{(N-1)W} \right\}. \end{aligned} \quad (4.12)$$

One thing to be noted here is that the average valence  $n_f$  approaches its saturated value as  $n_f = (N/2)(1 - \tilde{\varepsilon}_f/\Delta)$ . The numerical results demonstrate that the linear approximation has preserved important physics and is consistent with the solutions of the full MF equations. In figures 3, 4 and 5 we plot the temperature dependence of  $\varepsilon_f$ ,  $n_f$  and  $\tilde{\varepsilon}_f$ . The full MF theory is shown by the solid line and the linear approximations by the broken line. The curves were obtained for the following values of the input parameters:  $V = 1$  eV,  $E_0 = -0.5$  eV,  $W = 10$  eV,  $N = 6$  and  $s = 0$ . The temperatures corresponding to the transitions between regions I and II and regions II and III were 18.2 K and 48.7 K respectively for these input parameters. We see that the curves for  $\varepsilon_f$ ,  $n_f$  and  $\tilde{\varepsilon}_f$  go smoothly through these values. The agreement is exact at  $T = 0$  and good until regime III is reached. In the next section we see that the interesting physics is in regions I and II.

At high temperatures where the f level is weakly hybridizing, one would expect a localized approximation to be valid for  $n_f$ :

$$n_f \simeq \frac{N}{e^{\tilde{\varepsilon}_f/T} + 1}. \quad (4.13)$$

This may be solved for  $\tilde{\varepsilon}_f$ :

$$\tilde{\varepsilon}_f \simeq T \ln \frac{N - n_f}{n_f} \simeq T \ln(N - 1) \quad N \neq 2. \quad (4.14)$$

The agreement of the equation (4.14) with the MF solutions is very good at high temperatures; for  $T \gtrsim 300$  K the error is less than 1.5%.

The result for  $N = 2$  is different because  $\tilde{\varepsilon}_f \rightarrow 0$  as  $T \rightarrow T^*$  and hence  $\tilde{\varepsilon}_f$  has a maximum as shown in figure 5(b).

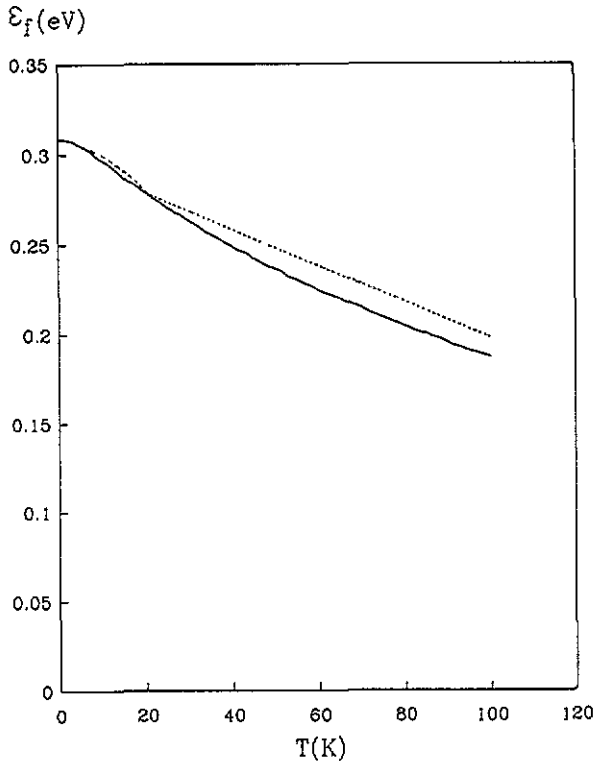


Figure 3. The effective f-level energy versus temperature for  $N = 6$ . The solid line indicates full MF solutions and the broken one shows the linear approximation. The interesting physics in this material occurs for  $T \lesssim 30$  K, where the agreement is quite good.

Equation (4.14) would give the following result as  $n_f \rightarrow 1$ :

$$\tilde{\epsilon}_f \simeq T(1 - n_f). \quad (4.15)$$

This is confirmed by solving equation (4.11) in the limit  $n_f \rightarrow 1$ . The different behaviour for  $\tilde{\epsilon}_f$  at high temperatures for  $N = 2$  compared with  $N \neq 2$  does not seem to show up in the thermodynamics.

