Magnetic instability of a highly degenerate Kondo lattice

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(Received 14 April 1986)

The large-degeneracy (N) limit of the periodic Anderson model is studied within a model in which the hybridization matrix elements $v_{k,m}$ are treated as angle dependent. The resulting effective heavy-fermion Fermi surface is multisheeted, with quasi-one-dimensional bands. A spin-density-wave instability with wave vector $2k_f$ is shown to arise below a critical value of the effective Schrieffer-Wolff coupling constant $J=v^2/|\varepsilon_f^0|$, where ε_f^0 is the unrenormalized f-level energy. The dependence of this critical coupling J_c on crystal field splitting is shown to be quite weak. For systems with J close to J_c, the effects of zero-point spin-density-wave fluctuations are shown to decrease the heavy-fermion mass at $T=0$. For increasing temperature, this decrease is rapidly washed out, leading to an initial increase of the low-temperature γ value. This behavior provides an interpretation of specific-heat observations in $CeAl_3$ and $CeCu_2Si_2$. The effect of applied field and pressure on the specific heat are discussed in the context of this theory.

I. INTRODUCTION

In studying the large N-limit[1] (N is the degeneracy of the localized levels) of a periodic Anderson lattice, the geometry of the resulting heavy-fermion Fermi surface will be strongly affected by the (k,m) dependence postulated for the hybridization matrix elements $v_{k,m}$. This is in contrast to the single-impurity problem where one imagines that spherical averaging implied by the point symmetry of the model will wash out details of this (k,m) dependence.

In this paper we will be concerned about the magnetic instabilities of the Anderson lattice problem in the limit that the unperturbed f state is well below the Fermi level—the "Kondo lattice" regime. We will be particularly interested in a spin-density-wave—type (SDW) instability, and consequently have chosen to study a model in which $v_{k,m}$ is strongly $\mathbf{k}$ dependent. The idea for the model comes from a consideration of the large l behavior of the matrix elements $v_{k,m}=\langle k\,|H_{\rm atom}|\,l,m\rangle$, where $|k\rangle$ is a plane-wave state, $|l,m\rangle$ is an atomic bound state, and $H_{\rm atom}$ is an effective one-electron Hamiltonian. For large N we are lead to consider large l, for which one can construct wave packets of atomic states $|l,M\rangle$ whose angular dependence is centered around a set of directions Ω_M, and which fall rapidly to zero outside a cone of solid angles $\delta\Omega$ subtending an area $4\pi/(2l+1)$ on the unit sphere.

With respect to this new basis, $v_{k,M}$ peaks for $\pm\hat{\mathbf{k}}$ pointing along Ω_M and falls rapidly to zero as the direction of $\hat{\mathbf{k}}$ goes outside the cone of angles $\delta\Omega$. So each atomic state $|l,M\rangle$ hybridizes with two opposing sectors of the free-electron Fermi surface. In the large-l limit, each of the 2 $(2l+1)$ localized states (including spin) therefore leads to a hybridized Hartree-Fock subband[2] (see below) which is highly oriented in k space, i.e., quasi-one-dimensional. In order to obtain consistency with the large-N limit of the single-impurity Kondo problem, it is found that the number of electrons in the conduction band, i.e., the volume of the Fermi sphere, must also scale with N, so that there are of order 1 conduction electron per subband per atom. This in turn implies that the Fermi surface overlaps $N/2$ extended Brillouin zones, so that, in a reduced-zone scheme, it becomes multisheeted. The main result of this paper is to show, using the $1/N$ expansion, that these quasi-one-dimensional subbands exhibit a spin-density-wave instability of wave vector $2k_F$ as the position of the unrenormalized f level, ε_f^0, is lowered relative to the Fermi level leading to a critical value of the dimensionless effective Schrieffer-Wolff coupling constant $J\rho=(v_{kM})^2\rho/|\varepsilon_f^0|$.

We also discuss the effect of splitting of the f degeneracy by a crystal field, on the critical J and investigate the behavior of the low-temperature specific heat as the instability is approached.

II. THE $N\rightarrow\infty$ LIMIT

Starting from the Coleman form[3] of the $U\rightarrow\infty$ Anderson lattice

$$H=\sum_{i,m}\varepsilon_f^0 n_{fiM}+\sum_k \varepsilon_k n_k+i\lambda\sum_{i,M}(b_i^\dagger b_i+f_{iM}^\dagger f_{iM})+\sum_i(b_i v_{M,k}/\sqrt{N}e^{i\mathbf{k}\cdot\mathbf{R}_i}f_{iM}^\dagger c_k+\text{H.c.})\,, \quad (1)$$

the $N\rightarrow\infty$ limit is defined by evaluating the path integral

$$Z=\int Dc\,Df\,Db\,D\lambda\, e^{-\int_0^\beta d\tau(c_k^\dagger\partial_\tau c_k+f_i^\dagger\partial_\tau f_i+H)} \quad (2)$$

using the method of steepest descent with respect to a spatially invariant mean boson amplitude $\langle\,|b|\,\rangle$ and chemical potential $\langle i\lambda\rangle=\varepsilon_f^R-\varepsilon_f^0$, where ε_f^R is a renormalized f level energy. We note that the local phase ϕ_i of the boson field $b_i=|b_i|e^{i\phi_i}$ may be absorbed into the local chemical potential $i\lambda_i$ following the argument of Read and Newns[4] and Coleman,[5] so that the location of the saddle point determines the mean boson amplitude. At the saddle point, the resulting model is that of a set of noninteracting hybridized bands which may be solved analytically using the ansatz of Sec. I for v_{kM}.

