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# Mixed-valence and Kondo lattice behaviour in the uranium heavy-fermion systems

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**Abstract.** The uranium heavy-fermion systems exhibit ‘Kondo-like’ behaviour even though the valence,  $n_f$ , is non-integral. Their low-temperature properties are characterised by a single small energy scale,  $T_K$ . We use a slave-boson treatment of the  $f^2$ – $f^3$  Anderson lattice to compute thermodynamic quantities including the Wilson ratio. We compute the frequency and energy-dependent charge and spin susceptibilities and show that at low temperature these have a Fermi-liquid form with a greatly enhanced electron mass. We show that the charge fluctuations are greatly suppressed relative to the spin fluctuations even for  $n_f \sim 2.5$  indicating that the spin fluctuations dominate the behaviour throughout the mixed-valence regime. Quasiparticle interactions are described by fluctuations in the boson fields about their mean-field values. To  $O(1/N)$  the interaction is due to charge fluctuations and gives rise to d-wave superconductivity. Corrections of  $O(1/N^2)$  are due to spin fluctuations. These change the results substantially and p-wave superconductivity may also be obtained.

## 1. Introduction

In this paper we consider the low-temperature properties of the uranium heavy-fermion compounds. Much theoretical attention has been given to the cerium compounds (for a review see e.g. Lee *et al* 1986) and it is our purpose to consider how far the microscopic picture which has been developed for these can be extended to the uranium systems. There are important physical differences. For uranium the two lowest ionic configurations are  $5f^2$  and  $5f^3$  both of which are magnetic. The uranium heavy-fermion compounds are strongly mixed valence ( $n_f \sim 2.5$ ). This is in contrast to the cerium compounds where the valence fluctuations are between  $f^1$  which is magnetic and  $f^0$  which is non-magnetic. Heavy fermion behaviour is observed here only in the Kondo limit, i.e. for  $n_f$  close to one. We note that there is an important difference concerning the Fermi surface. While calculations using the local density approximation (LDA) can be fitted to the de Haas–van Alphen data for the uranium systems this is not usually true of the cerium heavy-fermion systems (Springford 1989). Despite these differences the thermodynamic and transport properties are remarkably general (for a review see Stewart 1984). In particular we note the following universal features.

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1. The dimensionless ratio of the spin susceptibility,  $\chi_S$ , to the linear coefficient of the specific heat,  $\gamma$ , the 'Wilson ratio', is close to the free-electron value of one (see Lee *et al* 1986 for a plot of  $\gamma$  vs  $\chi_S$ ).
2. The low- $T$  resistivity,  $\rho$ , varies as  $AT^2$ , where  $A$  scales as  $\gamma^2$  (Kadowaki and Woods 1986).
3. The low- $T$  susceptibility also rises as  $T^2$ .
4. The specific heat of several of the compounds exhibits a rapid downturn with increasing temperature and can be fitted to  $C_V = \gamma T + \delta T^3 \ln T$ .

It has been suggested that the presence of a  $T^3 \ln T$  term in the specific heat and  $T^2$  contributions to  $\rho$  and  $\chi_S$  imply strong spin fluctuation effects and UPt<sub>3</sub> has sometimes been signalled out as being different to the other heavy-fermion compounds (Brodale *et al* 1986, Willis *et al* 1985). An analysis of the pressure-dependent data for UPt<sub>3</sub>, however, shows the existence of several 'scaling relations', i.e. the susceptibility, resistivity and the  $T^3 \ln T$  term in the specific heat all scale as  $(\gamma/\gamma(p=0))^n$  where  $n = 1, 2, 3$  respectively (Auerbach and Levin 1986a). It is these scaling relations that are difficult to explain in terms of a paramagnon theory. In liquid <sup>3</sup>He, for example, where spin fluctuation effects are known to be important, the Wilson ratio is strongly pressure dependent and  $\delta$  does not scale with  $\gamma^3$ . These features arise naturally when a slave-boson approach is used to treat the  $U = \infty$   $f^0$ - $f^1$  periodic Anderson model in the Kondo limit. This model describes a band of free electrons hybridising with a highly correlated band of  $f$  electrons and has been widely used as a starting point for microscopic theories of the heavy-fermion compounds (Millis and Lee 1987, Rasul and Desgranges 1986). This model is not, however, directly relevant for uranium.

Recently Rasul and Harrington (1987) (hereafter referred to as I) have considered an extension of the slave-boson method to describe the  $f^2$ - $f^3$  Anderson lattice providing a microscopic description of the uranium heavy-fermion compounds. The solution is more complicated and two boson fields are required to impose the constraint that  $2 \leq n_f \leq 3$ , i.e. we not only have to constrain  $n_f$  to being less than 3 but also greater than 2. Making a transformation to the radial gauge introduces two extra fields and we obtain four equations at mean-field level and a four by four matrix describing the fluctuations. This can be compared to cerium where only two mean-field equations are found and fluctuations are described by a  $2 \times 2$  matrix. The mean-field solution yields a renormalised band structure with heavy quasiparticles at the Fermi level. In contrast with cerium it is shown that the linear coefficient of the specific heat is enhanced throughout the mixed-valence regime.

The inclusion of fluctuations in the calculation leads to interactions between quasiparticles and enables physical quantities to be calculated to  $O(1/N)$ . It is then possible to show the presence of a  $T^3 \ln T$  term in  $C_V$ . This term does indeed scale with  $\gamma^3$  throughout the mixed valence regime, in agreement with experiment.

In this paper we consider a direct continuation of this work to calculate other thermodynamic quantities. At mean-field level we calculate the spin and charge susceptibilities,  $\chi_S$  and  $\chi_c$ . We show that  $\chi_S$  is also enhanced for all  $n_f$  giving a Wilson ratio of one and that  $\chi_c \ll \chi_S$ . The  $T^2$  term in  $\chi_S$  is also found and is seen to scale with  $\gamma^2$ . Going beyond the mean-field level we calculate the corrections to the Wilson ratio to  $O(1/N)$ . The resistivity can be found and varies as  $(T\gamma)^2$  as observed experimentally. The fluctuations also describe the dynamics of the system and further insight into the nature of the ground state is obtained by considering the energy- and frequency-dependent spin and charge susceptibilities. It can be shown that these have

the normal Fermi-liquid form for electrons with an enhanced mass. As in I we find close analogies between the mixed-valence behaviour of uranium and the behaviour of cerium in the Kondo limit. In both cases the behaviour is seen to be that of a Fermi liquid but with the unusual additional feature that the behaviour is determined by a single pressure-dependent energy scale.

We consider finally the superconducting properties. At low temperatures some of the heavy-fermion compounds including  $\text{UPt}_3$  and  $\text{URu}_2\text{Si}_2$  undergo a phase transition and become superconducting. The superconducting state is unconventional: a variety of experimental techniques show that the superconducting gap goes to zero at points or lines along the Fermi surface (Bishop *et al* 1984, Han *et al* 1986, Ott *et al* 1984) in contrast to normal superconductors where the gap is essentially isotropic. This suggests that the electrons are paired in a state of non-zero angular momentum. Furthermore the pairing mechanism is unlikely to be the conventional electron-phonon mechanism.

Using the slave-boson method we can consider the stability of the Fermi liquid to superconducting instabilities. For cerium it has been shown that to first order in  $1/N$  the interaction is via the exchange of spinless slave bosons (i.e. charge fluctuations) and is repulsive in the s and p channels but attractive in the d-wave channel for  $n_f$  close to one (Auerbach and Levin 1986b, Lavagna *et al* 1987). Terms of next order are, however, important as these involve spin fluctuations which are expected to have a significant effect (Houghton *et al* 1988). These terms do indeed dominate in the Kondo limit and p-wave superconductivity is also allowed. The attractive interaction is larger for the p-wave than the d-wave term so we expect to see p-wave superconductivity. We note in particular that superconductivity is obtained only in the Kondo limit.

Analogous calculations can be done for uranium. We show that there are important differences and a superconducting instability is found throughout the mixed-valence regime.

