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Theory of magnetic instabilities in heavy fermion compounds

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Abstract. In this paper we calculate the magnetic interactions between f electrons in the heavy fermion compounds using the slave boson approach to the periodic Anderson model. We show that at high temperatures we recover the RKKY interaction between local moments which may produce a magnetic transition with $T_N > T^*$. At low temperatures there is an additional part to the interaction which acts between the quasi-particles and allows magnetic transitions from within the heavy Fermi liquid state. The magnetic moment in the SDW state can be calculated and the possibility of small magnetic moments is discussed.

1. Introduction

The f electron metals exhibit a variety of ground states. In conventional systems, the RKKY interaction causes the local f moments to order below a critical temperature, T_N. It is well known, however, that in several of the Ce and U compounds the local moments are gradually compensated or 'screened' out leading to the formation of an enhanced mass Fermi liquid (see Coqblin *et al* (1990) for a list of magnetic and non-magnetic Ce compounds). These are the so-called 'mixed valent' or 'heavy fermion' compounds, which are characterized by a small energy scale, T^*. This heavy Fermi liquid may itself subsequently undergo a transition to a magnetic, superconducting or, in an applied magnetic field, metamagnetic state (see for example Taillefer *et al* (1990) for a review). With regard to the magnetic instabilities, it appears that we need to distinguish between two types of transition. A number of compounds including UPt_3 and URu_2Si_2, exhibit very weak magnetic transitions with T_N well below T^*, extremely small magnetic moments $\sim 0.01\ \mu_B$, which are correlated only over finite lengths and which in some cases may be characterized by incommensurate wavevectors. The magnetism is itinerant, arising out of the heavy quasi-particles rather than the local f moments. In UPt_3, however, we can replace 5% of the Pt by Pd or of the U by Th and obtain a robust antiferromagnetic state with a similar transition temperature to the pure compound but with long-range order and moments $\sim$ 30 times larger (Franse *et al* 1990). The difference in the ratio of the magnetic moment to T_N strongly suggests two different types of magnetic interaction. A similar effect is observed in other doped compounds such as $Ce(Cu_{1-x}Ni_x)_2Ge_2$ (Sparn *et al* 1990). The pure compounds UCd_{11} and U_2Zn_{17} also have a transition to an antiferromagnetic state with long range order and with reduced, but still reasonably large, magnetic moments

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$\sim$ 0.5–1.0 μ_B. In these cases the transitions are more reminiscent of local moment magnetism. Nonetheless, the magnetic state is unusual and, for example, there remains a large linear coefficient of specific heat as T goes to zero just as in the non-magnetic heavy fermion compounds (Broholm *et al* 1987). There appear to be three possible regions: (i) local moment magnetism, (ii) itinerant magnetism arising out of the heavy quasi-particles, and (iii) an intermediate region where both local and itinerant aspects are important.

Theoretically we expect the properties to be determined by the interplay of magnetic interactions and moment-compensating mechanisms. We define a quantity T_{N0}, the magnetic transition temperature in the absence of any moment-compensating mechanism and T_0^*, the characteristic temperature of the Fermi liquid state in the absence of magnetic interactions. Then in general we might expect that for $T_{N0} \gg T_0^*$ we obtain a magnetic ground state before the moment-compensating mechanism sets in, while for $T_0^* \gg T_{N0}$ the magnetic moments are compensated before the magnetic correlations become effective. The ground state, in this case, will be an enhanced mass Fermi liquid. Attempts to find a criterion to distinguish between these two regimes have been qualitatively successful (Doniach 1977, Jullien *et al* 1977 and Coleman 1983). This does not, however, account for the itinerant magnetism observed with very small magnetic moments.

In this paper we investigate the problem of Fermi liquid versus magnetic ground-state by using the slave boson approach to the periodic Anderson model (see for example Millis and Lee (1987) and Rasul and Desgranges (1986)). The mean-field approximation gives renormalized bands describing non-interacting quasi-particles with large effective masses. Fluctuations in the boson fields produce an interaction which couples to the hybridization and this will mediate the magnetic interaction via the conduction electrons. For this we need to look at processes in which at least two bosons are exchanged. A class of higher-order terms can then be defined and a ladder-type summation performed giving an RPA-type susceptibility. We consider the behaviour of the interaction in the high- and low-temperature limits. At high temperatures only the high-energy part of the boson propagator contributes. This describes the RKKY interaction between local f electrons. At $T = 0$, on the other hand, there is an important additional contribution from the low-energy part of the boson propagator. This interaction arises only between quasi-particles in the Fermi liquid regime. The full interaction, then, develops a temperature dependence around T^*. A similar approach has been considered by Doniach (1987) although he neglected the low-energy part. The form of the susceptibility has some similarities with that found from other approaches (Grewe and Welslau 1988, Grewe 1988, Kuramoto 1989 and Kuramoto and Miyake 1990).

We can now consider the conditions for a magnetic instability. We look first at the high-energy part of the interaction and calculate the critical 'Kondo coupling', J_c, as a function of the crystal field splitting, Δ, using the 'spin N' model, where N is the degeneracy of the f level. Looking first at $q = 0$, the results agree qualitatively with previous approaches, the major difference being that our model can be used to describe a spin density wave (SDW) instability. Next we consider ways of making our model more realistic and include the effects of:

(i) spin-orbit coupling. This has a significant effect on the value of J_c. As a function of N we now have NJ_c = constant, in contrast to previous results, and the dependence of J_c on Δ is expected to be smaller.

(ii) $q \neq 0$. Experimentally, the transitions are to an antiferromagnetic or incommensurate state and we consider the factors determining which transition in fact occurs. We show that this depends strongly on details of the band structure and band filling. We find large inter-band terms when $q = Q$, the 'nesting vector' which will give rise to a SDW gap opening between the two hybridized bands. This is in contrast to the SDW found by Doniach (1987) where the use of the spin N model lead to nearly half-filled bands with the gap opening in the middle of the bands.

