Mean-field results for the Kondo lattices at high magnetic fields

T. M. Hong* and G. A. Gehring
Department of Physics, The University, Sheffield S3 7RH, United Kingdom
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We generalize previous slave-boson mean-field calculations for the Kondo lattices to high magnetic fields, and derive analytic expressions for the Kondo energy when the hybridization matrix element is isotropic. For the anisotropic case, two metamagneticlike transitions are found, and their relative strength depends on the number of electrons participating in the hybridization per unit cell. We discuss the implications for this to the metamagneticlike transition and its related properties in heavy-fermion compounds. In particular, the relative motion of different spin bands is considered to reproduce the field dependence of the residual magnetoresistance.

I. INTRODUCTION

Many heavy-fermion compounds exhibit a metamagneticlike transition;[1,2] i.e., there is a peak in the susceptibility χ at some critical field H_M. This is not a conventional transition in the sense that there is no clear-cut critical temperature. When the temperature decreases, the peak becomes sharper and H_M decreases slightly, but the magnetization M at H_M remains roughly the same. Inelastic neutron-scattering (INS) studies[3] showed that there exists some magnetic correlations in these compounds, even when there is no long-ranged magnetic ordering, e.g., in $CeRu_2Si_2$. Since these correlations are quenched[3] close to the metamagneticlike transition, the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, which can[4] cause the correlations, is proposed by some authors[1,5] to be crucial for the transition.

Heavy-fermion compounds are characterized by a strong Coulomb repulsion at the impurity site, which can be enforced by forbidding double occupancy. The slave-boson method,[6] an exact treatment for this nonholonomic constraint, has been successfully applied to the system.[7] At the mean-field level, this method is able to produce many of the heavy-fermion properties except for the magnetic or superconducting ground states, which require the inclusion of higher-order fluctuations. In this paper we try to examine whether the quasiparticle interaction is crucial for the metamagneticlike transition. The existing mean-field equations,[6] obtained by a 1/(degeneracy) expansion of the slave-boson method for the periodic Anderson Hamiltonian, are employed and generalized to high magnetic field for a doublet ground state, which is common in the presence of the crystal field. When V is isotropic, we are able to solve the slave-boson mean-field equations[6] analytically and derive simple expressions for M and the Kondo temperature. For an anisotropic V, we numerically study the case with a doublet ground state and find two susceptibility peaks with their relative strength depending on the number of electrons participating in the hybridization per unit cell, n. Note that n includes the impurity f electron and is less than the total number of electrons in the unit cell because only those sheets of Fermi surface that cross the f-electron band can hybridize. Implications of this on the observed metamagneticlike transition and its related properties are discussed. In particular, the relative motion of different spin bands, which gives rise to two different conducting channels, is considered to reproduce the field dependence of the residual magnetoresistance. Note that, although we take the temperature to be zero in most of our calculations, the finite-temperature case can be easily considered.

II. MAGNETIZATION IN THE ISOTROPIC V CASE

Assuming a constant density of states for the bare conduction band ε_k, the standard slave-boson mean-field equations include[6]

$$n=\frac{1}{W}\int_{-W}^{W}d\varepsilon_k\frac{1}{4\pi}\int d\Omega[f(E_-)+f(E_+)]\,, \tag{1}$$

$$n_f=\frac{1}{W}\int_{-W}^{W}d\varepsilon_k\frac{1}{4\pi}\int d\Omega\left[\frac{\partial E_+}{\partial\varepsilon_k}f(E_-)+\frac{\partial E_-}{\partial\varepsilon_k}f(E_+)\right], \tag{2}$$

$$E_f+|E_0|=\frac{1}{W}\int_{-W}^{W}d\varepsilon_k\frac{1}{4\pi}\int d\Omega\,V^2(\theta,\phi)\frac{f(E_-)-f(E_+)}{E_+-E_-}\,, \tag{3}$$

where W is the conduction-band width, Ω is the solid angle at the azimuthal angles θ and ϕ, n_f is the mean f-electron occupation per impurity site, E_0 (E_f) is the bare (renormalized) f-electron one-body energy, $f(E)$ denotes the Fermi-Dirac distribution function, and the hybridized band energies are

$$E_{\pm}(\varepsilon_k,\theta,\phi) = \tfrac{1}{2}\{\varepsilon_k + E_f \pm [(\varepsilon_k - E_f)^2 + 4V^2(\theta,\phi)(1-n_f)]^{1/2}\} . \tag{4}$$