## 2. The slave-boson method

We take as our starting point an Anderson lattice in which the f occupation at each site is restricted to being between  $n$  and  $n + 1$  where  $n \neq 0$ . Two slave-boson fields are required to do this in contrast to the case of cerium where one suffices. The hybridisation term is modified to become

$$\sum_{ikm\sigma} V_{km\sigma} \exp(i\mathbf{k} \cdot \mathbf{R}_i) c_{k\sigma}^\dagger f_{im} a_i b_i^\dagger + \text{HC} \quad (2.1)$$

with the constraints

$$\sum_m f_{im}^\dagger f_{im} - a_i^\dagger a_i = Q_1 = n \quad (2.2)$$

$$a_i^\dagger a_i + b_i^\dagger b_i = Q_2 = 1. \quad (2.3)$$

Both  $Q_1$  and  $Q_2$  commute with the Hamiltonian and are therefore constants of the motion. For the case of uranium,  $n = 2$ , and we will use this from now on. We note, however, that the theory is easily generalised to arbitrary  $n$ . The presence of the two fields makes sure that the f occupation is both greater than 2 and less than 3. The treatment is simplified by assuming that both the c and f electrons can be labelled by a

single generalised spin index  $m$  where  $-J \leq m \leq J$  giving a degeneracy  $N = 2J + 1$ . We note that for a single cerium impurity the conduction electrons can in fact be expanded in eigenstates of total angular momentum and the procedure is correct whereas for the lattice problem it is more complicated and this becomes an approximation. For the uranium systems, however, even the one impurity problem is more complicated and the  $c$  electrons can only be labelled by  $m$  when  $j$ - $j$  coupling in the limit of zero  $j$ - $j$  coupling is used. It may be then that the approximation is worse for uranium than it is for cerium. Nonetheless, we would hope that it still captures the most important features.

Following I the partition function can be written in the following way

$$Z = \int_{-\pi/\beta}^{\pi/\beta} \frac{\beta d\lambda_1^i}{2\pi} \int_{-\pi/\beta}^{\pi/\beta} \frac{\beta d\lambda_2^i}{2\pi} \int Db^* Db Df^* Df Dc^* Dc Da^* Da \exp\left(-\int_0^\beta L(\tau) d\tau\right) \quad (2.4)$$

where

$$\begin{aligned} L(\tau) = \sum_i \left\{ b_i^\dagger(\tau) \frac{\partial}{\partial \tau} b_i(\tau) + a_i^\dagger(\tau) \frac{\partial}{\partial \tau} a_i(\tau) + \sum_m f_{im}^\dagger(\tau) \left[ \frac{\partial}{\partial \tau} + E_0 \right] f_{im}(\tau) \right. \\ \left. + i\lambda_1^i \left[ \sum_m f_{im}^\dagger(\tau) f_{im}(\tau) - a_i^\dagger(\tau) a_i(\tau) - 2 \right] + i\lambda_2^i [a_i^\dagger(\tau) a_i(\tau) + b_i^\dagger(\tau) b_i(\tau) - 1] \right\} \\ + \sum_{km} c_{km}^\dagger(\tau) \left[ \frac{\partial}{\partial \tau} + \epsilon_{km} \right] c_{km}(\tau) \\ + \sum_{ikm} [V_{km} \exp(i\mathbf{k} \cdot \mathbf{R}_i) c_{km}^\dagger(\tau) f_{im}(\tau) a_i(\tau) b_i^\dagger(\tau) + \text{HC}]. \quad (2.5) \end{aligned}$$

The radial ( $r, \rho$ ) and angular ( $\theta, \phi$ ) components of the boson fields can be separated via the following gauge transformations

$$b_i(\tau) = r_i(\tau) \exp(i\theta(\tau)) \quad (2.6)$$

$$a_i(\tau) = \rho_i(\tau) \exp(i\phi(\tau)) \quad (2.7)$$

$$f_{im}'(\tau) = f_{im}(\tau) \exp(i\theta_i(\tau) - i\phi_i(\tau)) \quad (2.8)$$

$$\lambda_1^i(\tau) = \lambda_1^i(\tau) + \dot{\theta}_i(\tau) - \dot{\phi}(\tau) \quad (2.9)$$

$$\lambda_2^i(\tau) = \lambda_2^i(\tau) + \dot{\theta}_i(\tau). \quad (2.10)$$

The effect of this is to introduce a 'temporal' dependence to the variables  $\lambda_1^i$  and  $\lambda_2^i$  which now become quantum fields, and to allow us to drop total derivative terms in the Lagrangian such as  $\rho\dot{\rho}$  and  $r\dot{r}$  through the imposition of periodic boundary conditions on the radial boson fields. This transformation enables us to avoid problems associated with infrared divergences which otherwise occur (Read 1985).

The partition function can then be written

$$Z = \int Df^* Df Dc^* Dc D\lambda_1 D\lambda_2 Dr D\rho \left( \prod_{it} r_i(\tau) \rho_i(\tau) \right) \exp\left(-\int_0^\beta d\tau L'(\tau)\right) \quad (2.11)$$

where the transformed Lagrangian is given by

$$\begin{aligned}
 L'(\tau) = & \sum_{km} c_{km}^\dagger(\tau) \left[ \frac{\partial}{\partial \tau} + \epsilon_{km} \right] c_{km}(\tau) + \sum_{im} f_{im}^\dagger(\tau) \left[ \frac{\partial}{\partial \tau} + E_0 + i\lambda_1^i(\tau) \right] f_{im}(\tau) \\
 & + \sum_{kmi} [V_{km} \exp(i\mathbf{k} \cdot \mathbf{R}_i) c_{km}^\dagger(\tau) f_{im}(\tau) r_i(\tau) \rho_i^\dagger(\tau) + \text{HC}] \\
 & + \sum_i \{ \rho_i^2(\tau) [i\lambda_2^i(\tau) - i\lambda_1^i(\tau)] + i\lambda_2^i(\tau) [r_i^2(\tau) - 1] - 2i\lambda_1^i(\tau) \}. \quad (2.12)
 \end{aligned}$$

The Lagrangian is now bilinear in the fermion fields and we can proceed to integrate these out by completing the square in the conduction electron fields. This leads to  $Z = Z_0 Z_f$  where  $Z_0$  is the partition function for free conduction electrons. The contributions to the effective action for  $Z_f$  can be separated into two parts :

1. the terms which come from imposing the constraint
2. a term quadratic in the f operators.

The f operators can also be integrated over leading to

$$\begin{aligned}
 Z_f = & \int D\rho_i D r_i \left( \prod_{i,\tau} \rho_i(\tau) r_i(\tau) \right) D\lambda_1 D\lambda_2 \exp \left( \sum \text{Tr} \ln A_{\mathbf{k}_1 \mathbf{k}_2}^m \right) \\
 & \times \exp \left( -\frac{1}{\beta^2} \sum_{\mathbf{k}\mathbf{k}'} \{ \rho(-\mathbf{k}') [-i\lambda_1(\mathbf{k}' - \mathbf{k}) + i\lambda_2(\mathbf{k}' - \mathbf{k})] \rho(\mathbf{k}) + r(-\mathbf{k}') i\lambda_2(\mathbf{k}' - \mathbf{k}) r(\mathbf{k}) \} \right. \\
 & \left. + i\lambda_2(\mathbf{k} = 0) + 2i\lambda_1(\mathbf{k} = 0) \right) \quad (2.13)
 \end{aligned}$$

with

$$\begin{aligned}
 A_{\mathbf{k}_1 \mathbf{k}_2}^m = & [\delta_{\mathbf{k}_1 \mathbf{k}_2} (-i\omega + E_0) + i\lambda_1(\mathbf{k}_1 - \mathbf{k}_2)] / \beta \\
 & + \frac{V^2}{\beta^4} \sum_{\mathbf{k}\mathbf{k}'_1 \mathbf{k}'_2} \rho(\mathbf{k}'_1) r(-\mathbf{k} + \mathbf{k}_1 - \mathbf{k}'_1) G_0(\mathbf{k}) r(\mathbf{k} - \mathbf{k}_2 - \mathbf{k}'_2) \rho(\mathbf{k}'_2) \quad (2.14)
 \end{aligned}$$

where  $G_0 = (i\omega - \epsilon_k)^{-1}$  and  $\mathbf{k}$  represents the four vector  $(k, i\omega)$ .  $(A_{\mathbf{k}_1 \mathbf{k}_2}^m)^{-1}$  denotes the Green function for f electrons with fluctuating f level position and mixing width.