We discuss qualitatively the effect that the low-energy part of the interaction will have on this picture. Here there is no simple dependence of the interaction on the bare parameters, though it will depend on the band structure and band filling. We show that at $q = 0$ this term alone is of the correct order of magnitude to produce a transition. Using simple quasi-1d bands we can investigate the q-dependence of the low energy terms and the possibility of an incommensurate value of q is suggested.

The magnetic transition temperature, T_N, due to the high-energy terms is then calculated as a function of J. Below a certain temperature, $T_m \sim T^*$, the magnetic susceptibility becomes temperature-independent and there are no transitions with T_N less than T_m. It is this temperature range, however, where the low-energy part of the interaction begins to play a role and we discuss the possibility that it is the temperature dependence of this which may drive the magnetic transitions from the quasi-particle regime.

Finally we consider the gap equation for the SDW arising from the high-energy terms. In a recent paper it was suggested that there was no non-trivial solution for this (Harigaya 1990). This is not what we find here and we discuss the reasons for the discrepancy. The magnetic moment, S, is calculated as a function of J, and it is seen that this is reduced for $T_N \sim T^*$. For transitions produced by the low-energy part of the interaction S is further reduced although we only obtain very small values for $T_N \ll T^*$. Special features of the band structure such as nesting may further reduce S in certain cases.

2. RPA form for the magnetic susceptibility

Using the slave boson approach, the periodic Anderson model with $U \rightarrow \infty$ can be reformulated to give an effective Hamiltonian (Millis and Lee 1987 and Rasul and Desgranges 1986)

$$H = \sum_{\sigma k} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{im} E_{0m} f^\dagger_{im} f_{im} + \sum_{k\sigma im} V_{\sigma m}(k) f^\dagger_{im} b_i c_{k\sigma} \exp(R_i k) + \text{h.c.} \tag{2.1}$$

subject to the constraint $n_{fi} + n_{bi} = 1$, where b_i is the 'slave boson' field which ensures that $n_{fi} < 1$. We note that strictly speaking this is only valid for the Ce compounds although we do not expect the reults for U to differ greatly (Evans and Gehring 1989). A convenient way of dealing with this is to write the path integral form for the partition function Z, where the constraint is taken care of by introducing a Lagrange multiplier $i\lambda$.

$$Z = \int_{-\pi/\beta}^{\pi/\beta} \frac{\beta d\lambda}{2\pi} \int Dc Dc^\dagger Df Df^\dagger Db Db^\dagger \exp\left[- \int_0^\beta d\tau L(\tau) + i\lambda(n_{fi} + n_{bi} - 1)\right] \tag{2.2}$$

where

$$L(\tau) = H(\tau) + \sum_{k\sigma} c^{\dagger}_{k\sigma} \frac{\partial c_{k\sigma}}{\partial \tau} + \sum_{im} f^{\dagger}_{im} \frac{\partial f_{im}}{\partial \tau} + \sum_{i} b^{\dagger}_{i} \frac{\partial b_{i}}{\partial \tau} \tag{2.3}$$

We write the boson field in terms of its phase and amplitiude, $b_i = \rho_i \exp(i\theta_i)$ and make the gauge transformation, $f_{im} \rightarrow f_{im} \exp(i\theta_i)$. The phase velocity, $\dot{\theta}_i = \partial\theta_i/\partial\tau$, then couples to the Lagrange multiplier giving, $i\lambda \rightarrow i\lambda + i\dot{\theta}_i(\tau)$. $i\lambda(\tau)$ now depends on imaginary time, τ, and acts as a boson field. The 'spin N' approximation in which $c_{k\sigma} \rightarrow c_{km}$ and $V_{\sigma m}(k) \rightarrow V$ is frequently made to simplify the calculation. The simplest approximation we can make is the 'mean-field' approximation where we replace $\rho_i(\tau)$ and $i\lambda_i(\tau)$ by their average values. This gives us an effective hybridization Hamiltonian with renormalized parameters, $V \rightarrow \tilde{V} = \rho V = (1 - n_f)^{1/2} V$ and $E_0 \rightarrow \epsilon_f = i\lambda + E_0$. ϵ_f acts as the characteristic energy scale in the system and can be identified with T^*. The problem reduces to one of non-interacting quasi-particles where the renormalized parameters are found by minimizing the free-energy and solving the mean-field equations. The quasi-particles have an enhanced mass given by $m^*/m = \tilde{V}^2/\epsilon_f^2 \sim 1/\epsilon_f$ which is large in the limit of E_0 being large and negative.

We can now calculate the f electron susceptibility in the m^{th} channel for a field along the z axis to be

$$\chi_{fm}(q, \nu) = \sum_{k} G_{fm}(k) G_{fm}(k + q) \tag{2.4}$$

where we have not included the magnetic moment. k is used to denote the four vector (k, ω). $G_{fm}(k)$ is the f electron Green function given by

$$G_{fm} = \sum_{\alpha=\pm} A_{-\alpha} [\omega - E_{\alpha}(k)]^{-1} \tag{2.5}$$

where $E_{\pm}(k)$ are the quasi-particle bands

$$E_{\pm}(k) = 0.5 \left[\epsilon_k + \epsilon_f \pm \sqrt{(\epsilon_k - \epsilon_f)^2 + 4\tilde{V}^2} \right] \tag{2.6}$$

and $A_{\mp}(k)$ are the f electron weights in the bands

$$A_{\mp}(k) = \frac{\partial E_{\pm}(k)}{\partial \epsilon_f} \tag{2.7}$$

We can now go beyond the mean-field theory and include fluctuations in the boson fields. There are two types of fluctuation corresponding to fluctuations in the amplitude and phase of the boson field. In k space we have $\rho(k) = \rho + \delta\rho(k)$ and $\lambda(k) = \lambda + \delta\lambda(k)$. The fluctuations to 1st order have been considered by several people and have been used to calculate the correction to the Wilson ratio, the T^2 term in the resistivity (Millis and Lee 1987), and the superconducting interaction in different angular momentum channels (Lavagna *et al* 1987). In all these calculations it is the fluctuations in the phase of the boson field, associated with enforcing the constraint at each site, which gives the dominant contribution.

