Spin-flip scattering of critical quasiparticles and the phase diagram of YbRh_{2}Si_{2}

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Spin-flip scattering of critical quasiparticles and the phase diagram of $YbRh_2Si_2$

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Several observed transport and thermodynamic properties of the heavy-fermion compound $YbRh_2Si_2$ in the quantum critical regime are unusual and suggest that the fermionic quasiparticles are critical, characterized by a scale-dependent diverging effective mass. A theory based on the concept of critical quasiparticles scattering off antiferromagnetic spin fluctuations in a strong-coupling regime has been shown to successfully explain the unusual existing data and to predict a number of so far unobserved properties. In this paper, we point out a new feature of a magnetic field-tuned quantum critical point of a heavy-fermion metal: anomalies in the transport and thermodynamic properties caused by the freezing out of spin-flip scattering of critical quasiparticles and the scattering off collective spin excitations. We show that a step-like behavior as a function of magnetic field of *e.g.* the Hall coefficient and magnetoresistivity results, which accounts quantitatively for the observed behavior of these quantities. That behavior has been described as a crossover line $T^*(H)$ in the $T-H$ phase diagram of $YbRh_2Si_2$. Whereas some authors have interpreted this observation as signaling the breakdown of Kondo screening and an associated abrupt change of the Fermi surface, our results suggest that the T^* line may be quantitatively understood within the picture of robust critical quasiparticles.

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I. INTRODUCTION

Quantum phase transitions in heavy-fermion compounds have attracted considerable interest over the last two decades. These systems exhibit deviations from the standard Fermi-liquid description of metals, as a consequence of the interaction of the fermionic (Landau) quasiparticles with bosonic critical spin fluctuations. The existence of phase transitions in these systems was proposed early on by Doniach[1], who argued that the competition of Kondo screening of the local moments and the (RKKY) interaction between them should lead to a quantum phase transition separating a paramagnetic from a (usually) antiferromagnetic phase. A full explanation of just how this happens is still lacking (for a review see Ref. 2). Therefore the discovery of a well-accessible quantum-critical regime in some heavy-fermion compounds has generated a good deal of research activity. In particular, $YbRh_2Si_2$ (YRS), which has a magnetic field-tuned quantum phase transition, has been studied extensively. Motivated by experimental observations of deviations from conventional quantum-critical behavior[2] at very low temperature in YRS, we have previously considered the interplay of fermionic (quasiparticle) and bosonic (spin fluctuations) critical behaviors and shown how this leads to *critical quasiparticles* with unconventional behavior in the critical region.[3] The behavior of several of the transport and thermodynamic properties in the critical regime were successfully accounted for on the basis of the critical quasiparticle theory, both in YRS[3,4] and $CeCu_{6-x}Au_x$.[5] In addition to the unconventional behavior in YRS as $T \to 0$, a crossover behavior in the Hall constant[6] and several other quantities[7] was observed along a line $T^*(H)$ in the temperature (T) - magnetic field (H) phase diagram, with the crossover width scaling as T. This T^* line begins at relatively high (T, H), monotonically decreases with decreasing magnetic field and apparently ends at the quantum critical point (QCP), which is accessed by tuning H to the critical field $H_c \approx 0.06$ T. A number of authors have interpreted this crossover as a signature of the breakdown of Kondo screening and a concomitant change of the Fermi surface[8–10].

In this paper, we propose an alternative explanation for the T^* line that is based on the theory[3,4] of well-defined critical quasiparticles with robust Kondo screening. The theory was originally developed for disordered systems, in which impurity scattering serves to distribute to the entire Fermi surface the critical renormalization of the quasiparticle effective mass. This results from interaction with antiferromagnetic spin fluctuations that in the pure case is important only at "hot spots" on the Fermi surface. Later, it was shown that exchange of pairs of AFM spin fluctuations, (*i.e.* energy fluctuations), carrying small total momentum leads to critical quasiparticles even for clean systems.[5] In both cases, there results scaling behavior of the free energy and transport properties that is characterized by fractional power laws in temperature and in the tuning parameter. In addition to the strong-coupling regime, the theory also applies in the conventional spin-density wave weak-coupling regime. In renormalization group language, the theory has two stable fixed points, at weak and at strong coupling. Thus, depending on the initial conditions at the temperature where the scaling towards lower temperatures begins, the system flows either to the weak-coupling or to the strong-coupling fixed point. The predictions of this the-

ory in the strong-coupling regime were found to be in excellent agreement with all available experimental data in cases where the system possesses additional fluctuations enhancing the effective mass in a singular way. In the case of $YbRh_2Si_2$, three-dimensional ferromagnetic fluctuations have been identified, leading to a logarithmic increase of the effective mass in temperature (which is weaker than the power-law increase eventually resulting from the strong-coupling theory of three-dimensional antiferromagnetic fluctuations at low T).