### 3. The mean-field solution

To proceed we now assume that the boson fields are essentially uniform spatially and temporally. The mean-field solution is found by taking  $r(\mathbf{k})$ ,  $\rho(\mathbf{k})$ ,  $\lambda_1(\mathbf{k})$  and  $\lambda_2(\mathbf{k})$  as constant and determining these by minimising the free energy with respect to them. We take

$$(\rho(\mathbf{k}), r(\mathbf{k}), \lambda_1(\mathbf{k}), \lambda_2(\mathbf{k})) = \beta \delta_{\mathbf{k}}(\rho, r, \lambda_1, \lambda_2) + (\delta \rho(\mathbf{k}), \delta r(\mathbf{k}), \delta \lambda_1(\mathbf{k}), \delta \lambda_2(\mathbf{k})) \quad (3.1)$$

and assume that  $\delta\rho(\mathbf{k})$  etc are small. To zeroth order in the fluctuations the free energy is given by

$$F_{\text{mf}} = \rho^2(i\lambda_2 - i\lambda_1) - 2i\lambda_1 - i\lambda_2 + i\lambda_2 r^2 + T \sum_{km} \ln H_m(\mathbf{k}) + \ln(i\omega - \epsilon_k). \quad (3.2)$$

Apart from the constant terms this is just the free energy of a band of  $c$  electrons plus a band of electrons with Green function

$$H_m(\mathbf{k}) = (-i\omega + \epsilon_f + \tilde{V}_{km}^2 G_0(\mathbf{k}))^{-1} \quad (3.3)$$

which can be written

$$H_m(\mathbf{k}) = \sum_{x=\pm} A_{-x} / (i\omega - E_x) \quad (3.4)$$

where

$$E_{m\pm}(k) = \frac{1}{2} \left\{ \epsilon_k + \epsilon_f \pm [(\epsilon_k - \epsilon_f)^2 + 4\tilde{V}_{km}^2]^{1/2} \right\} \quad (3.5)$$

$$A_{m\pm}(k) = -\frac{1}{2} \left( 1 \pm \frac{\epsilon_k - \epsilon_f}{[(\epsilon_k - \epsilon_f)^2 + 4\tilde{V}_{km}^2]^{1/2}} \right) \quad (3.6)$$

where  $\tilde{V}_{km}^2 = \rho^2 r^2 V_{km}^2$  and  $\epsilon_f = E_0 - i\lambda_1$ .

By minimising  $F_{\text{mf}}$  with respect to the four boson fields we obtain four mean-field equations which can be solved to find  $n_f$  and  $\epsilon_f$ .

We assume from now on that we can replace  $V_{km}^2$  by its average  $\langle V_{km}^2 \rangle = V^2$ , and take the conduction electron density of states,  $\rho_0$ , to be constant. This enables us to evaluate the integrals analytically at zero temperature. The following expressions were found in I

$$n_f = N\Delta / \pi\epsilon_f \quad (3.7)$$

$$\epsilon_f = E_0 + \frac{N\Delta_0}{\pi} (2n_f - 5) \ln(W/\epsilon_f) \quad (3.8)$$

where  $\Delta = (3 - n_f)(n_f - 2)\Delta_0 = \tilde{V}^2 \rho_0 / \pi$  and  $W$  is the conduction electron band width. We note that there is a symmetry between the two limits  $E_0 \rightarrow \pm\infty$ , i.e. between  $n_f \rightarrow 2$  and  $n_f \rightarrow 3$ . The behaviour in both these 'Kondo' limits is directly analogous to that obtained for cerium as  $n_f \rightarrow 1$ .

We can calculate the magnetic susceptibility from (3.2) by adding a term  $h \sum_{im} m f_{im}^\dagger f_{im}$  into the Hamiltonian. The effect is to change  $\epsilon_f \rightarrow \epsilon_f + hm$ . The free energy can be found and differentiating twice with respect to  $h$  gives  $\chi_S$ . We note that only the explicit dependence of  $F_{\text{mf}}$  on  $h$  has to be considered as we have  $\partial F_{\text{mf}} / \partial n_f = \partial F_{\text{mf}} / \partial \epsilon_f = 0$  from minimising the mean-field solution.

The expression for the free energy is:

$$F = \Delta F - i\lambda_1 n_f \quad (3.9)$$

where

$$\Delta F = T \sum_{k,i\omega} \sum_{m,x} \ln[i\omega - E_{mx}(k)] \quad (3.10)$$

where  $\alpha = \pm$  and  $E_{m\pm}(k)$  is found by replacing  $\epsilon_f$  with  $\epsilon_f + hm$  in  $E_{\pm}(k)$ . This describes the two renormalised bands. Using Poisson's formula we obtain

$$\Delta F = \sum_{m,\alpha,k} \int_{-\infty}^{\infty} d\epsilon f(\epsilon) \Theta[\epsilon - E_{m\alpha}(k)] \quad (3.11)$$

the sum over  $k$  can be performed giving

$$\Delta F = \rho_0 \sum_{m\alpha} \int d\epsilon f(\epsilon) \left( W + \epsilon + \frac{\tilde{v}^2}{\epsilon_f + hm - \epsilon} \right) \quad (3.12)$$

where  $f(\epsilon)$  is the Fermi function. We can now take the second derivative with respect to  $h$  and take the limit  $h \rightarrow 0$ . This leads to the following result at zero temperature

$$\chi_S = \frac{N\rho_0 g^2 \mu_B^2 J(J+1)}{3} \frac{m^*}{m} = \frac{g^2 \mu_B^2 J(J+1) n_f^2}{3N\Delta_0(3-n_f)(n_f-2)} \quad (3.13)$$

We can also add into the Lagrangian a term coupling the field to the conduction electrons. The effect is small the correction being of  $O(m/m^*)$ . We note that the contribution from the c electrons is approximately that which we would have expected from a normal unenhanced Fermi sea. This is precisely the result we obtain for a single impurity. In the case of a single impurity the picture we have is of the impurity spin being screened by a cloud of conduction electrons. We might then expect that polarising the f electrons by applying a magnetic field would lead to an opposite and almost equal change in the screening cloud to oppose the formation of a net magnetic moment. In fact this does not happen as a consequence of Anderson's compensation theorem (Anderson 1961). For the lattice the physical picture is different. There are not enough conduction electrons to screen each spin (Nozières 1985) and the loss of magnetic moment by the f electrons is better thought of in terms of them becoming part of the Fermi surface. The number of conduction electrons in the screening cloud can be shown to be  $\ll 1$  (Millis and Lee 1987). Even without the compensation theorem we would expect that the susceptibility of the conduction electrons differs little from the value in the absence of the f electrons. Recently experiments have been done on  $UBe_{13}$  in a magnetic field. Neutron scattering showed the induced polarisation to be very much smaller on the conduction electrons than on the uranium sites, in agreement with our result.

In I  $\gamma$  was calculated for zero temperature. Using their result the Wilson ratio, which is defined as  $R = \tilde{\chi}_S / \tilde{\gamma}$ , where  $\chi_S = [g^2 \mu_B^2 J(J+1)/3] \tilde{\chi}_S$  and  $\gamma = (\pi^2 k_B^2 / 3) \tilde{\gamma}$ , is equal to one giving a Landau parameter  $F_0^a = 0$ . This is the result expected for renormalised but non-interacting quasiparticles.

It is also possible to consider the low-temperature behaviour by expanding the Fermi function to order  $T^2$

$$f(\epsilon) = -\Theta(\epsilon) + \frac{1}{3} \pi^2 k_B^2 T^2 \delta'(\epsilon). \quad (3.14)$$

Using this in the expressions for  $n_f$  and  $\epsilon_f$  we can expand

$$n_f(T) = n_f(0) [1 + n_T (\pi k_B T / \epsilon_f)^2] \quad (3.15)$$



and

$$\epsilon_f = \epsilon_f(0)[1 + \epsilon_T(\pi k_B T / \epsilon_f)^2]. \quad (3.16)$$

If we assume that the Fermi level remains approximately constant then we find

$$n_T = \frac{1}{6}(5n_f - 12)(3 - n_f)(n_f - 2)g(n_f) \quad (3.17)$$

and

$$\epsilon_T = \frac{1}{3} - n_T(1 + a) \quad (3.18)$$

where

$$g(n_f) = \frac{1}{(n_f^2 - 6)^2 + n_f^2(3 - n_f)(n_f - 2) \ln W / \epsilon_f} \quad (3.19)$$

and

$$a = \frac{n_f(2n_f - 5)}{(3 - n_f)(n_f - 2)}. \quad (3.20)$$

We note that the  $T^2$  term in  $n_f$  is positive for  $n_f > 2.4$  and negative for  $n_f < 2.4$ . This can be understood in the following way.  $n_f = 2.4$  corresponds to the minimum in  $\gamma$ , therefore if  $n_f(0) > 2.4$  the entropy is increased and the free energy decreased as  $n_f$  increases towards 3. Similarly if  $n_f(0) < 2.4$  the entropy is increased as  $n_f$  decreases.