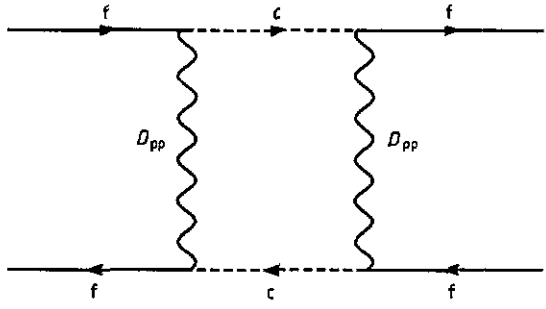

Figure 1. The first of the ladder diagrams contributing to $\chi_{fm}(q)$.

To this order then, fluctuations in the amplitude of the boson fields are relatively unimportant. It is these fluctuations, however, which we expect to mediate the inter-site magnetic interactions via the hybridization with the conduction electrons. Such interactions will only be generated by double exchange of bosons and we calculate now the contribution these terms make to the magnetic susceptibility.

Consider first the contribution from the diagram shown in figure 1. This gives

$$\chi_{fm2}(q) = V^4 \sum_{k,k',k''} G_{fm}(k)G_{fm}(k+q)D_{\rho\rho}(k-k'')G_{cm}(k'')G_{cm}(k''+q) \times D_{\rho\rho}(k''-k')G_{fm}(k')G_{fm}(k'+q) \tag{2.8}$$

where $G_{cm}(k)$ is the mean-field Green function for c electrons, $= \sum_{\alpha=\pm} A_\alpha[\omega - E_\alpha(k)]^{-1}$, and $D_{\rho\rho}(k)$ is the boson propagator for fluctuations in the amplitude of the boson field.

We assume that the wavevector dependence of the boson propagators is much smaller than the energy dependence. This is the 'local' approximation which is frequently used. We start by considering the sum over k. We have

$$F(q,\omega'') = \sum_k G_{fm}(k)G_{fm}(k+q)D_{\rho\rho}(\omega-\omega'') = \sum_{k,\alpha=\pm,\beta=\pm} \left(\frac{A_{-\alpha}(k)}{\omega - E_\alpha(k)}\right)\left(\frac{A_{-\beta}(k+q)}{\omega+\nu-E_\beta(k+q)}\right) D_{\rho\rho}(\omega-\omega''). \tag{2.9}$$

Performing the sum over ω then gives

$$F(q,\omega'') = \sum_{k,\alpha,\beta} \frac{A_{-\alpha}(k)A_{-\beta}(k+q)}{\nu + E_\alpha(k) - E_\beta(k+q)} \times \{f[E_\alpha(k)]D_{\rho\rho}[E_\alpha(k)-\omega''] - f[E_\beta(k+q]D_{\rho\rho}[E_\beta(k+q)-\omega'']\}. \tag{2.10}$$

From now on we consider $\nu = 0$. Taking the Fermi level to lie in the lower band the sum over k can be performed to give, at $q = 0$ and $T = 0$,

$$F(0,\omega'') = \chi_{fm}(0)D_{\rho\rho}(-\omega''). \tag{2.11}$$

Since most of the f electron weight is close to the Fermi level we expect a similar factorization to hold for $q \neq 0$ and finite temperatures giving

$$F(q,\omega'') \approx \chi_{fm}(q) D_{\rho\rho}(-\omega'') \tag{2.12}$$

quite generally. The full expression (2.8) therefore factorizes to give

$$\chi_{fm2}(q) = \chi_{fm}(q)\chi_{fm}(q)V^4 \sum_{k''} D_{\rho\rho}(-\omega'')D_{\rho\rho}(\omega'')G_{cm}(k'',\omega'')G_{cm}(k''+q,\omega'')$$

$$= \chi_{fm}^2(q) I(q)\,. \tag{2.13}$$

We can now write down a whole series of diagrams and perform a ladder summation giving an RPA type susceptibility

$$\tilde{\chi}_{fm}(q) = \frac{\chi_{fm}(q)}{1-\chi_{fm}(q)I(q)}\,. \tag{2.14}$$

We now discuss the behaviour of $I(q)$. We consider first the high-temperature limit. There is a problem here as the mean-field solution breaks down at a temperature T_c. We can in fact push T_c to being $\gg T^*$ by including the T dependence of the Fermi level and thus avoid the problem (Evans *et al* 1989). Alternatively we can follow the procedure used by Coleman (1987) and fix the mean-field parameters just below T_c and then continue to allow the temperature to increase. In either case at sufficiently high temperatures only the high-energy part of the boson propagator will contribute. $D_{\rho\rho}(\omega)$ is found from functional integral techniques and it is easily shown that (Houghton *et al* 1988)

$$D_{\rho\rho}(\infty) = 1/i\lambda \approx -1/E_0 \tag{2.15}$$

for all temperatures giving $I(q) = \chi_c V^4/E_0^2$.

At $T = 0$ the situation is more complicated. Most of the c electron weight lies relatively far from the Fermi level and c electrons near the Fermi surface have a weight $\sim m/m^*$. This may lead us to expect that the low-energy contribution to the interaction is small. However, at $T = 0$ we find (Rasul and Desgranges 1986)

$$D_{\rho\rho}(0) = 1/(2NV^2\rho_0) \tag{2.16}$$

where ρ_0 is the conduction electron density of states, assumed constant. We see that $D_{\rho\rho}(0) \gg D_{\rho\rho}(\infty)$ and despite the small weight of the low-energy c electrons, the low-energy part of the interaction cannot be neglected. To keep the calculation simple we split the sum over ω up into two parts, $|\omega| < \omega_c$ and $|\omega| > \omega_c$, where $\omega_c \sim \epsilon_f$. We assume that for $|\omega| < \omega_c$ we can replace $D_{\rho\rho}(\omega)$ by its value at $\omega = 0$ while for $|\omega| > \omega_c$ we can replace the boson propagator by its value in the high-energy limit. We obtain

$$I(q) = V^4\left[\chi_{cm}^{h}(q)D_{\rho\rho}(\infty)D_{\rho\rho}(-\infty) + \chi_{cm}^{l}(q)D_{\rho\rho}(0)D_{\rho\rho}(0)\right] \tag{2.17}$$

where

$$\chi_{cm}^{l}(q,0) = \sum_{k,|\omega|<\omega_c} G_{cm}(k,\omega)G_{cm}(k+q,\omega) \tag{2.18}$$

and

$$\chi^{h}_{cm}(q,0) = \sum_{k,|\omega|>\omega_c} G_{cm}(k,\omega)G_{cm}(k+q,\omega)\,. \tag{2.19}$$

It is easily shown that $\chi^{h}_{c}(0,0) = \rho_0$ while $\chi^{l}_{c}(0,0) \sim \rho_0 m/m^*$. Since the high-energy contribution to χ_c is so much bigger than the low-energy contribution it is insensitive to the value of ω_c. The low-energy part, however, has a spurious dependence on ω_c.