We argue here that the thermal activation of spin-flip excitations of critical quasiparticles in a non-zero magnetic field leads to a threshold behavior of transport properties as a function of magnetic field at fixed temperature. There are actually two types of processes contributing to this threshold behavior, which defines a crossover $T^*(H)$, Near the QCP, the switching on of spin-flip scattering leads to a step-like feature in the imaginary part of the critical component of the quasiparticle self energy [at a temperature $T_1^*(H)$], which by analyticity carries over to the real part and hence to the thermodynamic properties. The properties of this T_1^* line mirror those of the experimentally determined $T^*(H)$ line near the QCP. As we show below, the T_1^* line approaches the QCP following a fractional power law. In the temperature regime for which data are available at present, the asymptotic low temperature behavior has not yet been reached. Nonetheless, an evaluation of the T_1^* line using the available thermodynamic data approaches the QCP almost vertically in the $T-H$ phase diagram, as apparently observed for $T^*(H)$. This effect arises as a consequence of the unusual renormalization of the bare single quasiparticle Zeeman splitting $h_0 = g\mu_B H$. As we explain below, the magnetic field is screened by the Fermi liquid interaction, such that $h_0 \to h = R_{nl} h_0$, where $R_{nl}(T,H)$ is a generalized Wilson ratio (in the limit $H \to 0$, $R_{nl} \to R$, where R is the usual Wilson ratio). This renormalization of the Zeeman splitting played an important role in the interpretation of the linewidth of electron spin resonance (ESR) in YRS,[11,12] in that it increases the low temperature linewidth in the Fermi liquid regime by two orders of magnitude, in agreement with experiment.[13] Since the Wilson ratio R is found to tend to zero upon approaching the QCP, the renormalized Zeeman splitting of the quasiparticle energy is predicted to nearly vanish (the observed finite response to a magnetic field is accounted for by the noncritical, nonquasiparticle contribution). Consequently, the thermal energy required to flip the spin nearly vanishes as $H \to H_c$ and $T \to 0$, leading to a threshold anomaly at $T_1^*(H)$ the width of which goes to zero as well. At higher T the anomaly is rapidly washed out.

There exists, however, a second type of spin-flip excitation, the collective excitation observed in ESR experiments.[13,14] This excitation has also been seen in inelastic neutron scattering experiments.[15] The condition of thermal energy being equal to the ESR energy quantum ω_r defines a line $T_2^*(H)$ which we find coincides with the experimentally determined T^* line at higher T, H. At lower field the T_2^* line crosses the critical field at a non-zero temperature and therefore with a non-zero width. We therefore find a crossover behavior near the point where $T_1^*(H)$ and $T_2^*(H)$ meet.

In Sec. II, we review the reasons leading to a renormalization of the single-particle Zeeman splitting. In Sec. III, we calculate the imaginary part of the self energy of the critical quasiparticles and derive the threshold behavior at the line $T_1^*(H)$. This allows an approximate calculation of a step-like feature in the magnetoresistivity in Sec. IV and in the Hall coefficient in Sec. V, which is compared with experiment. Then we deduce the real part of the self energy using analyticity arguments, and therefore the quasiparticle weight factor Z. The effective mass ratio obtained from the relation $m^*/m = 1/Z$ allows the identification, in Sec. VI, of a step-like feature in the magnetic-field dependence of the specific heat and other thermodynamic quantities.

In Sec. VII, we calculate the contribution of thermal excitation of the ESR spin resonance to the imaginary part of the self energy. Using analogous arguments as in Sec. II, we derive the threshold contributions to the transport quantities along a line $T_2^*(H)$, defined by the scattering off the spin resonance.

We collect the results in Sec. VIII and compare the theoretically determined $T^*(H)$ line with the published experimentally-determined $T^*(H)$ and find excellent agreement.