There are two contributions to the  $T^2$  term for the susceptibility one comes from a  $T^2$  term in  $F_{mf}$  and the other from the  $T$  dependence of  $n_f$  and  $\epsilon_f$ . The susceptibility is given by

$$\chi_S = \chi_S(0) \left[ 1 + \left( \frac{\pi k_B T}{\epsilon_f} \right)^2 [1 - (n_T + 2\epsilon_T)] \right]. \quad (3.21)$$

In the two Kondo limits,  $n_f \rightarrow 2, 3$  we have  $\chi_S = \chi_S(0)[1 + \frac{2}{3}(\pi k_B T / \epsilon_f)^2]$  which is just what we have for cerium as  $n_f \rightarrow 1$ . However, in the middle of the valence regime we have  $\chi_S = \chi_S(0)[1 + \frac{1}{3}(\pi k_B T / \epsilon_f)^2]$  and the coefficient of the term in  $T^2$  changes by a factor of two as we go from the Kondo limit to the mixed-valence regime.

If we now allow the Fermi level to vary with temperature we find that this has a significant effect. We note that  $E_0$  is measured relative to the Fermi energy,  $\mu$ . For  $n_f(0) > 2.4$  an increase in  $T$  tends to increase  $n_f$  which lowers  $\mu$ .  $|E_0|$  decreases, leading to an increase in  $\epsilon_f$  tending to push  $n_f$  back towards the mixed-valence regime. This 'negative feedback' tends to stabilise  $n_f$  at its zero temperature value. A similar argument holds for  $n_f(0) < 2.4$ . A better approximation seems to be that  $n_f$  remains constant (numerical results confirm this). The expression for  $\chi_S$  is then modified by putting  $n_T = 0$ . This does not make a quantitative difference to  $\chi_S$  but means that  $\chi_S = \chi_S(0)[1 + \frac{1}{3}(\pi k_B T / \epsilon_f)^2]$  throughout the mixed-valence regime for both cerium and uranium systems. The coefficient of the term in  $T^2$  scales with  $\gamma^2$  in both cases.

The charge susceptibility can also be calculated. The static f-f charge susceptibility is found from  $\chi_c^f = dn_f/d\mu \simeq -dn_f/dE_0$  and is given by

$$\chi_c^f = \frac{\pi(n_f - 2)(3 - n_f)g(n_f)n_f^2}{N\Delta_0}. \quad (3.22)$$

This can also be compared to the corresponding result for cerium as  $n_f \rightarrow 1$  and it is seen that the behaviour in the Kondo limits,  $n_f \rightarrow 2, 3$  is similar. In the middle of the valence regime  $\chi_c^f$  depends on the value of  $W/N\Delta_0$  in contrast to the case of cerium where there is no such dependence. There are two possible approaches. (i) We can get an estimate for  $W/N\Delta_0$  from the experimental values of  $m^*/m$  and  $n_f$  and use our theoretical expression for  $m^*/m$  to find  $W$ . Using  $m^*/m = 200$  and  $n_f = 2.5$  gives  $W \sim 8N\Delta_0/\pi$ . (ii) Alternatively we can use the 'scaling limit'  $W \rightarrow \infty$ . This assumes that the value of  $W$  does not have a significant effect on any physical quantity. Using the first approach we find  $\chi_c$  for uranium  $\sim 0.2\pi/N\Delta_0$  which is similar in magnitude to that for cerium in the mixed valence regime. With  $W \rightarrow \infty$ ,  $\chi_c \sim (\ln W/N\Delta_0)^{-1} \sim 0$  for all  $n_f$ .

We note that the charge susceptibility remains much smaller than the spin susceptibility throughout the mixed-valence regime. This is in contrast to the case of cerium where as we move towards mixed valence the spin and charge susceptibilities become comparable.

$\chi_c^f$  can be rewritten in the following way

$$\chi_c^f = \frac{N\rho_0 m^*/m}{1 + F_f} \tag{3.23}$$

which defines a Landau parameter for the f electrons

$$F_f = (3 - n_f)^{-2} (n_f - 2)^{-2} g(n_f)^{-1} - 1. \tag{3.24}$$

$F_f$  is the only Landau parameter which is large and  $O(1/N)^0$ . The behaviour of  $\chi_c$  can be understood as follows.  $\chi_c = \partial n / \partial \mu$  where  $n$  is the number of electrons. For a system with a large density of f states at the Fermi level we might expect that a small change in  $\mu$  would give rise to a large change in  $n_f$  and hence a large value for  $\chi_c$ . This would be true if the bands were 'rigid'. It is clear, however, that that is not the case here; if it were we would be able to violate the constraint  $n_f < 1$  simply by adding more electrons to the system. The small value of  $\chi_c$  is then a consequence of the fact that the f-level resonance has to be 'pinned' to the Fermi level.

The charge susceptibility for the conduction electrons,  $dn_c/d\mu$ , can also be calculated. This gives a value  $N\rho_0$  which is what it would be in the absence of the f electrons. The total charge susceptibility  $\chi_c$  is given by the sum of the two individual susceptibilities,  $\chi_c = N\rho_0 + N\rho_0 m^*/m(1 + F_f)^{-1}$ . It might be thought that we can use this expression to obtain a single Landau parameter,  $F_0^s$ , for the whole system, i.e. write  $\chi_c = N\rho_0 m^*/m(1 + F_0^s)$ . This would give a value of

$$F_0^s = \frac{m^*}{m} \left( 1 + \frac{m^*}{mF_f} \right)^{-1} - 1 \tag{3.25}$$

as has been quoted elsewhere (Millis and Lee 1987). In fact work by Fulde *et al* (1988) on the Landau theory for a Fermi liquid in which there are two types of electrons suggests that there are two independent Landau parameters:  $F_h$  corresponding to the interaction between 'heavy' particles and  $F_l$  corresponding to the interaction between 'heavy' and 'light' particles. The formula they derive is

$$\chi_c = \frac{dn_h}{d\mu} + \frac{dn_l}{d\mu} = N\rho_0 \frac{1 + F_h + (1 - 2F_l)m^*/m}{1 + F_h - F_l^2 m^*/m}. \tag{3.26}$$

Putting  $F_l = 0$  and  $F_h = F_f$  clearly gives back our result. This point is further clarified by the calculation of the dynamic susceptibility in the next section.

We see that the spin susceptibility is essentially that of the f electrons while the charge susceptibility is essentially that of the c electrons. The quasiparticles can be thought of as having f spin and c charge and physical quantities coupling to the spin degrees of freedom will see fermions with a large mass enhancement while those that couple to the charge degrees of freedom will not see the large mass.

#### 4. Corrections to $O(1/N)$ and dynamics

The fluctuations around the mean-field level are important as they give us corrections to order  $1/N$  and also allow us to calculate the dynamics.

To Gaussian order in the fluctuations we expand the exponential keeping terms bilinear in the the deviations of the boson fields around the mean-field values. This gives

$$Z_G = \int D\rho Dr \left( \prod_{i\tau} \rho_i(\tau) r_i(\tau) \right) D\lambda_1 \lambda_2 \exp \left( -\frac{1}{\beta} \sum_{\mathbf{k}} q(-\mathbf{k})^T \mathbf{S}(\mathbf{k}) q(\mathbf{k}) \right) \quad (4.1)$$

where

$$q(\mathbf{k}) = (\delta\rho(\mathbf{k}), \delta r(\mathbf{k}), \delta\lambda_1(\mathbf{k}), \delta\lambda_2(\mathbf{k})). \quad (4.2)$$

$q^T(\mathbf{k})$  denotes the transpose of  $q(\mathbf{k})$  and  $\mathbf{S}(\mathbf{k})$  is the full  $4 \times 4$  boson propagator. We list the elements of  $\mathbf{S}(\mathbf{k})$  as derived in I.