Writing the resulting free energy in the form

$$\mathscr{F}=\sum_{k,M}\int^{E_F}d\varepsilon\int^{\varepsilon}d\omega[\delta(\omega-E_1)+\delta(\omega-E_2)]+i\lambda(\langle b^\dagger b\rangle-Q)\;, \tag{3}$$

where $E_{1,2}$ are the hybridized subband energies for a cone of k vectors hybridizing with a given M sublevel of the f states, given by

$$E_{1,2}=\frac{\varepsilon_k+\varepsilon_f^R}{2}\mp[(\varepsilon_k-\varepsilon_f^R)^2/4+v^2\langle b^\dagger b\rangle]^{1/2}/N \tag{4}$$

and Q is the f occupancy. Since the renormalized f level, and hence the hybridization gap lie above the Fermi level, the heavy-fermion properties are dominated by the lower subband, E_1, leading to

$$\mathscr{F}=\frac{V}{(2\pi)^3}\sum_M\delta\Omega\int^{\varepsilon_F}d\varepsilon\int^{\varepsilon}d\omega\,k(\omega)\left.\frac{d\varepsilon_k}{dE_1}\right|_{\omega}+i\lambda(\langle b^\dagger b\rangle-Q)\;.$$

Using

$$\varepsilon_k=E_1-\frac{V^2\langle b^\dagger b\rangle/N}{(E_1-\varepsilon_f^R)}\;,$$

and replacing $V/(2\pi)k(\omega)\delta\Omega$ by the density of conduction-band states, ρ, the leading contribution to $\mathscr{F}$ becomes

$$\mathscr{F}=-\Delta_0\langle b\rangle^2\ln(D/\varepsilon_f^R)+i\lambda(\langle b^\dagger b\rangle-Q)\;, \tag{5}$$

where $\Delta_0=v^2\rho$, D is the conduction-band depth, and ε_f^R is measured relative to the Fermi level. Note that, since $\delta\Omega=4\pi/(2l+1)\propto 1/N$, the assumption that ρ is N independent implies that the volume of the conduction-band Fermi sphere scales with N. Substituting $i\lambda=\varepsilon_f^R-\varepsilon_f^0$ and varying with respect to $\langle b^\dagger b\rangle$ leads to the saddle-point equation

$$\varepsilon_f^R-\varepsilon_f^0=\Delta_0\ln(D/\varepsilon_f^R)\;, \tag{6}$$

from which we recover the usual Kondo energy $\varepsilon_f^R=De^{-\varepsilon_f^0/\Delta_0}=T_K$, in the Kondo regime $\Delta_0/\varepsilon_f\ll 1$.

Variation with respect to λ or equivalently ε_f^R gives

$$\sum_M\langle n_M^f\rangle+\langle b^\dagger b\rangle=Q$$

leading to

$$\langle b^\dagger b\rangle=1/[1+(\Delta_0/T_K)]\approx\frac{T_K}{\Delta_0} \tag{7}$$

(setting $Q=1$), so that the width of the hybridization gap in (4) becomes of order

$$\left[\frac{v^2\langle b^\dagger b\rangle}{N}\right]^{1/2}\approx(T_K\rho^{-1}/N)^{1/2}\;.$$

III. MAGNETIC INSTABILITY OF THE KONDO LATTICE

In order to study the magnetic instability of the Kondo state, we need to look at effects of zero-point fluctuations, $\delta b=b-\langle\,|\,b\,|\,\rangle$ of the boson field, on the particle-hole propagators. For a spin-density-wave instability, the relevant channel involves a particle on one sheet of the Fermi surface and a hole on the opposing sheet. To leading order in $1/N$ the effects of the boson fluctuations may be estimated using ladder diagrams. These diagrams will not be included in the lowest-order terms of the $1/N$ expansion for the free energy. So the fermion and boson propagators used in the ladder diagram calculation should, strictly speaking, be renormalized by the usual $1/N$ corrections.

Since the bosons conserve the M-channel index, the ladder diagrams are labeled by the channel indices, M,M' of the particle and hole. The leading magnetic instability occurs in a given subband with $M'=-M$. We consider the limit where $\varepsilon_f^R-\varepsilon_f^0$, the energy needed to excite a boson amplitude fluctuation is taken $\gg T_K$. As shown by Read[6] and Coleman[7] the principal effect of the $1/N$ "bubbles" on the boson phase fluctuations is to introduce a long-time algebraic tail in the boson propagator. In this paper we make the assumption that, since the principal spectral weight of the boson fluctuations lies at high frequencies $\varepsilon_f^R-\varepsilon_f^0$, the effect of the infrared phase fluctuations on the relative energies between magnetic and nonmagnetic ground states will only become important right at the magnetic instability. Thus from the point of view of defining the phase diagram of the Kondo lattice, we assume that the phase fluctuations may be neglected. This point will be taken up again in the discussion.

With this assumption the boson exchange may be treated as instantaneous, with coupling constant $-v^2/N\,|\,\varepsilon_f^0\,|=J/N$. We now evaluate the ladder diagrams in the heavy-fermion limit $T_{kf}\ll 1$. In this limit (see Appendix) we find

$$\chi_{ff}(q)=[1-J^2/N^2\chi_{ff}^0(q)\chi_{cc}^0(q)]^{-1}\chi_{ff}^0(q)\;, \tag{8}$$

where χ_{ff}^0 and χ_{cc}^0 are diagonal parts of the hybridized electron-hole susceptibilities for f electrons and conduction electrons, respectively (see Fig. 1).

The response functions $\chi_{ff}^0(q),\chi_{cc}^0$ are calculated by integrating over the cone $\delta\Omega_M$ of particle and holes belonging to a particular subband:

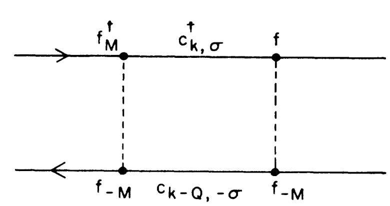

FIG. 1. Diagram contributing to the $f_M^\dagger f_{-M}$ particle-hole propagator.

$$\chi^0_{ff,M}(q)=\sum_{k,j,j'}\frac{n^{(j)}_{k,M}-n^{(j')}_{k-q,-M}}{E^{(j)}_{k,M}-E^{(j')}_{k-q,-M}}\,|\psi^{(j)}_f|^2\,|\psi^{(j')}_f|^2\,, \tag{9}$$

where $n^{(j)}_{k,M}$ is the Fermi occupation number for the particular band, either below or above the hybridization gap ($j=1,2$), with energy $E^{(j)}_{k,M}$. These functions have a quasi-one-dimensional peak at $q=2k_F$. For χ^0_{ff}, the dominant contributions come from the lower hybridized band, since, in the Kondo limit, the carriers have predominantly f character.