The interaction has naturally split into two terms, one coming from the high-energy part and the other from the low-energy part of the boson propagator. Using (2.15) and (2.16) gives at $T = 0$

$$I(q) = \left[\frac{V^4}{E_0^2}\chi^{h}_{c}(q) + \frac{1}{(2N\rho_0)^2}\chi^{l}_{c}(q)\right]. \tag{2.20}$$

We note that there are many other contributions to this order including those with single boson exchange, interactions with the other boson propagators, and terms involving off-diagonal susceptibilities, χ_{fc}. All of these have been considered and in the limits $n_f \to 1$ and $\rho_0 J \ll 1$ are negligible compared to (2.20).

The high-energy part of $I(q)$ can be written $I^{h}(q) \approx \rho_0 J^2$ where $J = V^2/E_0$. This is the only part of the interaction which survives to high temperature. The same term could in fact have been found by adding a term $J\boldsymbol{S}_f \cdot \boldsymbol{s}_c$ to the mean-field Hamiltonian and using the molecular field approximation. It describes coupling between nearly unrenormalized f electrons. As the temperature is reduced, the low-energy part of the interaction begins to play a role and the total interaction will increase.

Several papers have considered this problem from a different starting point (Grewe and Welslau 1988, Grewe 1988, Kuramoto 1989 and Kuramoto and Miyake 1990). They begin with a collection of single sites, then consider interactions between them mediated by the conduction electrons in an extension of either the non-crossing approximation or Fermi liquid theory. The full susceptibility so calculated has the form

$$\chi_f(q,\omega) = [\chi^{I}_{f}(\omega)^{-1} - K(q,\omega)]^{-1}\,. \tag{2.21}$$

$K(q,\omega)$ splits into two terms representing the high- and low-energy contributions as above. The high-energy term is of the form $K^h \sim \chi_B J^2$ and the low-energy term $K^l \sim \chi_B$, where χ_B is the band contribution to the susceptibility which appears to be similar to our χ_c. The differences with our approach are as follow:

(i) The zeroth order f electron susceptibility, χ^{I}_{f}, is calculated for the impurity so does not depend on q.

(ii) K^h and K^l are each proportional to the full 'band' susceptibility, χ_B, and not just a part of it as in our calculation.

(iii) In the results presented by Grewe(1988) he finds that for $T = 0$ $\chi_B \sim \rho_0 m/m^*$ which corresponds to our result for χ^{l}_{c}. The low-energy contribution to the interaction is therefore comparable to ours while the high-energy contribution is a factor m/m^* smaller.

At $T \gg T^*$, however, he obtains $\chi_B \sim \rho_0$ and the high-energy term is now similar to ours, the low-energy terms having gone to zero in both models.

The numerical prefactors are also different. Despite these discrepancies it is nonetheless interesting that such different approaches produce a final result with much in common.

3. The condition for a magnetic instability

3.1. $q = 0$

We consider here the condition for a magnetic instability by looking for zeros of the denominator of (2.14). We start by considering the case $q = 0$, which would lead to a ferromagnetic instability, and then consider under what conditions $\chi_f(q)\chi_c(q) > \chi_f(0)\chi_c(0)$ giving an antiferromagnetic or incommensurate ground state.

We look for instabilities driven by the high-energy part of the interaction and consider the equation

$$1 - J^2\chi_{fm}(0)\chi^h_{cm}(0)\,. \tag{3.1}$$

We have $\chi_{fm} \sim 1/\epsilon_f$ and $\chi^h_{cm} \sim \rho_0$ and (3.1) is similar to the condition arrived at from qualitative approaches where the ground state energies of a Kondo singlet and magnetically-ordered states are compared (Doniach 1977, Jullien *et al* 1977 and Coleman 1983).

We consider the $1/N$ model described in section 2 with $N = 6$ but with a crystal field splitting the originally degenerate f level into three doublets separated by energies Δ_1 and Δ_2 (Evans 1990). The magnetic instability will occur in the channel corresponding to the ground state doublet with energy ϵ_{f0}. We have $\chi_{f0} = \rho_0\tilde{V}^2/\epsilon^2_{f0}$ and $\chi^h_c = \rho_0$. The mean-field equations yield

$$E_0 = 2\rho_0 V^2 \ln\left(\frac{W^3}{\epsilon_{f0}\epsilon_{f1}\epsilon_{f2}}\right) \tag{3.2}$$

where $\epsilon_{f1} = \epsilon_{f0} + \Delta_1$ and $\epsilon_{f2} = \epsilon_{f0} + \Delta_2$. ϵ_{f0} is now given in terms of J and Δ_1 and Δ_2 and for given crystal fields we can calculate the critical value of J, J_c, for which (3.1) is satisfied at $T = 0$. For $J > J_c$ we obtain a Kondo liquid while for $J < J_c$ the ground state is magnetic. Putting $\Delta_2 = 2\Delta_1$ it is found that J_c increases at first rapidly with Δ_1 then begins to level off as seen in figure 2. We note that $\Delta_1\rho_0 = 0.06$ gives $\Delta_1/T^* = 12$ which is fairly typical for the heavy fermion compounds. Increasing Δ_1 reflects a decrease in the effective degeneracy so this behaviour is as expected from previous approaches. We show below, however, that with more realistic bands the behaviour is modified. We can also calculate the critical value of T^*. Defining $1/T^* = \gamma$ where γ is the linear coefficient of the specific heat we can calculate T^*_c. This decreases with Δ_1 as found by Doniach (1987).