$$\begin{aligned} S_{\rho\rho}(\mathbf{k}) &= i(\lambda_2 - \lambda_1) - \frac{NV^2r^2}{\beta} \sum_{\mathbf{k}_1} H(\mathbf{k}_1) G_c(\mathbf{k}_1 + \mathbf{k}) + NV^4\rho^2r^4T \sum_{\mathbf{k}_1} F(\mathbf{k}_1) F(\mathbf{k}_1 + \mathbf{k}) \\ S_{rr}(\mathbf{k}) &= \frac{\rho^2}{r^2} S_{\rho\rho}(\mathbf{k}) \\ S_{r\rho}(\mathbf{k}) &= \frac{\rho}{r} \frac{S_{\rho\rho}(\mathbf{k})}{2} - \frac{i\lambda_2 r}{\rho} \\ S_{\lambda_1\lambda_1}(\mathbf{k}) &= -\frac{NT}{2} \sum_{\mathbf{k}_1} H(\mathbf{k}_1) H(\mathbf{k} + \mathbf{k}_1) \\ S_{\lambda_1\rho}(\mathbf{k}) &= -i\rho + \frac{iNV^2r^2\rho T}{2} \sum_{\mathbf{k}_1} [F(\mathbf{k}_1) H(\mathbf{k}_1 + \mathbf{k}) + H(\mathbf{k}_1) F(\mathbf{k} + \mathbf{k}_1)] \\ S_{\lambda_1r}(\mathbf{k}) &= i\frac{\rho^2}{r} + \frac{\rho}{r} S_{\lambda_1\rho}(\mathbf{k}) \\ S_{\lambda_2\rho} &= i\rho \\ S_{\lambda_2r} &= ir \end{aligned} \quad (4.3)$$

where we have introduced the quantities

$$G_c(\mathbf{k}) = G_0(\mathbf{k}) - \tilde{V}^2 G_0^2(\mathbf{k}) H(\mathbf{k}) = -\sum_{\alpha} A_{\alpha}(\mathbf{k}) / (i\omega - E_{\alpha}(\mathbf{k})) \quad (4.4)$$

$$F(\mathbf{k}) = G_0(\mathbf{k}) H(\mathbf{k}) = -\sum_{\alpha} \alpha / (i\omega - E_{\alpha}(\mathbf{k})) (E_{+}(\mathbf{k}) - E_{-}(\mathbf{k})). \quad (4.5)$$

We can now evaluate the Gaussian functional integrals using the assumption that the fluctuations are locally cartesian

$$F_G = -\frac{1}{2}T \sum_k \ln[\det \mathbf{S}(k)] \quad (4.6)$$

The  $1/N$  corrections to the Wilson ratio can now be calculated. These are important as a diverging Wilson ratio would suggest a ferromagnetic instability. There are two types of corrections: (i) the expressions for  $n_f$  and  $\epsilon_f$  are modified to include terms of  $O(1/N)$ , and (ii) the Gaussian fluctuations introduce an extra part,  $F_G$ , to the free energy. The first type of corrections need not be evaluated explicitly as they cancel when the ratio  $\tilde{\chi}_S/\tilde{\gamma}$  is taken. The only term that contributes to the temperature dependence but not the field dependence of the free energy comes from the temperature dependence implicit in the frequency sum in the expression for  $F_G$

$$\begin{aligned} F_G &= \frac{1}{2\beta} \sum_{k,\omega} \ln[\det \mathbf{S}(k, \omega)] \\ &= \frac{1}{2} \sum_k \int \frac{d\omega}{2\pi} n_B(\omega) \tan^{-1} \frac{\text{Im} [\det \mathbf{S}(k, \omega)]}{\text{Re} [\det \mathbf{S}(k, \omega)]} \end{aligned} \quad (4.7)$$

where  $n_B(\omega)$  is the Bose function. For low  $T$  we can expand  $n_B(\omega)$ . To evaluate the term in  $T^2$  we only need to keep terms to  $O(\omega)$  in (4.7). The matrix elements of  $\mathbf{S}$  can be evaluated in the low- $\omega$  limit (see I) and the following expression for the Wilson ratio is found:

$$R = 1 + N^{-1} [1 - (3 - n_f)^2 (n_f - 2)^2 g(n_f)] + O(N^{-2}). \quad (4.8)$$

$g(n_f)$  is equal to  $n_f^{-2}$  in both Kondo limits and the behaviour of  $R$  is directly analogous to that for cerium. For  $W = 8N\Delta_0/\pi$ ,  $g(2.5) \simeq 0.9$  and  $F_0^a = -0.99/N$ , and as  $W \rightarrow \infty$ ,  $g \rightarrow 0$  and  $F_0^a = -1/N$ . We see that  $R$  does not differ appreciably from its Kondo limit value throughout the mixed-valence regime and to a very good approximation the Wilson ratio is pressure independent for all values of  $n_f$ . This can be compared to the result for cerium where for  $N = 6$   $R$  is reduced by  $\sim 5\%$  as  $n_f$  changes from  $\sim 1$  to 0.5 and for  $N = 2$  there is a reduction of  $\sim 20\%$ .

The expression for  $R$  is consistent with the *ansatz*

$$R = 1/(1 - N^{-1}) \quad (4.9)$$

which is the result obtained for a single cerium-type impurity in the Kondo limit. From this we see that the Fermi liquid is only unstable to ferromagnetism for  $N < 1$ . This is completely independent of the mass enhancement in contrast to results obtained from other theories (Coleman 1983, Rice and Ueda 1985), and suggests that the heavy-fermion systems are very stable to ferromagnetism which is confirmed by the fact that experimentally none of the compounds have a ferromagnetic ground state. We note that Millis and Lee (1987) calculate part of the  $O(1/N^2)$  term for cerium and show that this is not universal which suggests that the one impurity result will have to be modified for the lattice.

The dynamic properties of the system are of interest as they help clarify the nature of the Fermi-liquid ground state. The collective properties of the Fermi liquid are

related to the Bose fluctuations. We need to add into the free energy functional a 'source' term associated with the  $f$  occupations. The dynamic susceptibilities can then be calculated from a functional derivative of the full free energy. To calculate the spin susceptibility the term that is added into  $L'$  is

$$\int_0^\beta d\tau \sum_{im} m h_i(\tau) f_{im}^\dagger(\tau) f_{im}(\tau). \quad (4.10)$$

We can now define the spin susceptibility

$$\begin{aligned} \chi_{S_i}(\tau) &= \langle T_\tau M_z(R_i, \tau) M_z(0, 0) \rangle \\ &= \frac{\partial^2 \ln Z(h)}{\partial h_i(\tau) \partial h_0(0)} \end{aligned} \quad (4.11)$$

where  $M_z(R_i, \tau) = \sum_m m f_{im}^\dagger f_{im}$ . We note that the source currents enter in an identical way to  $i\delta\lambda_1(\mathbf{k})$ , apart from some constant terms. Transforming to  $\mathbf{k}$  space the result is

$$\tilde{\chi}_S(k, \omega) = 2S_{\lambda_1\lambda_1}(k, \omega) \quad (4.12)$$

for the spin susceptibility. Taking the limits  $k \rightarrow 0$  and  $\omega \rightarrow 0$  while keeping the ratio  $\omega/kv_F^*$  finite we obtain the following expression

$$S_{\lambda_1\lambda_1}(k, \omega) = \frac{N\rho_0}{2} \frac{m^*}{m} s\left(\frac{\omega}{v_F^*k}\right) \quad (4.13)$$

where  $v_F^*$  is the Fermi velocity and  $s(x)$  is the Lindhard function i.e.

$$s(x) = 1 - \frac{1}{2}x \ln \left| \frac{1+x}{1-x} \right| + \frac{1}{2}i\pi x \Theta(1-x). \quad (4.14)$$

This is exactly of the form expected for a non-interacting Fermi liquid with characteristic energy  $\epsilon_f$  and the same result is found for cerium.

The imaginary part of the susceptibility can be found. For  $\omega \rightarrow 0$  it is given by

$$\text{Im } \tilde{\chi}_S(k, \omega) = \frac{\omega}{2v_F^*k} \frac{1}{\epsilon_f} \Theta(v_F^*k - \omega). \quad (4.15)$$

This indicates that the  $f$  electrons are delocalised for times long compared with  $\epsilon_f^{-1}$ . This delocalisation means that the  $f$  electrons do not have to be screened individually by the conduction electrons as mentioned previously.

It can be seen that the Fermi-liquid relation

$$\lim_{\omega \rightarrow 0} \text{Im } \frac{\tilde{\chi}_S(k, \omega)}{\omega} = \frac{\pi k_F}{2Nk} \text{Re } \tilde{\chi}_S(0, 0)^2 \quad (4.16)$$

is satisfied. This relation is analogous to the Korringa relation for the single impurity which has been shown to hold exactly for the impurity Anderson model (Shiba 1975).