In the presence of an external magnetic field H, E_f becomes $E_f + mg\mu_B H$ for the doublet $m = \pm J$ and the right sides of the mean-field equations need to be averaged over m. In the above expression, J,g denote the total angular momentum and the Landé g factor of f electrons, and μ_B is the Bohr magneton. For convenience, we shall redefine $Jg\mu_B H$ as H.

For an isotropic hybridization matrix element, it has been shown[6] that the Kondo temperature, at zero field, equals

$$T_K(0) \approx W \exp\left[-\frac{W(\mu+|E_0|)}{V^2}\right] , \tag{5}$$

and the chemical potential μ can be determined by Eqs. (1) and (2) as

$$\mu = W(n-n_f-1) + O\left[\frac{V^2(1-n_f)}{W}\right] , \tag{6}$$

for all fields where, for an N-degenerate ground state, n is set equal to 2 (one conduction electron hybridizing with the one f electron). However, for $N=n$ the mean-field equations give the chemical potential lying in the hybridization gap and so heavy-fermion behavior is only found for $n < N$. In our case as $N=2$ we choose n to be *slightly*[8] less than 2. Note that W is the largest energy scale in the system (after the strong on-site repulsion is replaced by the no-double-occupancy constraint), and we shall neglect higher terms of order $(V/W)^2$, e.g., the second term in Eq. (6). As the field increases, μ always stays in the lower band for the $\downarrow$-spin electrons. But for the $\uparrow$-spin electrons, there are three regions that need to be distinguished. As shown in Fig. 1, μ initially lies in the lower band (region I); then it goes into the gap (region II) and eventually enters the upper band (region III) at large fields.

Numerical results for the isotropic case are shown in Fig. 2, in which E_f decreases much faster in region III than in regions I and II. Note that in region II, the hybridization gap is for the charge, not the spin, excitations, because, although the total number of electrons for each spin is fixed, the f electron can still transmute into the conduction electron, which has a smaller g value. But the transmution rate is very slow compared with the density-of-states effect in region III, and the magnetization curve in region II appears to be flat. These properties can be understood by the following analytic approximations.

For region I, it is straightforward to show that

$$1-n_f \approx \frac{T_K^2(0)}{T_K(H)}\frac{W}{V^2} , \qquad M \approx \frac{15}{7}\frac{H}{T_K(H)} , \tag{7}$$

for $J=\frac{5}{2}$ and $g=\frac{6}{7}$ (M is in units of μ_B) where

$$T_K(H) \equiv E_f - \mu \approx [T_K^2(0) + H^2]^{1/2} . \tag{8}$$

The crossover field at which μ enters region II is

$$H_{\mathrm{I,II}} \approx \frac{V^2}{W}(1-n_f)(2-n) \approx (2-n)T_K(0) . \tag{9}$$

Since $2-n$ is less than 0.2 for heavy-fermion compounds,[8] $T_K^2(0) \gg H_{\mathrm{I,II}}^2$ and $T_K(H) \approx T_K(0)$ in region I.