Writing

$$E^1(k^\pm)=E^1_F(\varepsilon^\pm_k-\varepsilon_F)\frac{\partial E^1}{\partial \varepsilon_k}$$

we find

$$\chi^0(2k_F)=\rho\,\frac{d\varepsilon}{dE^1}\bigg|_{\varepsilon_F}\frac{4\pi}{\delta\Omega}\int_0^{k_F}\frac{dp}{2k_F}\ln\left[\frac{2p/k_F}{2p/k_F+\delta\Omega/\pi}\right]$$

$$=\frac{\Delta_0\langle b\rangle^2}{NT_K^2}\left[1+\ln\left[\frac{2\pi}{\delta\Omega}\right]\right]$$

$$=\frac{1}{NT_K}[1+\ln(2\pi/\delta\Omega)]\,. \tag{10}$$

For χ^0_{cc}, the mixed propagator with the hole in the E^1_M subband and the particle in the E^2_M subband gives the dominant contribution. At the Fermi level these subbands are separated by an energy gap $E_{\rm gap}=T_K+\rho^{-1}/N$. Strictly speaking, the large-N limit would make $(T_K\rho)^{-1}/N$ tend to zero. However, for N large and finite, the magnetic instability occurs at a value of T_K for which $T_K\rho \ll 1/N$, hence in the vicinity of this phase boundary $E_{\rm gap}\approx\delta\rho^{-1}/N$, leading to $\chi^0_{cc}\cong\rho\ln(D/E_{\rm gap})=\rho\ln(ND\rho)$.

Taking $D\rho$ to be of order unity, the criterion for the spin-density-wave instability then becomes [from (8)]

$$\frac{J^2C}{N^2T_K\rho}\ln N[1+\ln(2\pi/\delta\Omega)]=1\,, \tag{11}$$

where C is a constant, leading to a critical value of the Kondo temperature, T_{Kc}, of

$$\frac{T_{Kc}}{D}\approx\frac{\tilde C}{N^2(\ln N^2)^2}=(\tilde C)2\times10^{-3} \tag{12}$$

for $N=6$, where $\tilde C$ is a coefficient which varies slowly with N. Equation (11) for the spin-density-wave instability is essentially equivalent to Eq. (14) of Read *et al.*[8] obtained from a comparison of the ground state of the Kondo metal with that of a fully magnetized antiferromagnet, apart from a slowly varying factor. In contrast to the latter treatment, the present approach leads to a switching on of the spin density wave through a second order transition.

IV. EFFECTS OF CRYSTAL FIELD SPLITTING ON THE MAGNETIC INSTABILITY

The strong dependence of the critical Kondo coupling on N, (12) naturally leads to the question of the effects of crystal-field splitting of the degeneracy, on the above results. This may be answered by adding a crystal-field term

$$H_x=\sum_{MM',i}\varepsilon^x_{MM'}c^\dagger_{fiM}c_{fiM'}\,, \tag{13}$$

to the basic model Hamiltonian (1).

$\varepsilon^x_{MM'}$ is assumed symmetric under $M\to -M$. Since the noninteracting conduction-electron energies are not affected by the crystal field, the hybridization does not mix levels $(M,-M)$ with $(M',-M')$. The mean-field Hamiltonian can now be diagonalized by taking linear combinations $c^\dagger_{fi\mu}=\sum_M\phi_{\mu M}c^\dagger_{fiM}$ which diagonalize (13), leading to linear combinations of subbands with renormalized f-level energies

$$\varepsilon^R_{f_\mu}=\varepsilon^R_f+\varepsilon^x_\mu\,, \tag{14}$$

where ε^R_f is an f-level renormalization common to all subbands and ε^x_μ are the eigenvalues of $\varepsilon^x_{MM'}$. The heavy-fermion density-of-states enhancement factor for the μ'th subband

$$\frac{d\varepsilon_k}{dE^\mu_1}=\frac{v^2\langle b^\dagger b\rangle/N}{(E_1-\varepsilon^R_f-\varepsilon^x_\mu)^2} \tag{15}$$

is now reduced somewhat for the higher lying subbands, and the renormalized f-level energy ε^R_f is now given in the Kondo limit by the solution of

$$\varepsilon^0_f\cong\Delta_0/N\sum_{\mu=1}^{N}\ln[D/(\varepsilon^R_f+\varepsilon^x_\mu)]\,. \tag{16}$$

For $N=6$, in a cubic crystal with the Γ_7 doublet state lowest, this gives

$$\varepsilon^0_f=\Delta_0\ln\{(D/\varepsilon^R_f)^{1/3}[D/(\varepsilon^R_f+\varepsilon^x)]^{2/3}\}\,. \tag{17}$$

Setting $\varepsilon^x/\varepsilon^R_f=\alpha$ one has $\varepsilon^R_f=T_K/(1+\alpha)^{2/3}$ which shows that for a system for which the crystal-field splitting is comparable to the Kondo temperature, the renormalized f-level energy is reduced by a factor ≈ 1.6.[9] Thus one may expect that increasing crystal-field splitting will tend to push the system across into the spin-density-wave magnetic phase. Nevertheless, in the Kondo metal state, the heavy-fermion specific heat still has a considerable contribution from the higher lying subbands: from (15) and a similar expression for $\langle n_{f\mu}\rangle$ leading to $\langle b^\dagger b\rangle\cong(1+\alpha)/(1+\alpha/3)\varepsilon^R_f/\Delta^0$ the linear electron specific-heat coefficient is given by

$$\gamma\propto\frac{1}{3\varepsilon^R_f}[1+2/(1+\alpha)^2]\,, \tag{18}$$

so that for $\alpha\approx1$, $\frac{1}{3}$ of the electronic specific heat would come from the Γ_8 quartet of subbands.