We now want to estimate  $T_L^*$  at which  $n_f \rightarrow 1$  and MF theory breaks down. In this limit  $\Delta^* = 4T_L^* \ln 2$  is given by

$$\Delta^* = \frac{N}{2} e(N-1)^{(2-N)/N} T_0 \exp\left(-\frac{\Delta^*(1-2/N)}{NV^2\rho_0}\right). \quad (4.16)$$

For the  $N = 2$  case we get  $T_L^* = (e/4 \ln 2) T_0 \cong 0.98 T_0$ . This is compared to the result from full MF theory  $T^* = 1.13 T_0$ . Thus we see that the linear approximation describes the physics of the system reasonably well for the high-temperature regimes.

The agreement at  $T = 0$  is exact and is very good in the temperature range where interesting phenomena occur.

## 5. Applications of the linear approximation

In this section we use the linear approximation to calculate the magnetic susceptibility and the heat capacity and compare the results with the full solution. A brief discussion of

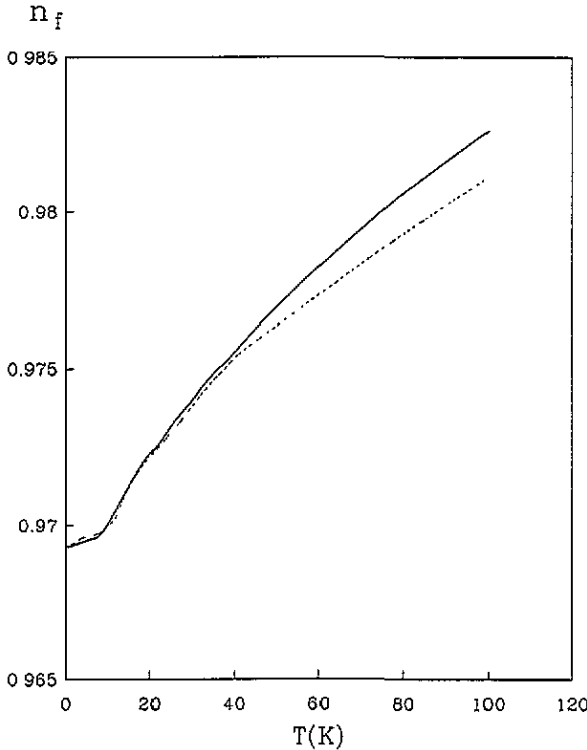


Figure 4. The number of f electrons per site versus temperature. The solid and broken lines have the same meaning as in figure 3. The interesting physics in this material occurs for  $T \lesssim 30$  K, where the agreement is quite good.

the magnetic susceptibility has been given before [11]. In a magnetic field  $E_{0m}$  becomes  $E_0 + g\mu_B mB$  and the susceptibility is found from

$$\chi = -(g\mu_B)^2 (\partial^2 F / \partial H^2)_{H=0}. \tag{5.1}$$

Using the linear approximation we find the following analytical expressions for  $\chi$ :

$$\chi = \rho_0 (g\mu_B)^2 \sum_{m=-J}^J m^2 \begin{cases} \tilde{V}^2 / (\tilde{\epsilon}_f^2 - \Delta^2) & \text{regime I} \tag{5.2} \\ \frac{1}{2\Delta} \left[ (N-1)W - \frac{\tilde{V}^2}{\tilde{\epsilon}_f + \Delta} \right] & \text{regime II} \tag{5.3} \\ NW/2\Delta - \tilde{V}^2 / (\Delta^2 - \tilde{\epsilon}_f^2) & \text{regime III.} \tag{5.4} \end{cases}$$

We plot  $\chi$  as a function of  $T$  in figure 6. As can be seen from the figure 6,  $\chi$  increases from the zero-temperature value  $\tilde{V}^2 / \tilde{\epsilon}_f^2$  quadratically in  $\Delta$  in regime I and has a maximum and crosses over to a Curie–Weiss regime in regime III. The solid line is the full MF result and the broken line is the linear approximation given by equations (5.2)–(5.4); the crossover occurs below  $T_K$  because  $\Delta$  is related to  $T$  by  $T \simeq 0.36\Delta$ . This is consistent with the numerical results of Evans *et al* [7]. We note that the boundary of regions I and II is at 18.2 K and II and III is at 48.7 K and thus the interesting behaviour is within regions I and II.