We consider now what happens when spin-orbit coupled bands are used (Zou and Anderson 1987). The conduction electrons now have their true spin σ and the hybridization matrix element depends on spin and wave vector, $V_{\sigma m}(k) = V_0 Y_{3m-\sigma}(k)\langle 3lm-\sigma, \frac{1}{2}\sigma \mid \frac{5}{2}m\rangle$, where $Y_{3m-\sigma}(k)$ is the spherical harmonic for $l = 3$ and $\langle 3lm - \sigma, \frac{1}{2}\sigma \mid \frac{5}{2}m\rangle = (4\pi)^{1/2}[(7 - 4\sigma m)/14]^{1/2}$ is the Clebsch–Gordan coefficient for spin-orbit coupled states with $j = \frac{5}{2}$ and $l = 3$. The simplest case is for $\Delta_1 = \Delta_2 = 0$ where it is easily seen that only two linear combinations of the f levels hybridize, the rest remaining localized at ϵ_f. The physical picture is, therefore, significantly different to that calculated within the 'spin N' model. The hybridization term is rewritten

$$\sum_{ki\sigma} 3^{1/2} V_0 f^\dagger_{i\sigma} b_i c_{k\sigma} e^{iR_i\cdot k} + \text{h.c.} \tag{3.3}$$

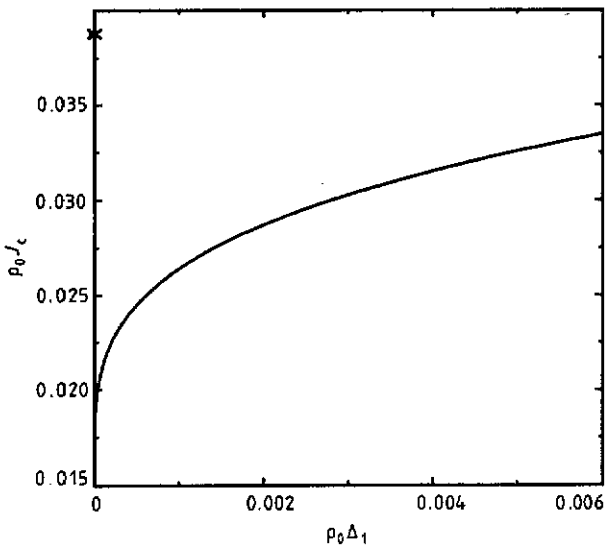

Figure 2. Critical value of $\rho_0 J_c$ versus $\rho_0 \Delta_1$ where $\Delta_2 = 2\Delta_1$. The cross indicates the result when spin-orbit coupled bands are used with $\Delta_1 = \Delta_2 = 0$.

where we have defined

$$f_{i\sigma} = \frac{1}{3^{1/2} V_0} \sum_m V_{m\sigma}(k) f_{im} \,. \tag{3.4}$$

We note that the hybridization is in this case isotropic and the large anisotropy considered by Doniach (1987) is not appropriate. Since only those f electrons which hybridize can take part in the RKKY interaction the susceptibility has a different form to (2.14) and we have for the full susceptibility, now including the magnetic moment,

$$\tilde{\chi}_f = \frac{\mu_p^2 \chi_f}{1 - (3J)^2 \chi_f \chi_c} + (\mu_T^2 - \mu_p^2)\chi_f \tag{3.5}$$

where μ_p is the magnetic moment for the quasi-particle bands which is only a fraction of the full moment, μ_T, with $\mu_p^2 = 0.18\mu_T^2$. We obtain an effective model with $N = 2$ and the criteria for instability is

$$1 - \frac{(3J_c\rho_0)^2}{2} \exp\left(-\frac{1}{3J_c\rho_0}\right) \tag{3.6}$$

which is very different to that calculated above. Solving this we find a value for J_c which is approximately 2 times larger. When we vary N we find NJ_c = constant, in contrast to the 'spin N' model where NJ_c decreased with increasing N. We note that previous calculations have concentrated on the one- and two-site terms (Doniach 1977, Jullien *et al* 1977 and Coleman 1983). For one or two impurities we can expand around the impurity sites and m is a good quantum number. For the lattice this is no longer valid and different results are obtained. We note that the magnetic moment in the magnetic state would be small, i.e. $< \mu_p$.

For non-zero crystal field splittings the problem is harder and calculating the quasi-particle bands involves solving a quartic equation. If Δ is sufficiently large, however, we can approximate the lower quasi-particle band by that calculated as if the c electrons hybridized only with the ground state doublet. The only difference with the 'spin N' model is that V is now anisotropic (Evans 1990). We do not expect this to alter the results greatly and the effect of including spin-orbit coupling at large Δ will be smaller than for $\Delta = 0$. The dependence of J_c on Δ will then be smaller than that shown in figure 2.