The spin-density-wave instability will occur in the particle-hole channel for the lowest lying subbands. Equation (11) now becomes

$$\frac{(1+\alpha)}{(1+\alpha/3)}\frac{J^2\rho}{N}\frac{C}{N\varepsilon^R_f}(\ln N)[1+\ln(2\pi/\delta\Omega)]=1\,. \tag{19}$$

Solving (19) together with (17) numerically (Fig. 2), one finds that the value of T_{Kc} at the instability phase boundary is still strongly suppressed by the effects of orbi-

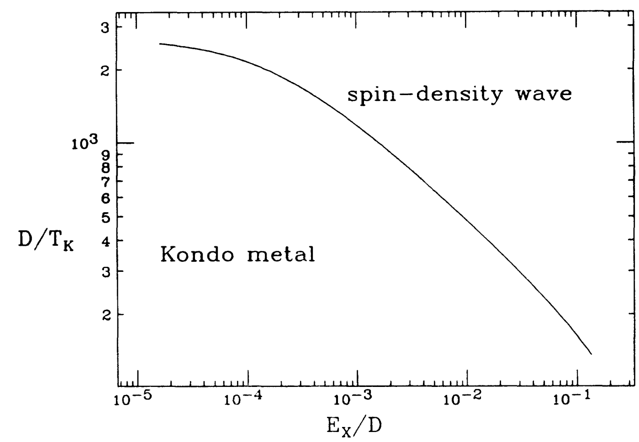

FIG. 2. Dependence of the critical heavy-fermion mass ($\simeq 1/T_K$) on crystal field. The constant in Eq. (11) has been arbitrarily set to 0.3.

tal degeneracy even when the crystal field is an order of magnitude larger than T_{Kc}. Put another way, the maximum heavy-fermion C/T value, which occurs for coupling constant J just above the critical value, will be lowered as ε^x increases. Thus the value of the crystal-field splitting energy may be expected to be one of the significant factors determining whether a given heavy-fermion compound will have a Kondo or magnetic ground state.

V. EFFECT OF SPIN-DENSITY-WAVE FLUCTUATIONS ON THE SADDLE-POINT EQUATIONS

In the $N\rightarrow\infty$ limit, the system is modeled by a set of narrow hybridized bands of noninteracting heavy Fermions. The low-temperature specific heat is given by the Sommerfeld formula

$$\gamma \underset{N\rightarrow\infty}{\propto} N(\varepsilon_F)=N\rho\, d\varepsilon/dE_1=1/T_K \tag{20}$$

(neglecting crystal field effects). In order to estimate the contribution to the free energy from the zero-point spin-density-wave fluctuations in the region of the instability, a random-phase-approximation (RPA)—like term needs to be added. As the magnetic phase boundary is approached, this contribution turns out to affect the saddle point Eqs. (6) and (7) in a singular way. There are also corrections of $O(1/N)$ which do not reflect the spin density wave instability and which we ignore for the purposes of this discussion.[10]

Within the ladder-diagram approximation (using the $T_K\rho \ll 1$ limit outlined in the Appendix), we write, following Brenig *et al.*[11]

$$\Delta F=-\sum_q \int_0^\infty d\omega\left[\tfrac{1}{2}+n(\omega)\right] \times\left[\arctan\left[\frac{J_{\rm eff}v}{1-J_{\rm eff}u}\right]-J_{\rm eff}v\right], \tag{21}$$

where $J_{\rm eff}=[(v^2/\varepsilon_f^0)^2\rho/N^2]\ln N$ is the effective magnetic coupling constant [corresponding to the spin-spin coupling in a Ruderman-Kittel-Kasuya-Yosida (RKKY) calculation]. u and v are the real and imaginary parts of $\chi^0_{ff}(q,\omega)$. The ω and q dependences of χ^0_{cc} vary on the energy scale of the bare conduction band, rather than on the heavy-fermion energy scale, so have been ignored. The saddle-point equations for ε_f^R and $\langle b^\dagger b\rangle$ now become

$$-v^2\rho\ln(D/\varepsilon_f^R)+\lambda-1/\langle b^\dagger b\rangle\Delta F'=0\,, \tag{22a}$$

$$\langle b^\dagger\rangle(v^2\rho/\varepsilon_f^R+1)-Q+2/\varepsilon_f^R\Delta F'=0\,, \tag{22b}$$

where the variation of ΔF with respect to $\langle b^\dagger b\rangle$ and ε_f^R arises from its dependence on the heavy-fermion density of states factor $d\varepsilon/dE_1$

$$\frac{d}{d\langle b^\dagger b\rangle}\frac{d\varepsilon}{dE_1}=\frac{1}{\langle b^\dagger b\rangle}\frac{d\varepsilon}{dE_1}\,,\qquad \frac{d}{d\varepsilon_f^R}\frac{d\varepsilon}{dE_1}=-\frac{2}{\varepsilon_f^R}\frac{d\varepsilon}{dE_1}\,, \tag{23}$$

and $\Delta F'$ is defined by $d(\Delta F)/d(d\varepsilon/dE_1)$. It will turn out that $\Delta F'$ is positive, so that the effect of $\Delta F'$ is to *increase* the effective Kondo temperature of the system at $T=0$, i.e., to *reduce* the heavy-fermion specific-heat enhancement via (20). There is also a paramagnon-type mass enhancement from the T^2 term in the low-temperature expansion of ΔF. This will also be proportional to $1/T_K$. To estimate $\Delta F'$ in (22) we expand $u(Q,\omega)$ about its maximum at $\mathbf{Q}=2k_F\mathbf{e}$ to obtain, for small $q=|\mathbf{Q}-2k_F\mathbf{e}|$,