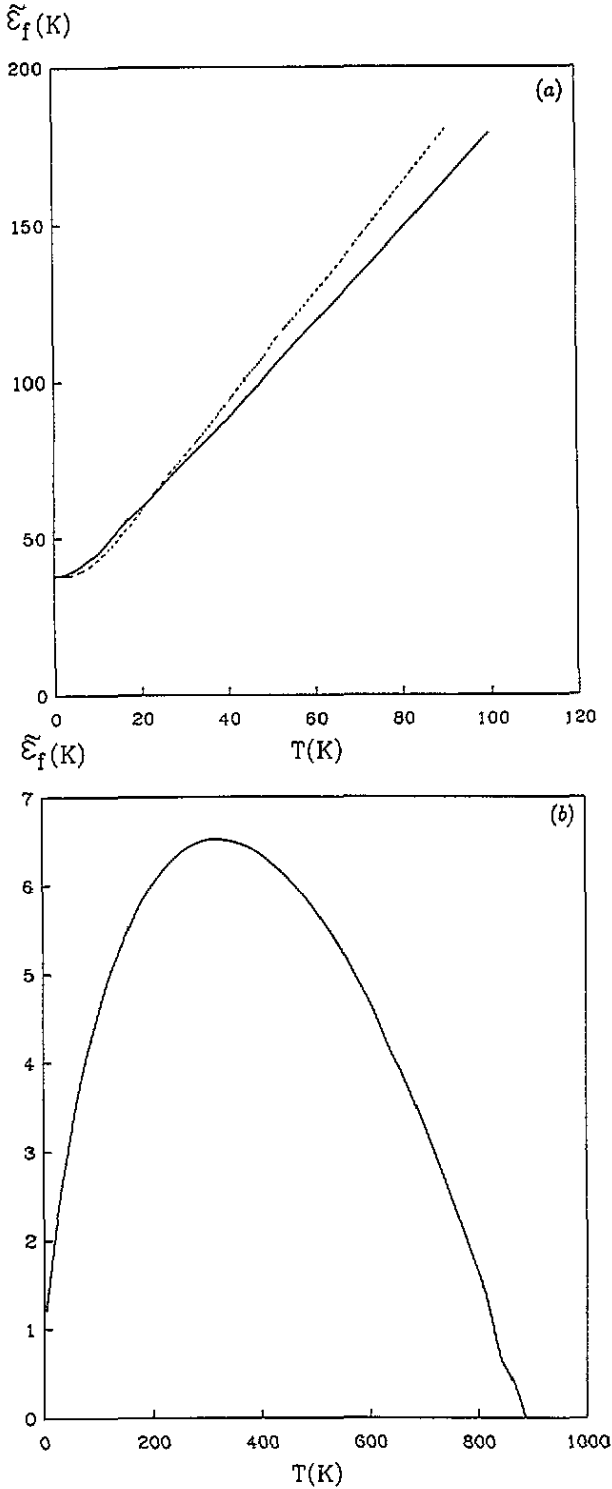


Figure 5. The effective f-level energy measured relative to the Fermi energy as a function of temperature. (a)  $N = 6$ . The interesting physics in this material occurs for  $T \lesssim 30$  K, where the agreement is quite good. (b)  $N = 2$ . The solid and broken lines have the same meaning as in figure 3.

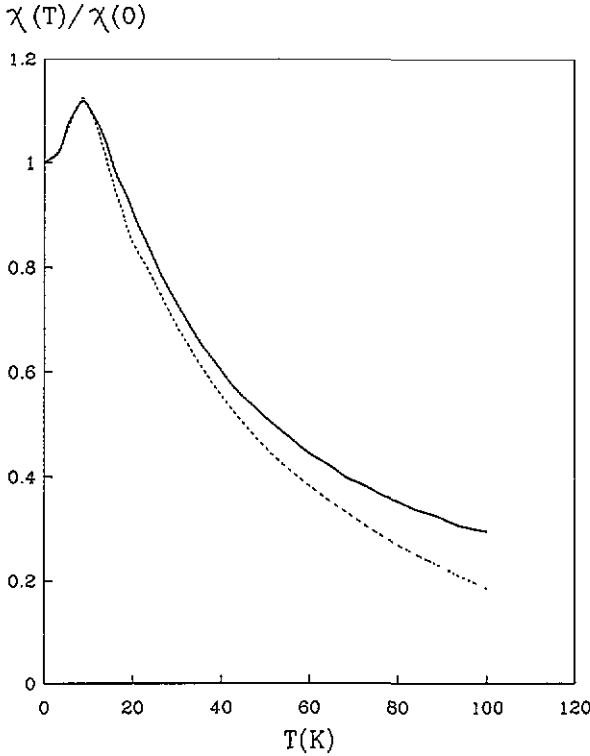


Figure 6. The magnetic susceptibility calculated as a function of temperature for both the full MF theory (solid line) and linear approximation (broken line). Note that for the given choice of parameters the boundary of regions I and II is at  $T = 18.2$  K and for regions II and III it is at  $48.7$  K.