3.2. $q \neq 0$

Experimentally the f electron compounds have antiferromagnetic fluctuations or undergo transitions to an antiferromagnetic or incommensurate state. We want now to consider the criteria (3.1) for $q \neq 0$. We assume a tight binding form for ϵ_k for a simple cubic lattice. Nesting properties will be associated with the vector $Q = (\pi/a, \pi/a, \pi/a)$. For the high-energy part of the interaction we consider what happens at $q = Q$. This gives $\epsilon_{k+Q} = -\epsilon_k + \mu$ where μ is the centre of the c electron band relative to the Fermi level. For simplicity we approximate the density of states by a constant, ρ_0, and consider isotropic hybridization. The results turn out to depend sensitively on the total number of electrons. In order to have metallic behaviour we need to take the total number of electrons, n_T, as being < 2. This can arise if, for example, more than one c electron band crosses the Fermi level. For $n_T = 1.95$ we find $\chi_f(Q)/\chi_f(0) = 0.48$ and $\chi_c^h(Q)/\chi_c(0) = 3.8$. We see that there is a tendency to antiferromagnetism rather than ferromagnetism which is due to the increase of χ_c^h with q. We emphasize that the intra-band contribution to $\chi_f(Q)$ is negligible compared to the inter-band term and the latter is so large due to the proximity of the upper and lower band edges. A magnetic instability will give rise to a spin density wave which will widen the gap between the two bands. This is very different to the situation described by Doniach (1987) where he assumes 1c electron and $2/N$ f electrons per sub-band. For large N the bands are close to half-filling and in this case the biggest contribution to $\chi_f(Q)$ comes from the intra-band terms, and the gap would open within the lower band. As we decrease the filling from two the antiferromagnetic terms fall off very quickly and for $n_T = 1.89$ the tendency to ferromagnetism becomes larger than that to antiferromagnetism. There are several other factors which can influence the relative tendency to antiferromagnetism compared to ferromagnetism. Using the tight-binding density of states Kaga (1990) showed that $\chi_f(Q)/\chi_f(0) \approx 2.6$ implying a greater tendency to antiferromagnetism than the calculation here, although he did not calculate χ_c. Furthermore, in our model there is a gap in the quasi-particle density of states. This is rather artificial. We can eliminate the gap in a number of ways, for example by including a k-dependent hybridization (Gumhalter and Zlatic 1990) or a small amount of direct f–f hopping (Harrington *et al* 1988). This significantly increases the value of $\chi_f(Q)/\chi_f(0)$.

We want now to consider the low-energy part of the interaction, I^l. We note that the value of χ^l_{cm} is not very well defined as it depends on the value of ω_c. Taking $\omega_c = \epsilon_f$ we find for $q = 0$ and $N = 2$, $\chi_f \chi_c^l D^2_{\rho\rho}(0) \approx 1/4$ which is too small to drive the transition by itself although this term increases rapidly as we increase ω_c. We do not expect to be able to rely on the absolute value and the important feature is that it is of the correct order of magnitude. In this case the value of the interaction is not determined in a simple way by the bare parameters of the model, in contrast to the high-energy terms, although it will depend on the details of the band structure.

We now want to consider what happens for finite values of q. Here the results of Grewe and Welslau (1988) lead us to expect that I^1 may peak for an incommensurate value of q. There are two competing factors. The gap, $E_+(k+q) - E_-(k)$, with k close to the Fermi level is initially large, and this tends to decrease with increasing q becoming $\sim \epsilon_f$ for $q = Q$. At the same time the c electron weight in the relevant part of the upper band, which is ~ 1 for $q = 0$, becomes smaller eventually becoming $\sim m/m^*$ for $q = Q$. This combination produces a peak at an incommensurate value of q. This can be checked using simple, periodic quasi-one-dimensional bands given by $\epsilon_k = -W + (2Wa/\pi)k$ for $0 \leqslant k \leqslant \pi/a$ and $\epsilon_k = -W - (2Wa/\pi)k$ for $-\pi/a \leqslant k \leqslant 0$. We then have $\epsilon_{k+q} = \epsilon_k + \epsilon_q$. We consider the inter-band contribution to $\chi_c^1(q)$ which we expect to dominate. Within the approximation, χ_{cm}^1 peaks for $\epsilon_q \sim 0.5W$. We note that this value is much bigger than the one found by Grewe and Welslau (1988). The maximum value of $\chi_c^1(q)$ is about a factor 4 greater than that at $q = 0$ and so appears to be about the right order of magnitude to drive the transition. We also need to calculate the q-dependence of χ_f, a feature that the theory of Grewe and Welslau cannot take into account. We expect $\chi_f(q)$ to increase monotonically with q (Auerbach *et al* 1988). Depending on the relative magnitudes of the increases in χ_f and χ_c^1 we may obtain either a commensurate or an incommensurate transition.

We can now calculate the antiferromagnetic transition temperature T_N. This will depend on the form of $\chi_f(q,T)$. We start by considering the T-dependence of $\chi_f(0,T)$. In general this has a small peak after which it falls off as $1/(T+\theta)$ where $\theta > 0$. We can approximate the T dependence of χ_f by $\chi_{fm} = 1/[N(T+\theta)]$ for $T > T_m$ and χ_{fm} = constant for $T < T_m$ where T_m is the position of the peak. For the mixed-valent compounds $T_m \sim T^*/2$ and $\theta \sim T^*/3$ (Laurence *et al* 1981). It is not as clear that these relations are obeyed in the heavy fermion compounds although we expect them to hold approximately (see e.g. Stewart 1984 for a review).

With this form for $\chi_f(T)$, the equation for T_N becomes very simple with

$$2T_N = J^2\chi_c - T^* \tag{3.9}$$

for $T_N > T_m$ and T_N falling to zero when $T_N = T_m$. This is shown in figure 3 for $T_m = T^*/3$ assuming a ground state doublet with $\Delta_1 = 10\epsilon_{f0}$ and $\Delta_2 = 2\Delta_1$. We note that this part of the interaction cannot produce transitions from within the Fermi liquid regime. The phase diagram is essentially the same as that obtained by previous calculations (e.g. Coqblin *et al* 1990).

The calculated temperature-dependence of $\chi_f(Q)$ is similar. There is no peak but $\chi_f(Q,T)$ has a plateau up to a certain temperature, T_{mQ}, before falling off as $1/(T+\theta_Q)$, where $\theta_Q \sim T_{mQ} \sim T_Q^*$ and T_Q^* is the inverse of $\chi_f(Q)$ at $T = 0$. The phase diagram will be similar to that in figure 3.

We can now look at the low-energy terms. We assume that it is possible to obtain $1 < \chi_f(q,0)\chi_c^1(q,0)/(2N\rho_0)^2$. In this case the interaction falls off with temperature. T_N will increase with the increase of the quantity $\chi_f(q,0)\chi_c^1(q,0)/(2N\rho_0)^2$ above the critical value of 1 and we will always have $T_N < T^*$. This gives a possible explanation for the low-temperature itinerant magnetic phase. We note that in this case it is the T-dependence of the interaction $I^1(q)$ rather than the T-dependence of the susceptibility which drives the transition. This has been predicted by fitting experimental data for U_2Zn_{17} to a susceptibility of the form (2.14) (Broholm *et al* 1987).