$$u(q,\omega)\cong A\frac{d\varepsilon}{dE}[1-a(q/k_F)^2+b(T\rho)^2+\cdots] \tag{24}$$

and

$$v(q,\omega)\cong B\omega\rho\frac{d\varepsilon}{dE}\,, \tag{25}$$

where A and B, a and b are constants, and $\mathbf{e}$ is a unit vector spanning a subband Fermi surface (note $B\propto k_F/Q$). In performing the integration over ω, we need to cut off the integral at frequencies above which electron-hole pair density of states contributing to $v(q,\omega)$ loses its heavy-fermion mass enhancement. These will be determined by values of E_1 beyond which the hybridization crosses over to the bare conduction-band density of states, determined from Eq. (4) to be

$$\omega_{\rm max}\cong\left[\frac{v^2\langle b^\dagger b\rangle}{N}\right]^{1/2}\cong\left[\frac{T_K D}{N}\right]^{1/2}.$$

Writing $\kappa_0^2=(1-J_{\rm eff}A\,d\varepsilon/dE)=1-\tilde{J}_{\rm eff}$ which tends to zero as the magnetic phase boundary is approached, the leading contribution to $\Delta F'$ is found to be

$$\Delta F'=\sum_q A/2[1-a(q/k_F)^2]\ln\{1+X^2[1+Y(q/q_{\rm max})]^2\} \tag{26}$$

where

$$X=\frac{\tilde{J}_{\rm eff}}{2A\kappa_0^2}\frac{\omega_{\rm max}}{k_F^2}\,,\quad Y=\frac{\tilde{J}_{\rm eff}}{\kappa_0^2}a(q_{\rm max}/k_F)^2\,.$$

We now work in a limit where $X/Y \propto (T_K/ND)^{1/2} \ll 1$. In this limit $\Delta F'$ has the asymptotic form

$$\Delta F' \sim X^2/Y^{3/2} \propto \frac{\tilde{J}_{\rm eff}}{\kappa_0^2}(\omega_{\max}/k_F^2)^2 . \quad (27)$$

Substituting $\omega_{\max}^2 = v^2/N\langle b^\dagger b\rangle$, we find for the modified saddle-point equations

$$\langle b^\dagger b\rangle \sim \frac{\varepsilon_f^R}{v^2\rho}\left[\frac{1}{1+N\left[\dfrac{\tilde{J}_{\rm eff}}{1-\tilde{J}_{\rm eff}}\right]^{1/2}}\right]$$

and (28)

$$T_K \sim D\exp\left[\frac{-\varepsilon_f^0 + c/N\Delta^0\rho\left[\dfrac{\tilde{J}_{\rm eff}}{1-\tilde{J}_{\rm eff}}\right]^{1/2}}{\Delta^0\rho}\right]$$

$$= T_K^0 \exp\left[\frac{c}{N}\left[\frac{\tilde{J}_{\rm eff}}{1-\tilde{J}_{\rm eff}}\right]^{1/2}\right] .$$

Thus the limit $X/Y \ll 1$ is justified provided κ_0^2 is not too small. Equation (28) shows that the effect of precursor zero-point spin-density-wave fluctuations is to increase T_K, i.e., to reduce the heavy-fermion effective mass as the magnetic phase boundary is approached.

VI. TEMPERATURE DEPENDENCE OF THE LOW-TEMPERATURE SPECIFIC HEAT

The principal effect of finite temperature will be to *weaken* the spin fluctuation effects by driving the system away from the SDW instability via

$$\kappa_0^2(T) = 1-\tilde{J}_{\rm eff}(T) \simeq \kappa_0^2(0) + (T/T_s)^2 + \cdots \quad (29)$$

from (24). Here T_s is introduced as a scale temperature. From (24) we may write

$$J_{\rm eff}(T) = J_{\rm eff}(0)[1-(T/T_1)^2 + \cdots] ,$$

where T_1 is a temperature scale set by the Fermi-liquid properties of the heavy fermions, excluding spin-density-wave fluctuations. Hence

$$T_s = \kappa_0 T_1 = [1-\tilde{J}_{\rm eff}(0)]^{1/2} T_1 \quad (30)$$

defines a new, reduced, temperature scale, relative to that appropriate for the "normal" heavy-fermion Fermi liquid. Because this temperature dependence occurs in the exponential in (28), it should dominate the low-temperature behavior relative to explicit T^4 terms in the low-temperature expansion of F. Hence at low temperatures we expect to see the dominant temperature dependence of the specific heat come from the temperature dependence of T_K. Setting

$$F_2 \simeq -\frac{m^*}{m} T^2/T_K(T) , \quad (31)$$

where m^*/m includes the effects of paramagnon mass enhancement, we have

$$C/T = -\frac{\partial^2 F}{\partial T^2} = \gamma(0)\left[1 - \frac{2T}{T_K}\frac{\partial T_K}{\partial T} + \frac{T^2}{T_K^2}\left[\frac{\partial T_K}{\partial T}\right]^2 - \frac{T^2}{2T_K^2}\frac{\partial^2 T_K}{\partial T^2}\right] . \quad (32)$$