Similarly for region II, we obtain

$$1-n_f \approx T_K(0)\frac{W}{V^2} , \qquad M \approx \tfrac{15}{7}(2-n) , \tag{10}$$

$$T_K(H) \approx T_K(0) - H . \tag{11}$$

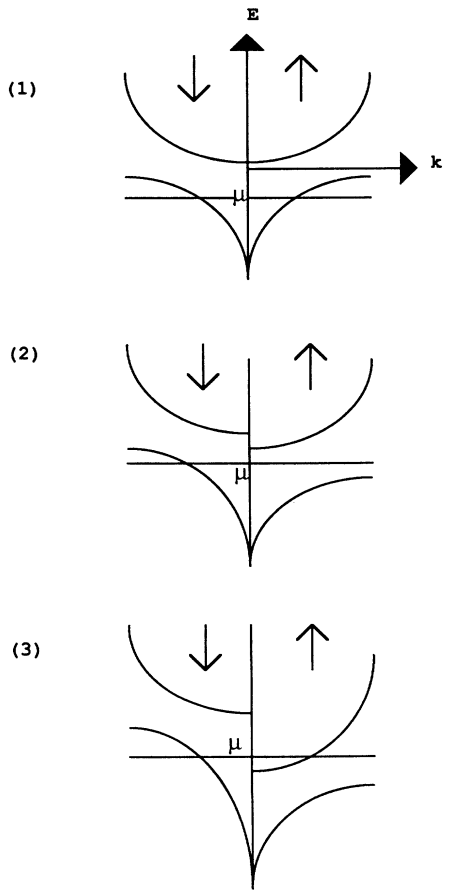

FIG. 1. Three regions are distinguished for the isotropic-V case, according to the relative position of the chemical potential to the dispersion bands (the $\uparrow$-spin bands are on the right).

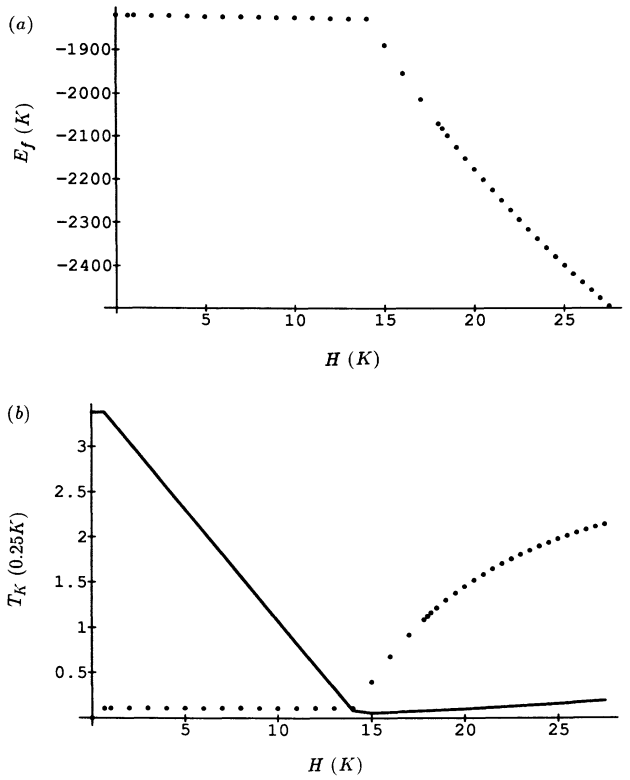

FIG. 2. Isotropic-V case: (a) Field dependence of E_f with $n=1.95$, $W=50\,000$ K, $V_0^2/W=1000$ K, $E_0=-10\,000$ K, and $T_K(0)=13.5$ K. (b) Field dependence of T_K (solid line) and $M(\mu_B)$ (dotted line). Critical fields for the crossover between regions are 0.7 and 14 K.

The critical field at which μ goes into region III equals

$$H_{\mathrm{II,III}} \approx \frac{V^2}{W}\frac{1-n_f}{n-1} \approx \frac{T_K(0)}{n-1} , \tag{12}$$

which, not surprisingly, is roughly $T_K(0)$ or half of the gap energy.