In the following section we derive the gap equation for the spin density wave state and calculate the magnetic moment.

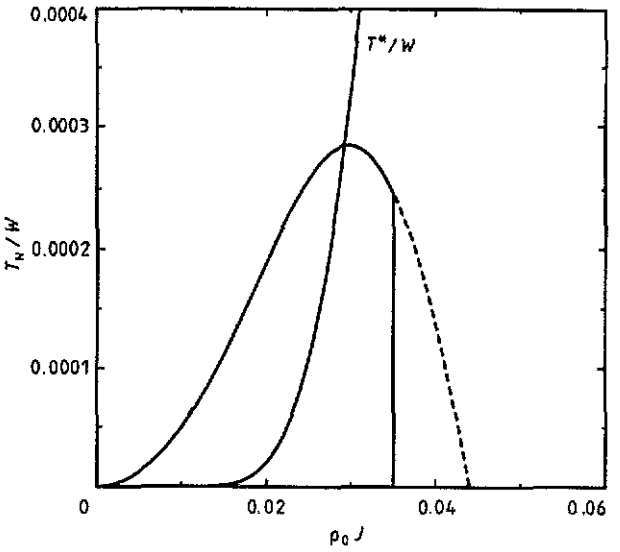

Figure 3. The magnetic transition temperature, T_N/W, and T^*/W versus $\rho_0 J$ for $\Delta_1 = 10\,T^*$, $\Delta_2 = 2\Delta_1$ and $T_m = T^*/3$. The dotted line shows the curve for $T_m = 0$.

4. The spin density wave state

We now calculate the gap equation for the spin density waves below the magnetic transition. This problem has previously been considered by Harigaya (1990) where it was claimed that there was no non-trivial solution. He considered, however, diagrams describing only single boson exchange. Corresponding terms for the susceptibility were found to be negligible compared to the two-boson exchange. He also neglected the upper band terms which we have seen give the dominant contribution to the antiferromagnetic susceptibility. Considering first the high-energy part of the interaction, we wish to calculate $S = \sum_{k\sigma} \tilde{G}^{+-}_{f\sigma}(k)$ where $\tilde{G}^{+-}_{f\sigma}(k)$ is the anomalous propagator given by the Fourier transform of $\langle T_\tau f_{k,\sigma}(\tau) f^\dagger_{k+Q,-\sigma}(0)\rangle$ and where calculating the spin for the f electrons rather than the quasi-particles should not alter the final result. We have treated the f electron ground state doublet as having spin σ. Defining $G^{++}_{f\sigma}$ as the Fourier transform of $\langle T_\tau f_{k\sigma}(\tau) f^\dagger_{k\sigma}(0)\rangle$ and $G^{--}_{f\sigma}(k)$ as the Fourier transform of $\langle T_\tau f_{k+Q-\sigma}(\tau) f^\dagger_{k+Q-\sigma}(0)\rangle$, we use the diagrams shown in figure 4 to give the following relations

$$\tilde{G}^{++}_{f\sigma}(k) = G^{++}_{f\sigma}(k) + \tilde{G}^{+-}_{f\sigma}(k)\Sigma^{-+}_{f\sigma}(k)G^{++}_{f\sigma}(k) \tag{4.1}$$

$$\tilde{G}^{+-}_{f\sigma}(k) = \tilde{G}^{++}_{f\sigma}(k)\Sigma^{+-}_{f\sigma}(k)G^{--}_{f\sigma}(k) \tag{4.2}$$

where $G^{++}_{f\sigma}$ and $G^{--}_{f\sigma}$ are the unperturbed propagators and $\tilde{G}^{++}_{f\sigma}$ and $\tilde{G}^{--}_{f\sigma}$ the perturbed propagators in the presence of the spin density wave. $\Sigma^{+-}_{f\sigma}(k)$ is the anomalous self-energy which we approximate by the diagram in figure 4(*c*) involving double boson exchange. This gives

$$\Sigma^{+-}_{f\sigma}(k) = \sum_{k'k''} G^{++}_{c\sigma}(k') D_{\rho\rho}(\omega' - \omega'') \tilde{G}^{+-}_{f\sigma}(k'') D_{\rho\rho}(\omega'' - \omega') G^{--}_{c\sigma}(k'). \tag{4.3}$$

This factorizes in a similar way to (2.8). We consider the static-order parameter $\Sigma^{+-}_{f\sigma}(k,0)$ and then also neglect the k dependence giving $\Sigma^{+-}_{f\sigma}(k) = \Sigma_f$. We obtain the following self-consistency equation

$$\Sigma_f = J^2 \Sigma_f \tilde{\chi}_f(\Sigma_f) \tag{4.4}$$

where

$$\tilde{\chi}_f(\Sigma_f) = \sum_{k,\omega} \frac{G^{++}_f(k) G^{--}_f(k)}{1 - \Sigma_f^2 G^{++}_f(k) G^{--}_f(k)} . \tag{4.5}$$

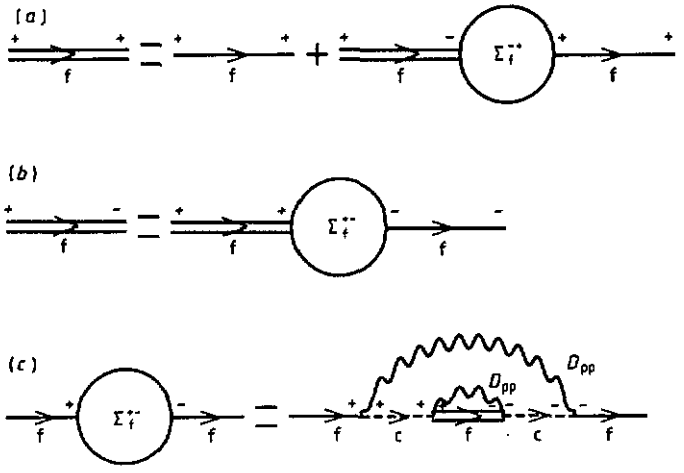

Figure 4. The diagramatic representation of the Dyson equations (*a*) (4.1) and (*b*) (4.2). Single lines represent unrenormalized electron propagators and double lines the renormalized propagators. (*c*) The gap equation for the SDW.