Substituting the exponential dependence from (28) thus leads to

$$C/T = \gamma(0)\left[1 + \frac{5}{2}\frac{\tilde{c}^2}{(1+t^2)^{3/2}} + \frac{1}{2}\frac{\tilde{c}^2 t^4}{(1+t^2)^3} - \frac{3}{4}\frac{\tilde{c}t^4}{1(1+t^2)^{5/2}}\right] , \quad (33)$$

where we have set $t = T/T_s$, $\tilde{c} = C/N[\tilde{J}_{\rm eff}/(1-\tilde{J}_{\rm eff})]^{1/2}$. Thus remarkably, the low-temperature γ value is predicted to *increase* with increasing temperature (Fig. 3). Moreover, the shape of the curve looks strikingly linear at $T \lesssim T_s$, in agreement with experiment. As the temperature increases, the decrease of F due to explicit T^4 and higher terms will be expected to take over, leading to a maximum in C/T versus T at low temperatures. To model this behavior, we need to include an explicit dependence of the free energy T^4 and higher-order terms. A five-parameter fit to the data[12] for $CeAl_3$ (Fig. 4) is given by the following somewhat arbitrary model for the free energy:

$$F_4 = -\frac{m^*}{m}\frac{1}{T_K(T)}\frac{T^2}{[1+(T/T_1^2)-(T/T_2^4)]} , \quad (31a)$$

where $T_k(T)$ is defined using Eqs. (28) and (29). The tem-

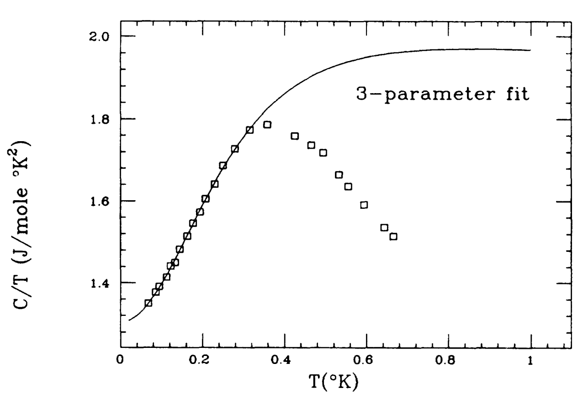

FIG. 3. Three-parameter fit of the low-temperature formula for C/T from (33) to data (Ref. 12) for $CeAl_3$. The spin-density-wave fluctuation scale temperature is found to be 0.361 K, and $\tilde{C}=0.381$. A similar fit (not shown) can be made to data for $CeCu_2Si_2$.

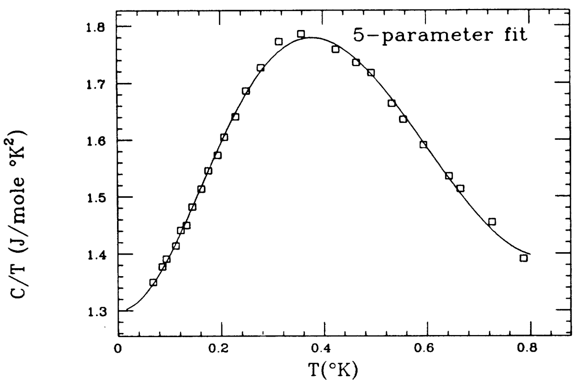

FIG. 4. Fit of the five-parameter formula for C/T derived from (31a) by differentiating twice, to data (Ref. 12) for $CeAl_3$. In this fit T_s is found to be 0.365 K, while T_1 and T_2 are 1.53 and 2.25 K, respectively.

perature dependence of the specific heat is obtained by differentiation of (31a) as in Eq. (32). Using the fitted parameters and Eq. (30) we find $\kappa_0^2 \approx 0.055$ for $CeAl_3$. In this interpretation of the data, the observed low-temperature increase is due to a washing out of the incipient SDW fluctuations (which tend to suppress the heavy-fermion mass) with increasing temperature, while the decrease in C/T at higher temperatures is due to temperature dependence of the normal heavy Fermi liquid parameters (excluding the magnetic fluctuations).

VII. LOW-TEMPERATURE BEHAVIOR OF THE SUSCEPTIBILITY

The low-temperature suppression of the specific heat by SDW fluctuations will also be expected to show up in the susceptibility. However, since higher lying crystal-field multiplets will contribute significantly to χ, particularly for anisotropic compounds such as $CeAl_3$ and $CeCu_2Si_2$, where the susceptibility transverse to the c axis will involve mixing of different crystal-field-split pieces of Fermi surface, the temperature-dependent effects discussed in the last section may be expected to show up considerably weakened in the susceptibility of a polycrystalline sample.[13]

Close to $T=0$, for G along the c axis, we approximate χ by

$$\chi_{c_{\rm axis}} = \sum_m \frac{(g\mu_B m)^2}{[T_K(T)+\varepsilon_m]} = \tfrac{1}{2}(g\mu_B)^2 \left[\frac{9}{T_K(T)} + \frac{26}{T_K(T)+\varepsilon^x} \right] , \quad (34)$$

where we have taken the ground-state doublet to be $m=\frac{3}{2}$ and the excited state doublets (treated as degenerate) to be $m=\frac{1}{2}$ and $\frac{5}{2}$. Although the resulting temperature is generally like the measurements for $CeAl_3$, the overall increase between 0.03 and 0.5 K is predicted too high (of order 18%) compared with the measured values[14] which show only a 2% increase between these temperatures. This may be partly due to the polycrystalline nature of the sample. However, this discrepancy does point to a quantitative limitation of the present approach.