At low temperatures the MF solutions obtained here always exhibit a maximum and therefore a fit to the experiments can be obtained only for systems which show the maximum of the susceptibility at finite temperature. A monotonically decreasing  $\chi$  is obtained if anisotropic hybridization is included as is the case where an  $N$ -fold-degenerate  $f$  level hybridizes with a doubly degenerate conduction band [12]. The Curie-like behaviour at high temperatures is interesting because in the MF approximation the full periodic Anderson lattice is mapped onto a non-interacting Fermi gas. It arises in the theory as formulated here because of the form of the density of states and its unusual temperature dependence. It is an indication that the MF theory is giving a good account of the behaviour in the temperature regime  $T_K < T < T^*$ , which for our parameters is  $38 \text{ K} \lesssim T \lesssim 780 \text{ K}$ , and that the observation of a classical Curie-Weiss susceptibility should not be taken as proof that the  $f$  electron is no longer part of the Fermi liquid.

We can use the simple approximation appropriate for a localized level to estimate  $\chi$ :

$$\tilde{\epsilon}_f/T \simeq \ln(N - 1). \tag{5.5}$$

It is straightforward to obtain

$$\chi = \frac{(g\mu_B)^2}{T} \sum_{m=-J}^J m^2 \frac{e^{\tilde{\epsilon}_f/T}}{(e^{\tilde{\epsilon}_f/T} + 1)^2} \simeq \frac{(g\mu_B)^2}{T} \sum_m m^2 \frac{(N - 1)}{N^2}. \tag{5.6}$$

We examine the Curie constant which may be obtained from the localized level approximation equation (5.6) and regime III result given by equation (5.4). The classical result is

$$C_{\text{cl}} = \frac{1}{3}J(J+1)(g\mu_B)^2. \quad (5.7)$$

Both equations (5.6) and (5.4) give a Curie constant of this form (when we use  $N = 2J + 1$ ) but with correction factors. These are  $(N - 1)/N$  and  $N/(8 \ln 2)$  respectively. We see that the linear theory is becoming relatively inaccurate at high temperatures. It is not surprising that the localized level approximation gives a good result for the Curie constant.

The high-temperature expression for  $\chi$  is not exactly of a Curie-Weiss form but it does tend to  $1/T$  at high temperatures from below.

Plots of  $\chi^{-1}$  in the high-temperature regime for the full and linear theory give a good fit to a straight line and the same Curie-Weiss constant of  $\theta = -20$  K over the temperature range around 80 K. In fact the plot is not linear and gives a value of  $\theta$  closer to  $-5$  K if evaluated between 40 and 60 K. This is what one would deduce from equation (5.4):

$$\theta \cong -T_K/(2N \ln 2) \sim -5 \text{ K}.$$

The linear theory may also be used to obtain the electronic specific heat, but it is not helpful to do so because the analytic expressions for the internal energy are very cumbersome to differentiate. In figure 7 we show the full MF specific heat. At high temperatures we may use the approximation of sharp maximum in the density of states giving an effective energy,  $\tilde{\epsilon}_f$ . This leads to the following expression for the internal energy:

$$U = U_{\text{cond el}} - E_0(1 - n_f) \quad (5.8)$$

where  $E_0$  is the bare f level. The contributions to the specific heat divided by  $T$  from this result is shown in figure 7. (This would be difficult to observe experimentally because of the contribution from phonons.)

## 6. Discussion

In this paper we have shown how the MF theory of the periodic Anderson model may be used to obtain a good understanding of heavy-fermion materials over the temperature range over which their properties change from that characteristic of localized classical spins to that of a Fermi liquid.

We found a striking difference between the temperature dependence of the impurity and lattice problems in this treatment. For an impurity the temperature at which the MF theory fails  $T^*$  is very close to the Kondo temperature defined at low temperatures,  $T_K^I$ . For a lattice this is not true; the effective Kondo temperature  $\tilde{\epsilon}_f$  is much less than  $T^*$ . Physically this means that the Kondo resonance becomes less well defined for  $T \gtrsim T_K$  but that the sharp features in the density of states for the lattice problem persist up to  $T \simeq T^*$ . Experimentally the thermodynamics of heavy-fermion compounds is similar to that of Kondo impurities—this is because the thermodynamics is determined by an integral of the density of states with the smeared Fermi function.