Calculating  $\chi_S(k, \omega)$  to higher order in  $1/N$  is difficult, but assuming that  $R$  is of the form given by equation (4.9) suggests that the susceptibility is given by

$$\tilde{\chi}_S(k, \omega) = N\rho_0 \frac{m^*}{m} \frac{s(x)}{1 + F_0^2 s(x)} \quad (4.17)$$

where  $F_0^a = -N^{-1}[1 - (3 - n_f)^2(2 - n_f)^2g(n_f)]$  and  $x = \omega/v_F^*k$ .

Since  $-1 < F_0^a < 0$  the denominator does not vanish for any  $x$  and the only contribution to the imaginary part of  $\chi_S$  comes from the imaginary term in  $s(x)$ . There is no sharply defined collective mode and as already pointed out no magnetic instability. There will however be a maximum in  $\text{Im}\chi_S$  for frequencies in the vicinity of which  $\text{Re}[1 + F_0^a s(x)]$  vanishes. We expect a broad resonance characteristic of a damped collective mode. We note that the value of  $1/N$  is important in determining the behaviour. For large  $N$  the damping is very strong and  $\chi_S$  differs little from the result for a non-interacting Fermi liquid. For cerium the smallest value for  $N$  is 2 and even for this there is no pronounced peak and the spin fluctuations are not very strong. It is interesting to compare with the results for liquid  $^3\text{He}$  with which analogies have been made. The susceptibility is again of the above form with  $F_0^a > -1$ . In this case, however,  $F_0^a$  is close to  $-1$  and the susceptibility differs greatly from the non-interacting one (Leggett 1975). In contrast to the heavy-fermion systems the imaginary part of the susceptibility is strongly peaked at low frequencies,  $\omega \sim v_F^*k(1 + F_0^a)$ , and although the peak still does not represent a real propagating excitation it is reasonable to think of it as representing a sort of quasidelementary excitation, a 'paramagnon'. We note that it is unclear how the introduction of a realistic atomic coupling scheme for uranium and a proper treatment of the higher order terms would alter our result. Nonetheless, the experimental results which show  $R \sim 1$  are in good agreement with our calculation and it may be that a more accurate calculation would not change things very much.

The charge susceptibility can be calculated in a similar way. We add a term

$$\int_0^\beta d\tau \sum_{im} g_i(\tau) f_{im}^\dagger(\tau) f_{im}(\tau) \tag{4.18}$$

into  $L'$  and define

$$\begin{aligned} \chi_{ci}(\tau) &= \langle T_\tau \delta n_f(R_i, \tau) \delta n_f(0, 0) \rangle \\ &= \frac{\partial^2 \ln Z[h]}{\partial g_i(\tau) \partial g_0(0)} \end{aligned} \tag{4.19}$$

where  $\delta n_f(R_i, \tau)$  is the f electron density at site  $i$ . This leads to

$$\chi_c^f(k, \omega) = \frac{2\rho^2 r^2 S_{\lambda_1 \lambda_1}(k, \omega)}{\det S(k, \omega)}. \tag{4.20}$$

This can be rewritten in terms of the boson propagators

$$\chi_c^f(k, \omega) = 4\beta\rho^2 \langle \check{\rho}(k, \omega) \check{\rho}(-k, -\omega) \rangle = 4\beta r^2 \langle \check{r}(k, \omega) \check{r}(-k, -\omega) \rangle. \tag{4.21}$$

This illustrates that there is a close connection between the fluctuations in the boson fields,  $\rho$  and  $r$ , and the density fluctuations.

In the low- $k$  and low- $\omega$  limits  $\chi_c^f$  reduces to

$$\chi_c^f = N\rho_0 \frac{m^*}{m} \frac{s(x)}{1 + F_f s(x)}. \tag{4.22}$$

Again this has a Fermi-liquid form. We note that the linear dependence of  $\det \mathbf{S}$  on  $s(x)$  only arises from an exact cancellation of terms  $O(s(x)^2)$ . From this the imaginary part at low energies can be calculated

$$\text{Im } \chi_c^f(k, \omega) = \frac{\omega}{2v_F^* k \epsilon_f} F_f^{-2} \Theta(v_F^* k - \omega) \quad (4.23)$$

which is very much smaller than  $\text{Im } \tilde{\chi}_S$ . Again the following equation holds

$$\lim_{\omega \rightarrow 0} \text{Im } \frac{\tilde{\chi}_c^f(k, \omega)}{\omega} = \frac{\pi k_F}{2Nk} \text{Re } \tilde{\chi}_c^f(0, 0)^2 \quad (4.24)$$

where  $\chi_c^f = N \tilde{\chi}_c^f$ .

The total charge susceptibility can be found and is given by

$$\chi_c = N \rho_0 \frac{m^*}{m} \frac{s(x)}{1 + F_f s(x)} + N \rho_0 s(x). \quad (4.25)$$

Again this is consistent with the result of Fulde *et al* (1988) and does not imply a single Fermi-liquid parameter  $F_0^s$ , which can only be defined for small  $x$ . Although superficially the expressions for  $\chi_S$  and  $\chi_c$  look similar the fact that the Fermi-liquid parameters are so different leads to very different behaviour. In particular we note that the denominator will vanish for some  $x = x_0$  indicating the presence of a collective mode. Since  $F_f$  is large we can approximate

$$\chi_c = K_s x_0^2 / (x_0^2 - x^2) \quad (4.26)$$

where  $K_s = N \rho_0 (m^*/m) (1 + F_f)^{-1}$  and  $x_0^2 = \frac{1}{3} (1 + F_f)$  where  $K_s$  is the static compressibility and  $x_0 v_F^*$  is the speed of ordinary hydrodynamic sound. This has a zero sound mode at frequencies  $\omega = x_0 v_F^* k$ . This is, however, the result for a *neutral* Fermi liquid and to obtain a realistic result we need to include the long-range part of the Coulomb repulsion. For a normal Fermi liquid we expect that including the Coulomb repulsion replaces the zero sound mode which has  $\omega = ck$  with a plasma mode at frequencies  $\omega = \omega_p = (4\pi n e^2 / m)^{1/2}$ . A proper calculation does indeed show the presence of such a plasma mode with  $n = n_c$  and  $m$  unenhanced i.e. the mode we would expect for the conduction electrons alone. In addition, though, there is also found a 'heavy-fermion' plasma mode at frequencies  $\omega \sim T_K$  (Millis *et al* 1987).

For a single impurity the following exact result holds between  $\tilde{\chi}_S$ ,  $\chi_c^f$  and  $\tilde{\gamma}$  (Yoshimori 1976)

$$\tilde{\gamma} = [\tilde{\chi}_c^f + (1 - N^{-1}) \tilde{\chi}_S]. \quad (4.27)$$

If we substitute in the values calculated above we can deduce a value for  $R$ . We obtain the same value that we found previously verifying that the relationship holds for the lattice also at least to  $O(1/N)$ .

It appears then that the low- $T$  and low-frequency properties are just those of a Fermi liquid with energy scale  $\epsilon_f$  exactly as was found for cerium. Despite the apparent extra complexity of the equations for uranium, the expressions for  $\chi_S$  and  $\chi_c$  reduce to the same form as was found for cerium, i.e. they have the same  $k$  and  $\omega$  dependence.

We can also calculate the temperature-dependent resistivity,  $\rho(T)$ . The electric field only couples to the c electrons (the f electrons are dispersionless) and the resistivity

arises from the scattering off the Bose fluctuations. Two methods have given the same results for cerium. We can use an analogy with paramagnon theory where the resistivity arises from the scattering off spin fluctuations (Jullien *et al* 1974, Auerbach and Levin 1986b). Alternatively we can compute the c electron Green function to  $O(1/N)$  and find the scattering rate from the imaginary part of this. We note that in a Gallilean invariant theory the second procedure would not be correct. In general we can only obtain reliable results from the two-particle Green function. Here, however, the f electrons are dispersionless and the model is not Gallilean invariant. It is argued by Millis and Lee (1987) that essentially the correct result can be obtained just using the c electron self-energy.