VIII. EFFECTS OF APPLIED MAGNETIC FIELD, PRESSURE, AND DISORDER ON THE LOW-TEMPERATURE SPECIFIC HEAT

In the $N\to\infty$ limit, an applied magnetic field will alter the saddle-point equations by splitting the degeneracy of the hybridized Fermi surface. Because of spin-orbit coupling, this will in general complicate the simple model assumed for the hybridized bands in this paper. In order to get a qualitative idea of the effects of the field, we ignore these complications and simply take the bare f-orbital energies to be $\varepsilon_{fm}^0 = \varepsilon_f^0 + hm$, where $h = g\mu_B H$ (for zero crystal-field splitting). The $N\to\infty$ saddle point is obtained from

$$F = \sum_m \frac{\rho v^2 \langle b^\dagger b \rangle}{N} \ln \left[\frac{D}{\varepsilon_{fm}^R} \right] + (\varepsilon_f^R - \varepsilon_f^0)(\langle b^\dagger b \rangle - Q) , \quad (35)$$

where $\varepsilon_{fm}^R = \varepsilon_f^R + hm$. Deriving with respect to $\langle b^\dagger b \rangle$ and ε_f^R and expanding to order $(h/T_K)^2$, we find

$$\varepsilon_f^R = T_K(0)[1+\tfrac{1}{2}(h/T_K)^2 B_2] , \quad (36)$$

where $B_2 = (1/N)\sum_m m^2$, $T_k(0) = D\exp(-\Delta^0/|\varepsilon_f^0|)$, and

$$\langle b^\dagger b \rangle = \frac{T_k(0)}{\Delta^0}[1-\tfrac{1}{2}(h/T_k)^2 B_2] . \quad (37)$$

In this limit, the specific heat is given by the density of states at the Fermi level:

$$C/T = \sum_m v^2 \frac{\langle b^\dagger b \rangle}{N} \frac{1}{(\varepsilon_{fm}^R)^2} = \frac{1}{T_k(0)}[1+\tfrac{3}{2}(h/T_k)^2 B_2] . \quad (38)$$

Thus the effect of the applied field is to increase *both* the effective Kondo temperature *and* the zero-temperature specific heat.

Turning now to the effect of the magnetic field on the SDW instability, we note that this involves a transfer of a heavy fermion from one side of the Fermi surface, spin-orbit index m, to the other side, spin-orbit index $-m$. This results in

$$\chi_{ff}^0(Q,h) = \sum_{\mathbf{p}} \frac{f(E_{1,\mathbf{p}+\mathbf{Q},m}) - f(E_{1,\mathbf{p},-m})}{E_{\mathbf{p},-m} - E_{\mathbf{p}+\mathbf{Q},m}} . \quad (39)$$

For small h, the principal field dependence $\chi_{ff,m-m}^0$ in a given m channel comes from the asymmetry in the heavy-fermion density of states on going from the $-m$ to $+m$ subbands. This leads to

$$\chi_{ff,m-m}^0(Q,h) = \chi_{ff}^0(Q,0) \frac{2dE/d\varepsilon|_{h=0}}{dE^1 d\varepsilon|_m + dE^1/d\varepsilon|_{-m}} = \chi_{ff}^0(Q,0)\frac{\langle b^\dagger b \rangle|_h / \langle b^\dagger b \rangle|_0}{1+2(hm/T_K)^2} = \chi_{ff}^0(Q,0)\frac{[1-\frac{1}{2}(h/T_K)]^2 B_2}{1+2(hm/T_K)^2} . \quad (40)$$

Hence an applied magnetic field pushes the system away from the SDW phase boundary. This is consistent with the discovery of a field-driven phase transition in $CePb_3$ by Lin *et al.*,[15] where a transition is seen from a SDW phase at low fields to a Kondo phase above 5 T. It is also consistent with data of Bredl *et al.*[16] on the field dependence of the low-temperature specific heat of $CeCu_2Si_2$ and $CeAl_3$ where the effect of an applied field is to increase C/T at $T=0$, but to diminish the rate of increase of C/T with T as the field is increased. As κ_0^2 increases due to the applied field, the spin-fluctuation-induced increase in T_K derived in Sec. VI is diminished, thus leading to a less rapid rise in C/T versus T in an applied field.

The SDW Kondo lattice phase boundary should also be pressure dependent. The general effect of pressure will be to increase the hybridization matrix elements, v, hence to increase the basic Kondo temperature T_K. This will have the effect of simultaneously *decreasing* the heavy-fermion density of states, hence decreasing C/T at $T=0$, and pushing the system away from the SDW phase boundary. As with the applied field, the latter effect will tend to diminish the low-temperature increase of C/T versus T, but in contrast to the case of the applied field, the $T=0$ intercept for C/T will be expected to fall with increasing pressure, rather than to rise. This appears consistent with data of Brodale *et al.*,[12] although the data do not yet extend to low enough temperatures (or to small intermediate pressures) to verify the $T=0$ decrease of C/T.

Finally, the introduction of a small amount of lattice disorder by alloying may be expected qualitatively to lead to a broadening out of the quasi-one-dimensional peak in $\chi^0_{ff}(Q)$ at $Q=2k_F$. This will also push the system away from the SDW phase boundary, hence diminish the low-temperature rise of C/T. The heavy-fermion density of states will be expected to be less sensitive to disorder, so that the basic T_K should not vary so rapidly with mean free path.

IX. EFFECTS OF THE MAGNETIC INSTABILITY ON SUPERCONDUCTIVITY OF A KONDO LATTICE SYSTEM

The same boson fluctuations which lead to the SDW instability via particle-hole coupling, will induce superconductivity in the particle-particle channel. The effective electron-electron coupling energy involves excitation across the hybridization gap into conduction electron states above the heavy-fermion hybridized bands, leading to

$$V^{\text{eff}}_{\text{el-el}} \cong \left[\frac{v^2}{N\varepsilon_f^0}\right]^2 \frac{1}{2E_{\text{gap}}} = \frac{J^2\rho}{2N^3} \ . \tag{41}$$

In computing the particle-particle propagator, care must be taken to avoid putting two fermions on the same site. This tends to favor the antisymmetric (p-wave-like) superconducting state (Czycholl and Doniach[17]).