We can understand this as follows. In both the impurity and lattice problem we can define a temperature,  $T_0 = We^{E_0/N\rho V^2}$ , which is defined in terms of the bare parameters of the Anderson Hamiltonian. The high-temperature limit  $T^*$  is of the order of  $T_0$ . The

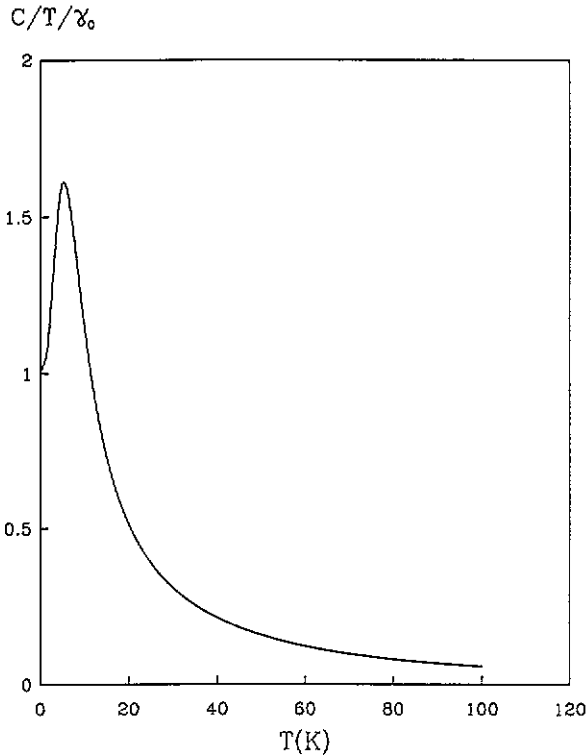


Figure 7. The MF theory for the specific heat divided by  $T$ .

difference between the lattice and the impurity cases arises at low temperatures because the energy of the localized level should be measured relative to the chemical potential. The chemical potential vanishes at  $T^*$  and is always zero for the impurity problem. For the lattice problem  $\mu$  rises at low temperature as  $n_f$  falls. Equation (3.2) for  $T_K$  may be written in a way which makes this more transparent:

$$T_K = \bar{\varepsilon}_f = \varepsilon_f^0 - \mu = W e^{-\bar{\varepsilon}_f W / V^2} e^{(E_0 - \mu) W / V^2}.$$

In all cases the factor  $e^{-\bar{\varepsilon}_f W / V^2}$  is close to unity. In the lattice problem the increase of  $\mu$  as  $n_f$  drops below unity causes  $T_K$  to be far below  $T_0$  as discussed in section 3. The linear approximations to the Fermi function which are used here are shown to give a very easy way of obtaining the interesting thermodynamic quantities for heavy-fermion materials. This also leads to an increased understanding. The peaks in  $\chi$  and  $\gamma$  may be understood in terms of the contrasting behaviour for regions I and III. Furthermore the appearance of the classical behaviour in region III may be related to the particular form of the density of states. We showed that the approximate constancy of  $\bar{\varepsilon}_f / T$  as temperature is varied leads to a Curie law and a constant specific heat.

We found that the magnitude of the temperature at which the true classical behaviour appears to set in depends on a temperature  $\tau$  as well as the Kondo temperature for an impurity,  $T_0$ . We also found that for an impurity the value of the effective Kondo temperature  $\bar{\varepsilon}_f = \varepsilon_f - \mu$  falls with increasing temperature; however, for the lattice  $\bar{\varepsilon}_f$  rises with temperature (for  $N = 2$  it passes through a maximum).



We have shown that the high-temperature behaviour may be understood in terms of a Fermi liquid at elevated temperature.

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### References

- [1] Steglich F 1993 *Physica B* **186–8** 1083
- [2] Coleman P 1987 *Phys. Rev. B* **35** 5072
- [3] Rasul J W and Desgranges H U 1986 *J. Phys. C: Solid State Phys.* **19** L671
- [4] Millis A J and Lee P A 1987 *Phys. Rev. B* **35** 3394
- [5] Bickers N E 1987 *Rev. Mod. Phys.* **59** 845
- [6] Harigaya K 1990 *J. Phys.: Condens. Matter* **2** 3259
- [7] Evans S M M, Chung T and Gehring G A 1989 *J. Phys.: Condens. Matter* **1** 10473
- [8] Evans S M M 1989 *Thesis* Oxford University
- [9] Matschke M and Entel P 1990 *Z. Phys. B* **78** 431
- [10] Wachter P 1992 *Solid State Commun.* **84** 25
- [11] Hong T M, Gehring G A and Wojciechowski R 1993 *Physica B* **186–8**
- [12] Evans S M M 1992 *Europhys. Lett.* **17** 469
- [13] Hong T M and Gehring G A 1992 *Phys. Rev. B* **46** 231