Finally, for region III,

$$1-n_f \approx (2-n)-\frac{|E_0|}{W}+\frac{V^2}{2W^2}\ln\frac{W^3}{V^2 T_k(H)} ,$$

$$M=\frac{15}{7}\left[1-(1-n_f)\frac{2HW/V^2}{[1+(2HW/V^2)^2]^{1/2}-1}\right] , \tag{13}$$

$$T_K(H)=\frac{1}{2}\left\{-\frac{V^2}{W}+\left[\left[\frac{V^2}{W}\right]^2+4H^2\right]^{1/2}\right\} . \tag{14}$$

Above the critical field

$$H^* \approx W\exp\left[-\frac{W(n-2)+|E_0|}{V^2/W}\right]$$

[note that this is equal to the $T_K(0)$ value in Eq. (5) for $n_f=1$], n_f approaches unity and the mean-field approximation breaks down.

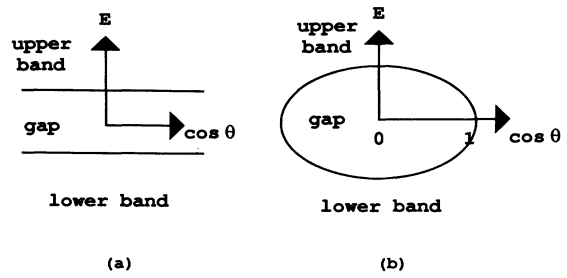

FIG. 3. (a) Energy bands for an isotropic V are plotted as a function of $\cos\theta$, where θ is the azimuth angle. (b) Same plot for an anisotropic $V(\theta)$ of the form in Eq. (15). The band gap centers at E_f (or $E_f \pm H$ in the presence of applied field), and its width equals $V^2(\theta)(1-n_f)/W$. The gap width in (b) is largest at $\cos\theta=0$ and vanishes at $\cos\theta=\pm 1$.

III. MAGNETIZATION IN THE ANISOTROPIC V CASE

For the $m=\pm\frac{5}{2}$ doublet ground state of the Ce-based compounds, it has been argued[9] that $V(\theta)$ assumes the anisotropic form

$$V(\theta)=\sqrt{(15/8)}V_0(1-\cos^2\theta) , \tag{15}$$

where θ is the azimuthal angle. The hybridization gap is plotted schematically in Fig. 3. It is hard to solve the mean-field equations analytically because of the complication caused by the angular averaging. There are in general four different regions as shown in Fig. 4. Results for small n values 1.6, 1.7, and 1.8 are plotted in Fig. 5. The susceptibility enhancement at the peak relative to the zero-field value is 1.31, 2.45, and 1.54 individually—strongest at $n=1.7$ as obtained by Ref. 9. The critical field $H_{c1}\approx T_K(0)$ corresponds to when μ *partially* enters the upper $\uparrow$-spin band except for $n=1.6$, for which H_{c1} situates before entering. Note that when n increases for the same energy parameters, as in Fig. 5(b), H_{c1} decreases, but $H_{c1}/T_K(0)$ increases [because $T_K(0)$ de-

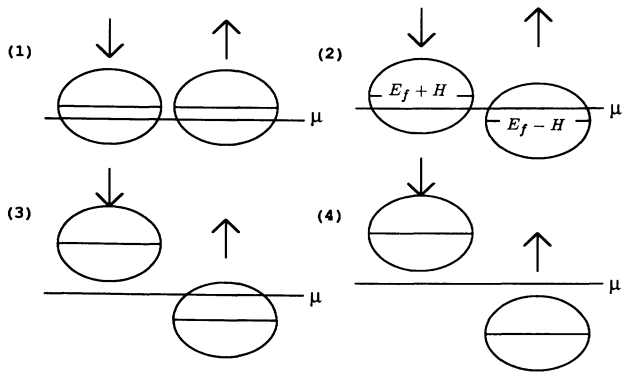

FIG. 4. As the field increases, different regions are distinguished according to the relative position of the chemical potential to different spin bands (the $\uparrow$-spin bands are on the right). The long horizontal line denotes the position of the chemical potential, and the short horizontal lines mark the centers for each spin gap.