In both cases we need expressions for  $\langle \tilde{a}(\mathbf{k})\tilde{a}(-\mathbf{k}) \rangle$ ,  $\langle \tilde{a}(\mathbf{k})i\tilde{\lambda}(-\mathbf{k}) \rangle$  and  $\langle i\tilde{\lambda}(\mathbf{k})i\tilde{\lambda}(-\mathbf{k}) \rangle$  where  $a(\mathbf{k})$  and  $\lambda(\mathbf{k})$  are the two boson fields which occur in the cerium problem. We can see how these differ in the case of uranium by noting that we need to replace  $\tilde{a}(\mathbf{k}) \rightarrow r\tilde{\rho}(\mathbf{k}) + \rho\tilde{r}(\mathbf{k})$  and  $i\tilde{\lambda}(\mathbf{k}) \rightarrow i\tilde{\lambda}_1(\mathbf{k})$ . The propagators we need are as follows

$$\langle (r\tilde{\rho}(\mathbf{k}) + \rho\tilde{r}(\mathbf{k}))(r\tilde{\rho}(-\mathbf{k}) + \rho\tilde{r}(-\mathbf{k})) \rangle = \frac{(2n_f - 5)^2 S_{\lambda_1 \lambda_1}(\mathbf{k})}{\det \mathbf{S}(\mathbf{k})} \quad (4.28)$$

$$\langle (r\tilde{\rho}(\mathbf{k}) + \rho\tilde{r}(\mathbf{k}))i\tilde{\lambda}_1(-\mathbf{k}) \rangle = \frac{(5 - 2n_f)^2 S_{\rho \lambda_1}(\mathbf{k})/r + (5 - 2n_f)\rho^3/r}{\det \mathbf{S}(\mathbf{k})} \quad (4.29)$$

$$\langle i\tilde{\lambda}_1(\mathbf{k})i\tilde{\lambda}_1(-\mathbf{k}) \rangle = \frac{((2n_f - 5)^2 S_{\rho \rho}(\mathbf{k})/r^2 + 2r^2 i\lambda_2)}{\det \mathbf{S}(\mathbf{k})}. \quad (4.30)$$

As  $n_f \rightarrow 2, 3$  we can see that the expressions for the bose propagators become exactly equivalent to those for cerium as  $n_f \rightarrow 1$  and the same expression for the resistivity is found. If we put  $n_f = 2.5$  then we see that again things simplify greatly. The only propagator to survive is

$$\langle i\tilde{\lambda}_1 i\tilde{\lambda}_1 \rangle = 2r^2 i\lambda_2 / (2i\lambda_2 \rho r S_{\lambda_1 \lambda_1} + \rho^6 / r^2). \quad (4.31)$$

Substituting this into the expression derived by Millis and Lee (1987) gives the same result as before when expressed in terms of  $\epsilon_f$  with corrections of the order  $(\ln W/N\Delta_0)^{-1}$ . We therefore see that for uranium as well as for cerium the resistivity is given by  $\rho = AT^2$  where  $A$  scales as  $\gamma^2$ .

## 5. The superconducting instability

We can study the stability of the normal heavy-fermion state against pair formation by calculating the quasiparticle-quasiparticle scattering amplitude for particles of opposite momenta near the Fermi surface. This is related to the two-particle irreducible vertex function  $\Gamma$ , which is obtained from the two-particle correlation function

$$\langle T_\tau d_{k'm}^-(\tau_1) d_{-k'm'}^-(\tau_2) d_{-k'm'}^+(\tau_3) d_{k'm}^+(\tau_4) \rangle \quad (5.1)$$

on amputating the external legs. Here the  $d^-$  are the quasiparticle creation and annihilation operators for the lower band, i.e. the linear combinations of c and f which diagonalise the Hamiltonian at mean-field level.

By considering the  $\omega \rightarrow 0$  limit of  $\Gamma$  evaluated on the Fermi surface and projected onto Legendre polynomials, the scattering amplitudes,  $A_l^{as}$  can be calculated.



$\Gamma$  can be evaluated using standard functional integral methods (Sherrington 1971). The Lagrangian  $L'$  can be written  $L' = L_0 + L_1$  where  $L_0$  contains the mean-field terms and  $L_1$  the fluctuations. This is substituted into  $\exp[-\int_0^\beta d\tau L'(\tau)]$  which occurs in the expression for  $Z$ .  $\exp[-\int_0^\beta d\tau L_1(\tau)]$  can then be expanded and the averages evaluated in the standard way. Evaluating the correlation function leads to the following expression for  $\Gamma$

$$\begin{aligned} \Gamma &= \frac{1}{N} [(1 - (3 - n_f)^2 (n_f - 2)^2 g(n_f)) \left\{ \left[ 1 + \frac{\alpha v(x) n_f r^2 \rho^2}{4} \left( (5 - 2n_f) - \frac{1}{3} n_f \ln \frac{W}{\epsilon_f} \right) g(n_f) \right] \right. \\ &\quad \left. - \frac{\alpha v(x) n_f^2}{12} (5 - 2n_f)^2 g(n_f) \right\} \\ &= \frac{1}{N} \left[ 1 - (3 - n_f)^2 (n_f - 2)^2 g(n_f) - \frac{v(x) \alpha j(n_f)}{12} \right] \end{aligned} \quad (5.2)$$

where  $\alpha = n_f/N$ ,  $x = k/2k_F$  and  $v(x) = (1/x) \ln |(1+x)/(1-x)|$ .  $j(n_f)$  is a complicated but slowly varying function of  $n_f$ .  $j(n_f) = 1$  in the two Kondo limits,  $j(2.5) \simeq 0.98$  for  $W = 8N\Delta_0/\pi$  and tends to one for  $W \rightarrow \infty$ . From this expression we can calculate the scattering amplitudes,

$$A_l^a = -\frac{m}{m^*} \frac{2l+1}{2k_F^2} \int_0^{2k_F} dk \Gamma(k, 0) P_l \left( 1 - \frac{k^2}{2k_F^2} \right) k \quad (5.3)$$

$$A_0^s = \delta_{l,0} + A_0^a. \quad (5.4)$$

We see that they are almost identical to the values obtained for the Kondo limit for cerium.

$$A_0^a = \frac{-1}{N} + \frac{(3 - n_f)^2 (n_f - 2)^2 g(n_f)}{N} \quad (5.5)$$

$$A_0^s = 1 + A_0^a \quad (5.6)$$

$$A_1^a = A_1^s = -0.10 \alpha j(n_f)/N \quad (5.7)$$

$$A_2^a = A_2^s = 0.064 \alpha j(n_f)/N. \quad (5.8)$$

The  $A$  are related to the Landau parameters in the following way

$$A_l^{a,s} = \frac{F_l^{a,s}}{1 + F_l^{a,s}/2l + 1} \quad (5.9)$$

We note that this gives the same value for  $F_0^a$  as was found before. It is not clear what we should take for  $F_0^s$  and a more general relation relating  $A$  to  $F_h$  and  $F_l$  appears to be needed.

The fact that the  $l = 2$  parameters are attractive suggests the presence of d-wave pairing as was found for cerium. We note that for cerium  $A_2 \rightarrow 0$  as  $n_f \rightarrow 0$  while here it remains approximately constant throughout the mixed-valence regime. It has been shown by Lavagna *et al* (1987) that if the long-range part of the Coulomb repulsion is also included then an extra term  $O(m/m^*)$  is introduced and as we move towards the mixed valence regime the superconducting transition disappears. The combination of

$A_2$  remaining approximately constant and  $m^*/m$  remaining large throughout the mixed-valence regime means that this does not occur in the present case and superconductivity is possible for all  $n_f$  between 2 and 3.

At leading order in  $1/N$  the particles interact via exchange of a single zero-frequency boson (charge fluctuations). It has been suggested by Houghton *et al* (1988) that an essential part of the physics is still missing. Spin fluctuations which are expected to play an important role are completely neglected when we work to this order. We need then to include terms to  $O(1/N)^2$ . We follow the procedure used by Houghton *et al* (1988) and consider taking the large- $\omega$  limit of the boson propagators. The only terms that survive are  $\langle \tilde{p}\tilde{p} \rangle$ ,  $\langle \tilde{p}\tilde{r} \rangle$  and  $\langle \tilde{r}\tilde{r} \rangle$ . If we do this we find the contribution to the vertex function to order  $1/N^2$  is

$$\Gamma(x) = (J_0/N)^2 \left( 1 + \frac{1-x^2}{2x} \ln \left| \frac{1+x}{1-x} \right| \right). \quad (5.10)$$

In the two Kondo limits  $(J_0/N)^2 = (V^2/E_0)^2$  which is precisely the result for cerium. In the middle of the valence regime

$$(J_0/N)^2 \simeq \frac{V^4}{(N\Delta_0/\pi \ln W/\epsilon_f)^2}. \quad (5.11)$$

The expressions for the scattering amplitudes are modified to give

$$A_1^{\text{a.s.}} = \frac{1}{N^2} \left[ -0.10n_f j(n_f) + 0.23N \left( \frac{J_0\rho}{N} \right)^2 \frac{W}{\epsilon_f} \right] \quad (5.12)$$

$$A_2^{\text{a.s.}} = \frac{1}{N^2} \left[ 0.064n_f j(n_f) + 0.036N \left( \frac{J_0\rho}{N} \right)^2 \frac{W}{\epsilon_f} \right]. \quad (5.13)$$

The relative values of the first and second terms depends on the parameters we use. Certainly in the Kondo limits p-wave superconductivity is allowed and d-wave superconductivity is allowed throughout the mixed-valence regime. If we take  $W = 8N\Delta_0/\pi$  and  $N = 6$  then as we approach the mixed-valence regime  $A_1$  changes sign and p-wave superconductivity is not allowed. Other parameters can, however, be chosen which do not give this change of sign. For example with  $W = 16N\Delta_0/\pi$  and  $N = 4$ , p-wave superconductivity dominates even for  $n_f \sim 2.5$ . In view of the approximations we have used our results are not likely to be very accurate and the situation in the mid-valence region is not clear. We note that experimentally it appears that the superconductivity is more likely to be p wave than d wave and our results do not contradict this.