In general (4.5) is relatively complicated. We can, however, make several approximations. The dominant contribution to the susceptibility comes from the inter-band terms with energies close to the Fermi level. We can, therefore, approximate as follows: $G^{++}_f(k) = A_-(k)[\omega - E_+(k)]^{-1}$ and $G^{--}_f(k) = A_+(k+Q)[\omega - E_-(k+Q)]^{-1}$. The quasi-particles are then defined by the poles of

$$[\omega - E_+(k)][\omega - E_-(k+Q)] = A_-(k) A_+(k+Q) \Sigma_f^2 . \tag{4.6}$$

We can approximate the factors A_α by their values at the Fermi level to give

$$[\omega - E_+(k)][\omega - E_-(k+Q)] = \Sigma_f^2 \tag{4.7}$$

which has solutions $\tilde{E}_\pm(k)$. We need also to calculate n_f and ϵ_f self-consistently in the presence of the spin density wave. These are given by

$$n_f = \sum_{k,\alpha=\pm} \frac{\partial \tilde{E}_\alpha(k)}{\partial \epsilon_f} \frac{1}{\omega - \tilde{E}_\alpha(k)} \tag{4.8}$$

and

$$\epsilon_f = E_0 + \sum_{k,\alpha=\pm} \frac{\partial \tilde{E}_\alpha(k)}{\partial \rho^2} \frac{1}{\omega - \tilde{E}_\alpha(k)}. \tag{4.9}$$

We can now calculate the spin as a function of J. We expect $\Sigma_f \tilde{\chi}_f(\Sigma_f)$ to be an approximately universal function of Σ_f/T_Q^*. We can then solve for $(\Sigma_f/T_Q^*)(T_Q^*/J^2) = \Sigma_f \tilde{\chi}_f(\Sigma_f)$ to give Σ_f as a function of J^2/T_Q^* and hence S as a function of J. We take $\chi_c^h(Q) = \rho_0$ and assume crystal field splitting $\Delta_1 = 10\,T^*$ and $\Delta_2 = 2\Delta_1$. The results are shown in figure 5. We see that for the values of J for which $T_N > T^*$, S is close to unity while as T_N approaches T^*, S is less than unity. S gets cut off for the value of J corresponding to T_{mQ} and $S \ll 1$ cannot be achieved.

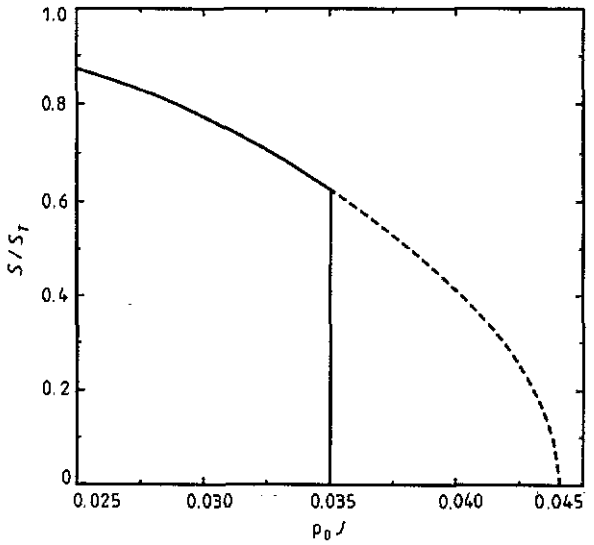

Figure 5. The magnetic moment S/S_T, where S_T is the maximum polarization of the f electron ground state doublet, in the SDW state at $T = 0$ as a function of $\rho_0 J$. The parameters are as in figure 3.

Again we can consider what happens if the low-energy term is itself large enough to produce the transition. As $I^l(q)$ increases above one S will increase from 0. Very small values for S will only be found when $I\chi_f$ is very close to 1 which will correspond to $T_N \ll T^*$. The result will, however, depend on the band structure. In the case of UPt_3 it has been suggested that nesting of the Fermi surface results in much smaller moments than expected (Miyake and Kuramoto 1990).

5. Conclusion

In this paper we have considered how fluctuations in the slave boson field give rise to magnetic interactions between the quasi-particles derived from the mean-field theory. An RPA form for the susceptibility is found. The interaction, $I(q)$, separates

naturally into low- and high-energy parts. The high-energy part describes the conventional RKKY interaction between local moments at high T which may produce an instability for $T_N > T_m$. The same effect could be found by treating low-order perturbation processes and the criteria for instability is similar to that found by classical approaches which describe the competition between the magnetic interaction-energy and the energy of the Kondo singlet. Certain differences in the details of the solution are, however, found when spin-orbit coupled bands are used. A self-consistent equation for the total spin in the SDW state is derived and the total magnetic moment shown to be close to uninty for $T_N \gg T^*$, then decreasing as T_N approaches T^*.

The low-energy part has previously been neglected. Despite the fact that the c electrons mediating the interaction only have a weight $\sim m/m^*$ near the Fermi energy, the largeness of the boson propagator at $\omega = 0$ means that the low-energy contribution to the interaction cannot be neglected. This describes interactions between quasiparticles well into the Fermi liquid state and disappears at high temperatures. This term alone is of the right magnitude to drive the transition giving the possibility of magnetic instabilities arising from the Fermi liquid state with $T_N < T^*$. In this case it is the T-dependence of the interaction rather than the susceptibility which drives the transition. An incommensurate value for q appears to be possible within a simple model. The magnitude of S will depend on the ratio T_N/T^* suggesting that very small values of S will only be observed for $T_N \ll T^*$, which is not the case experimentally. The details of the band structure will, however, also play a role and may contribute to reducing S in certain cases. We note that our calculations are of a model nature only and quantitative results are not expected.

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