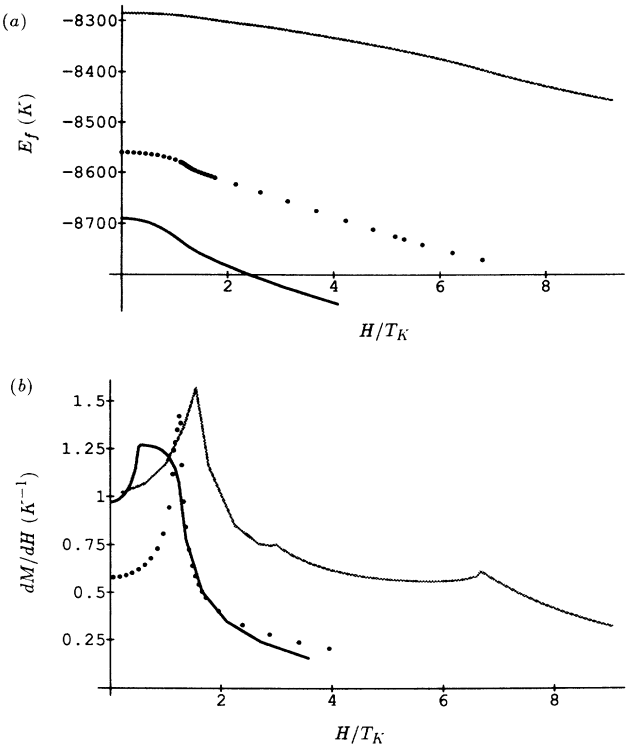

FIG. 5. For the anisotropic $V(\theta)$ defined in Eq. (15): (a) Field dependence of E_f for $n=1.6$ (solid line), 1.7 (dotted line), and 1.8 (grey line) with the same parameters: $W=50\,000$ K, $V_0^2/W=200$ K, $E_0=-10\,000$ K, and $T_K(0)=48.1$, 17.6, and 2.38 K individually. (b) Field dependence of the susceptibility which, for clarity, has been multiplied by 80, 26, and 10 for each n case.

creases faster with n]. For larger n values (we take $n=1.9$ and 1.95 in Fig. 6), the susceptibility enhancement at H_{c1} diminishes (1.22 and 1.09 individually), while a second susceptibility peak starts to appear at $H_{c2}=10T_K(0)-100T_K(0)$. The critical field H_{c2} corresponds to when μ *totally* enters the upper ↑-spin band. Since it is hard to determine n experimentally,[10] the choice of n is somewhat arbitrary. But experimentally[2] the magnitudes of the critical field and the Kondo temperature are roughly the same, and there is only one transition, so that H_{c1} in the small-n case seems to be a better candidate[11] for the real transition.

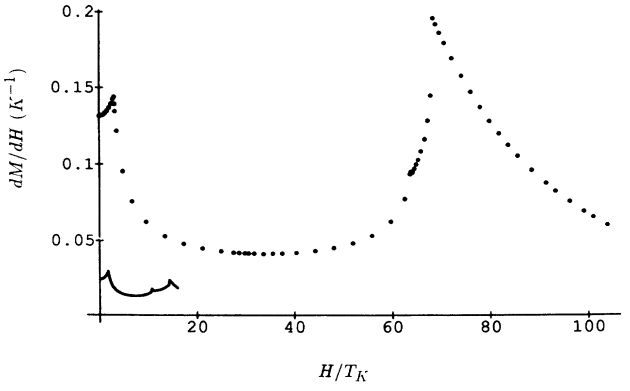

FIG. 6. Same plots as Fig. 5(b) with $V_0^2/W=1000$ K for $n=1.9$ [solid line, $T_K(0)=0.42$ K] and 1.95 [dotted line, $T_K(0)=4.81$ K].