## 6. Conclusion

We have considered the extension of the slave-boson method to the uranium heavy-fermion systems. Our main conclusion has been that despite the physical differences the properties of the uranium lattice throughout the mixed-valence regime are very similar to those for the cerium lattice in the Kondo limit,  $n_f \rightarrow 1$ . Even for  $n_f \sim 2.5$  the energy scale,  $\epsilon_f$ , remains small as has also been found using a variational technique for the one impurity problem (Yafet *et al* 1985, Nunes *et al* 1985). The properties

of the uranium lattice are considerably more complicated than those for cerium and are described by four mean-field equations and sixteen boson propagators compared to two and four for cerium. We might expect, and do indeed find, very complicated expressions arising. When we take the Kondo limits,  $n_f \rightarrow 2$  or  $3$ , however, the results reduce to a form which is directly analogous to that for cerium as  $n_f \rightarrow 1$ . As we move into the mixed-valence regime we need to add only small corrections of the order  $(1/\ln(W/\epsilon_f))^{-1}$  to the Kondo-limit results.

We note that when we are very close to the Kondo limit  $n_f \rightarrow l$ , we would expect the behaviour to be independent of the value of  $l$ , i.e. when fluctuations to the alternative valence state are greatly suppressed it should not matter whether that valence state is or is not magnetic. This is precisely what we find. The case of cerium is different to that of uranium as in the former case there is a crossover between two very different types of behaviour as we vary  $n_f$  from 1 to 0, while for uranium the behaviour at the two ends of the permitted valence regime is identical. It is therefore not very surprising that the properties of uranium change less as we approach the mixed-valence regime than those of cerium. It is remarkable, though, that the properties in fact change so little.

The 'scaling' relations which are observed experimentally for  $\text{UPt}_3$  are shown to be a direct consequence of 'Kondo lattice'-like behaviour. In particular we have calculated the Wilson ratio to leading and next leading order in  $1/N$  and shown that this has a similar form to that for cerium and is independent of pressure. The resistivity is found to vary as  $AT^2$  where  $A$  scales as  $\gamma^2$ .

The energy- and frequency-dependent susceptibilities have been shown to have the same  $k$ - and  $\omega$ -dependence as for cerium and the dynamic properties are just those of a Fermi liquid with enhanced electron mass. This can be compared to results for a single impurity using a variational technique to calculate  $\chi_S(\omega)$  (Evans and Gehring 1989). There it was found that the results for an impurity fluctuating between two magnetic valence states were qualitatively different to those for cerium. In particular two peaks were seen in  $\text{Im}\chi_S(\omega)$  compared to only one for cerium, the second peak being a direct consequence of the fact that both valence states are magnetic. There is experimental evidence that the neutron spectrum for cerium is qualitatively different to that for thulium which can be thought of as fluctuating between  $f^1$  and  $f^2$ , the thulium compound having an inelastic peak which is not present for cerium (Holland-Moritz 1983). Although the variational calculation has not been explicitly performed for the thulium lattice we would expect the second peak to be found in this case also. It is unclear why the slave-boson method presented here, which is easily extended to the case of thulium, does not give this feature.

Finally we have considered the superconducting instability. We show the importance of including terms of order  $1/N^2$ . In the two Kondo limits,  $n_f \rightarrow 2$  or  $3$  we find that both p- and d-wave superconductivity are allowed and the p-wave terms dominate, as has been found for cerium as  $n_f \rightarrow 1$ . In the middle of the valence regime d-wave superconductivity is certainly possible. The sign of the p-wave interaction depends on the parameters used and it is difficult to make a firm conclusion. Nonetheless this is an important result. For the cerium compounds the superconducting instability is quickly lost as we move away from  $n_f \sim 1$  and there is no superconductivity in the mixed-valence regime. Experimentally this is confirmed by the fact that none of the mixed-valence cerium compounds have a superconducting ground state. The behaviour of cerium cannot help us deduce what we expect to find for uranium for  $n_f \sim 2.5$ . Our results show that we in fact do still get a superconducting instability for

uranium throughout the mixed-valence regime but the symmetry of this depends on the parameters used.

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### References

- Anderson P W 1961 *Phys. Rev.* **124** 41  
Auerbach A and Levin K 1986a *Phys. Rev. B* **34** 3524  
— 1986b *Phys. Rev. Lett.* **57** 877  
Brodale G E, Fisher R A, Phillips N E, Stewart G R and Giorgi A L 1986 *Phys. Rev. Lett.* **57** 234  
Bishop D J, Varma C M, Batlogg B, Bucher E, Fisk Z and Smith J L 1984 *Phys. Rev. Lett.* **53** 1009  
Coleman P 1983 *Phys. Rev. B* **28** 5255  
Evans S M M and Gehring G A 1989 *J. Phys.: Condens. Matter* **1** 3095  
Fulde P, Keller J and Zwicknagl G 1988 *Solid State Phys.* **41** 1  
Han S, Ng K W, Wolf E L, Millis A, Smith J L and Fisk Z 1986 *Phys. Rev. Lett.* **57** 238  
Holland-Moritz E 1983 *J. Magn. Magn. Mater.* **38** 253  
Houghton A, Read N and Won H 1988 *Phys. Rev. B* **37** 3782  
Jullien R, Beal Monod M T and Coqblin B 1974 *Phys. Rev. B* **9** 1441  
Kadowaki K and Woods S B 1986 *Solid State Commun.* **58** 507  
Lavagna M, Millis A J and Lee P A 1987 *Phys. Rev. Lett.* **58** 266  
Lee P A, Rice T M, Serene J W, Sham L J and Wilkins J W 1986 *Comment. Condens. Matter Phys.* **12** 99  
Leggett A J 1975 *Rev. Mod. Phys.* **47** 331  
Millis A J and Lee P A 1987 *Phys. Rev. B* **35** 3394  
Millis A J, Lavagna M and Lee P A 1987 *Phys. Rev. B* **36** 864  
Nozières P 1985 *Ann. Phys., Paris* **10** 19  
Nunes A C, Rasul J W and Gehring G A 1985 *J. Phys. C: Solid State Phys.* **18** L873  
Ott H R, Rudiger H, Rice T M, Ueda K, Fisk Z and Smith J L 1984 *Phys. Rev. Lett.* **52** 1915  
Rasul J W and Desgranges H U 1986 *J. Phys. C: Solid State Phys.* **19** L671  
Rasul J W and Harrington A P 1987 *J. Phys. C: Solid State Phys.* **20** 4783  
Read N 1985 *J. Phys. C: Solid State Phys.* **18** 2651  
Rice T M and Ueda K 1985 *Phys. Rev. Lett.* **55** 995  
Sherrington D 1971 *J. Phys. C: Solid State Phys.* **4** 414  
Shiba H 1975 *Prog. Theor. Phys.* **54** 967  
Springford M 1989 private communication  
Stewart G R 1984 *Rev. Mod. Phys.* **56** 755  
Willis J O, Thompson J D, Fisk Z, de Visser A, Franse J J M and Menovsky A 1985 *Phys. Rev. B* **31** 1654  
Yafet Y, Varma C M and Jones B 1985 *Phys. Rev. B* **32** 360  
Yoshimori A 1976 *Prog. Theor. Phys.* **55** 67