To make a very rough comparison between the magnetic and superconducting ground state energies we set

$$E_{\text{BCS}} = -T_K \exp(-T_K/V^{\text{eff}}_{\text{el-el}}) \tag{42}$$

and compare with the RKKY energy

$$E_{\text{RKKY}} \cong -\frac{1}{2}\frac{J^2\rho}{N^2} \ . \tag{43}$$

Since we have shown that the magnetic instability condition $E_{\text{RKKY}} < T_K$ is qualitatively justified by the more detailed discussion of the SDW character of the instability given in this paper, we conclude that the small gain in energy due to Bardeen-Cooper-Schrieffer (BCS) pairing will always loose out in the end to the magnetic energy as ε_f^0 is made more negative ($J\rho$ decreasing). However, one cannot exclude a small region of the phase diagram, close to the SDW-Kondo phase boundary where the two instabilities may be in competition.

X. DISCUSSION AND BREAKDOWN OF THE LADDER APPROXIMATION AT THE MAGNETIC-NONMAGNETIC PHASE BOUNDARY

As the SDW phase boundary is approached, $\kappa_0 \to 0$, the spin fluctuations start to compete strongly with the heavy-fermion mass renormalization: from (28) this occurs for $\kappa_0 \lesssim 1/(\ln D/T_k)$. Under these conditions the neglect of infrared phase fluctuations of the boson field (Sec. III) clearly becomes unjustified since the SDW fluctuation energies are now approaching zero and a consistent treatment of both the Kondo renormalization and the spin-density-wave critical point (at $T=0$) is needed. This presents an interesting problem in that the arguments of Beal-Monod and Maki[18] and Hertz[19] that the upper critical dimension of a Hubbard-type system is reached at $T=0$ (3 space and 1 time dimensions) may be invalidated by the existence of the Kondo fluctuations which are inherently of a two-dimensional character for individual f sites. What happens in the Kondo lattice is not clear, but the above argument suggests that the Kondo fluctuations will remain relevant in this case.

Away from the phase boundary, on the SDW side, we expect that a saddle-point treatment analogous to that given in this paper will still work, and that the system will exhibit a combination of SDW and heavy-fermion character.[20] Close to the phase boundary, the f moments will be reduced,[21] but will increase with decreasing J, along with a corresponding reduction in heavy-fermion mass (increasing T_K) as the Fermi surface becomes reduced in area due to the SDW gap.

ACKNOWLEDGMENTS

The author thanks T. M. Rice, P. Coleman, E. Edelstein, J. Flouquet, and N. E. Phillips for helpful conversations. Part of this work was performed at the Lab León Brioullin, Centre d'Etudes Nucléaires de Saclay. The author thanks M. Lambert and Rhadakrishna for their hospitality and support. He also acknowledges the stimulating environment of the Aspen Center for Physics and the partial support of the National Science Foundation, Grant No. DMR 83-05723.

Note added: Since writing this paper, the author has learned of work by Rasul and Desgranges,[22] in which a low-temperature increase of C/T with T for the Kondo lattice has been predicted without consideration of a magnetic instability.

APPENDIX

The purpose of this appendix is to discuss the approximations leading to the SDW instability criterion Eq. (11). Because of the hybridization term in the $N \rightarrow \infty$ limit effective Hamiltonian, the electron-hole pair propagators are not diagonal in the original f and c representation but also contain off-diagonal or "anamalous" contributions. For this reason, the susceptibility function defined in Eq. (9) is in general 4×4 matrix $\chi_{\alpha\beta}(q)$ in which the suffix α denotes four possible particle-hole channels: $|f^\dagger f\rangle$, $|f^\dagger c\rangle$, $|c^\dagger f\rangle$, $|c^\dagger c\rangle$. Because of our basic assumption that the dominant spectral weight for boson-fluctuation exchange between the particle and hole may be treated as ω and k independent, the ladder diagrams may be summed by the simple RPA equation

$$\chi_{\alpha\beta}(Q) = \chi_{\alpha\beta}(Q) + \sum_{\gamma\delta} \chi^0_{\alpha\gamma} \frac{v^2}{N\varepsilon_f^0} \varepsilon_{\gamma\delta} \chi_{\delta\beta} ,$$

where $\varepsilon_{\gamma\delta}$ is the anti-unit-matrix

$$\begin{bmatrix} 0001 \\ 0010 \\ 0100 \\ 1000 \end{bmatrix}$$

resulting from the form of the original Anderson hybridization coupling. The SDW instability is now determined by the criterion that the smallest eigenvalue of the matrix

$$\underline{A} = \frac{v^2}{\varepsilon_f^0} \sum_{\delta} \chi^0_{K\delta} \varepsilon_{\delta\gamma}$$

equal unity. Since we are interested in the heavy-fermion limit $|\varepsilon_f^0| \ll \Delta_0$, we can classify the matrix elements of the particle-hole response function $\chi^0_{\alpha\beta}$ in powers of $(T_K\rho)^{-1}$, where ρ is the unhybridized conduction-band density of states. Estimates for the diagonal elements denoted by χ^0_{ff} and χ^0_{cc} in Sec. III are given in Eqs. (10) and preceding Eq. (11). There are also diagonal elements $\chi^0_{fc,fc}$ and $\chi^0_{cf,cf}$ which may be estimated to be of order ρ using $|\psi_c^1|^2 \simeq (\varepsilon_f^R - \varepsilon_k)^2/\gamma^2 \cong NT_K\rho$. Off-diagonal elements $\chi^0_{fc,ff}, \chi^0_{ff,cf}$ are of order $\rho/(NT_K\rho)^{1/2}$ and $\chi^0_{cf,cc}, \chi^0_{cc,cf}$ are of order $\rho(NT_K\rho)^{1/2}$. In the limit $T_K\rho \ll 1$, the matrix $\underline{A}^2$ corresponding to the exchange of two bosons illustrated in Fig. 1 has diagonal elements which dominate over the largest off-diagonal elements by a factor of order $1/(T_K\rho)^{1/2}$. Therefore, in this limit $(1-\underline{A})^{-1} = (1-\underline{A}^2)^{-1}(1+\underline{A})$ may be represented in terms of the approximately diagonal matrix $\underline{A}^2$, leading to the criterion in Eq. (11).

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