IV. FIELD DEPENDENCE OF THE RESIDUAL MAGNETORESISTANCE

The magnetoresistance at low temperatures, $\rho_0(H)$, is observed[2] to have a higher saturation value than $\rho_0(0)$ [in contrast with the otherwise similar $\gamma(H)$ relation] in $CeRu_2Si_2$. This is consistent with the two-"band" (↑- and ↓-spin quasiparticles) nature of the system, which predicts[12] that

$$\frac{\rho_0(H)-\rho_0(H=0)}{\rho_0(H=0)} = \frac{\sigma_\uparrow\sigma_\downarrow(\beta_\uparrow-\beta_\downarrow)^2H^2}{(\sigma_\uparrow+\sigma_\downarrow)^2+H^2(\beta_\uparrow\sigma_\uparrow+\beta_\downarrow\sigma_\downarrow)^2}>0\ , \quad (16)$$

where σ denotes the conductivity. We define β by $\beta\equiv e\tau/(m^*c)$, where τ is the mean free time and m^* the effective mass of the quasiparticles. Both σ and β are inversely proportional to m^* and the density of states, D, at the chemical potential. Since the magnetization principally comes from the f electrons, assuming "rigid" bands,

$$\begin{aligned} &\frac{M(H+\Delta H)-M(H)}{2}\approx D_\uparrow(H)\Delta E_\uparrow=D_\downarrow(H)\Delta E_\downarrow\ , \\ &\Delta E_\uparrow+\Delta E_\downarrow=2\,\Delta H\ , \\ &D_\uparrow+D_\downarrow=\gamma\ , \end{aligned} \quad (17)$$

where ΔE is the energy shift of the chemical potential due to the field increment ΔH and γ denotes the linear temperature coefficient of the specific heat. We can then express D in terms of the susceptibility $\gamma(H)$ and $\chi(H)$ as

$$\begin{aligned} D_\uparrow&=\frac{\gamma}{2}\left[1+\left[1-\frac{\chi}{\gamma}\right]^{1/2}\right]\ , \\ D_\downarrow&=\frac{\gamma}{2}\left[1-\left[1-\frac{\chi}{\gamma}\right]^{1/2}\right]\ . \end{aligned} \quad (18)$$

Simple analyses show that Eq. (16) increases like H^2 initially and saturates at large fields to a constant value depending on χ/γ. Using the experimental data[13] for γ and χ/γ, we calculate Eq. (16) to obtain Fig. 7, which shows a maximum at $H_M=7.8$ T for $CeRu_2Si_2$ in line with the experiments.[2]

However, this $\rho_0(H)$ dependence is not found[14] in CeB_6, $CeAl_2$, and $CeCu_2$, which also exhibit a metamagneticlike transition. This is probably caused by their antiferromagnetic ordering at low temperatures, which becomes more important than the two-band effect; thus the magnetoresistance increases when small fields disrupt the antiferromagnetic ordering and drops at higher fields to a lower value than at zero field when spins eventually order ferromagnetically (since the ↑-spin electrons are not scattered).

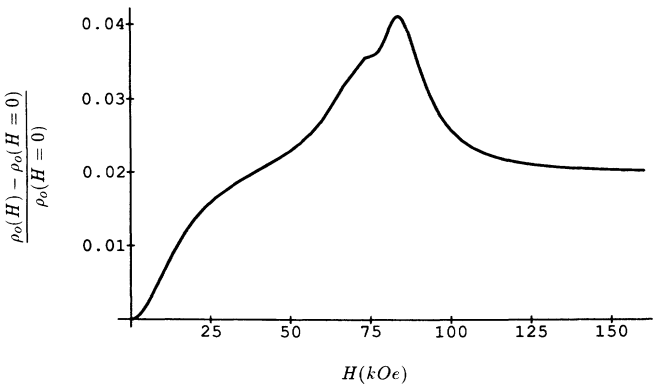

FIG. 7. Field dependence of the residual magnetoresistance for $CeRu_2Si_2$ by use of the two-band model (see text).

We have checked that the coexistence of heavy and light quasiparticles[15] in $CeRu_2Si_2$, as seen in the de Haas–van Alphen effects,[16] is unable to give the right $\rho_0(H)$ dependence. This is supported by the same experiments in $CeAl_2$, which also exhibits a metamagnetic behavior and an even wider distribution of masses,[16] but has the same $\rho_0(H)$ dependence[14] as in CeB_6. Note that[2] a positive magnetoresistance does not necessarily imply metamagnetic behavior, as is the case[14] for $CeCu_6$, because the ground-state degeneracy and the actual form of $V(\theta,\phi)$ are important to obtain the latter behavior. Alternatively, Haen *et al.* have proposed[2] the transition from nonmagnetic to magnetic impurities to be the cause.

V. OTHER TRANSITION-RELATED PROPERTIES

Experimentally,[2] the critical field is observed to increase slightly with finite temperature. This is in line with our calculations, for which, for the parameter ranges in Fig. 5, H_{c1} increases by 0.03% at $T=0.01$ K. From INS studies[3] the intrasite Kondo screening remains constant throughout the metamagnetic transition, while $\chi(H=H_M)$ follows[2] roughly a Curie-Weiss law. This is similar to previous numerical work[17] which shows that when the contribution to n_f from the upper hybridization band becomes appreciable at finite temperatures, χ behaves like a Curie-Weiss type, although n_f is still less than 1. We expect the same property in the magnetic-field case.

Further consistency comes from the pressure dependence of the magnetoresistance[18] which obeys the scaling behavior[19] at zero field, but becomes insensitive to pressure at the critical field, though relatively more sensitive at low pressures. The latter is expected because the critical fields, discussed in Sec. III, correspond to when μ either lies in the middle of the gap or totally leaves the gap region (for one of the spins). The density of states at those positions is least enhanced,[20] and therefore the pressure dependence via the state density is limited. Presumably, the over-spill states (in the gap), driven by higher-order fluctuations and thermally excited quasiparticle states, contribute to the weak dependence on low pressure. When the pressure increases, the gap widens up and these effects become less important.

VI. CONCLUSION

In conclusion, we have generalized the slave-boson mean-field equations to high magnetic fields and derived analytic expressions for T_K when the hybridization matrix element is isotropic. Using the anisotropic $V(\theta)$ for the $m=\pm\frac{5}{2}$ doublet ground state, we find two metamagmeticlike transitions with their relative strength depending on the number of electrons participating in the hybridization per unit cell. The identification of this to the experimentally observed transition can explain, as noted by Ref. 9, why the magnetization at the transition is insensitive to external conditions.[21] In addition, the relative motion of different spin bands can be used to reproduce the observed field dependence of the residual magnetoresistance. We also discuss the consistency of this mean-field picture with other transition-related properties. Note that we assume the antiferromagnetic correlations to play a passive role, which can be included, within the slave-boson approach, either by calculating higher-order fluctuations or via the depletion theorem of Nozières.[22] The suppression[3] of these antiferromagnetic correlations at high fields is regarded as *a consequence rather than a cause* of the transition. As several authors have emphasized,[5,9] the ferromagnetic functions while able to enhance the metamagnetic behavior, which subsequently shifts H_M to a lower value, do not trigger it. Although we have no convincing evidence for there being an incomplete hybridization gap, which is crucial to the above discussion, optical reflectivity[23] experiments in $CeCu_2Si_2$ (of the same tetragonal $ThCr_2Si_2$ structure as $CeRu_2Si_2$), UPt_3, and other heavy-fermion samples support such a view.

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*Permanent address: Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 30043, Republic of China.

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[20]*Except* when μ lies in the gap region, the angular averaging of the mean-field equations can be shown to be equivalent to replacing $V(\theta,\phi)$ by its root-mean-square value over the Fermi surface, V_0. When μ is about to leave the gap totally for the $V(\theta)$ in Eq. (15), the density of states at μ is small because it lies at the edge of the gap with $V(\theta=\pi/2)=(15/8)V_0$, while the resonance peak is only roughly of width for $V=V_0$.

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