We summarize our findings in Sec. IX and give a critical evaluation of the interpretation of the T^* line as corroborating the picture of critical quasiparticles

II. RENORMALIZATION OF THE ZEEMAN SPLITTING

A. Fermi liquid theory

The single particle Green's function in a magnetic field has the form

$$G_\sigma(k,\omega;H) = \frac{1}{\omega - \epsilon_k + \sigma h/2 - \Sigma_\sigma(k,\omega;H)} \qquad (1)$$

Here $h = R_{nl} h_0$ and $h_0 = g\mu_B H$ where R_{nl} is the renormalized Wilson ratio formulated as follows: The external field is screened by the molecular field $h_0 \to h_0(1 - f^a M/H)$, where $M = \sum_\sigma \int d\omega \int d^d k (2\pi)^{-d} \sigma G_\sigma(k,\omega;H)$ is the spin polarization and f^a is the (Landau quasiparticle) spin exchange interaction. In this paper, we consider a three-dimensional metal, with critical fluctuations also in $d = 3$. In the limit $H \to 0$, or more generally, if M is linear in H, we have $M = \chi H$. Using the Fermi liquid expression for the spin susceptibility[16] (in appropriate units) $\chi = \partial M/\partial H = N_0^*/(1+F^a)$, where $F^a = N_0^* f^a$ is the Landau parameter in the spin channel

and N_0^* is the quasiparticle density of states, we then get $h = h_0/(1+F^a) = Rh_0$, where $R = \chi/N_0^* = 1/(1+F^a)$ is the usual Wilson ratio. Now, in the case of non-zero magnetic field $R_{nl} = 1 - f^a\chi b$, where $b = (M/H)/\chi$. Here $\chi = \partial M/\partial H$ is the differential susceptibility at finite field H. Expressing $f^a\chi = F^a/(1+F^a) = 1-R$, we finally get

$$h = h_0[1 + (R-1)b] = h_0 R_{nl} \tag{2}$$

The static screening changes the applied field h_0 to h everywhere, so that we shall use the screened field in place of the bare field from now on. The screening factor R_{nl} (nl stands for "nonlinear screening") is expressed in terms of the Wilson ratio R and b, the ratio of nonlinear and differential susceptibility. Here, $R = \alpha_R \chi T/C$, with $C/T = \gamma$, the specific heat coefficient, $\alpha_R = (2\pi k_B/3g\mu_B)^2$, and $g = 3.6$ is the g-factor. The experimental data show that $b > 1$, always. and $b(H)$ is an increasing function of H, since the slope of $M(H)$ becomes smaller for increasing $H - H_c$. The nonlinearity of M thus weakens the increase of R with decreasing field towards H_c .

Expanding the dynamic part of the self energy at small ω and defining the quasiparticle (qp) Z-factor as $Z^{-1} = [1 - \partial\Sigma(k,\omega;0)/\partial\omega]$, we find

$$G_\sigma(k,\omega;h) = \frac{Z}{\omega - \epsilon_k^* + Z_{h\sigma}(\sigma h/2) + i\Gamma}, \tag{3}$$

where $\Gamma = Z\mathrm{Im}\Sigma$ and

$$Z_{h\sigma} = \frac{1 - \sigma[\Sigma_\uparrow(k,0;h) - \Sigma_\downarrow(k,0;h)]/h}{[1 - \partial\Sigma(k,\omega;0)/\partial\omega]_{\omega=0}} \tag{4}$$

$$\epsilon_k^* = Z[\epsilon_k + \frac{1}{2}(\Sigma_\uparrow(k,0;h) + \Sigma_\downarrow(k,0;h))] \tag{5}$$

In the limit of $h \to 0$ we may use the relation

$$\lim_{h\to 0} 2\sigma\partial\Sigma_\sigma(k,0;h)/\partial h = \lim_{\omega\to 0}\partial\Sigma(k,\omega;0)/\partial\omega, \tag{6}$$

to find $Z_{h\sigma} = 1$. So, the coupling of qp spins to the external field is only renormalized by the molecular field. This is in accord with the statement that Landau quasiparticles have the same quantum numbers as bare particles, and therefore the qp spin is a conserved quantity.

B. Renormalization of the Zeeman splitting of critical quasiparticles near a field-tuned QCP

The above relation of the two derivatives of the self energy with respect to h and ω does not hold generally in non-zero magnetic field. This can be seen by analyzing any diagram of the self energy $\Sigma_\sigma(\omega)$ in terms of bare Green's functions in the following way: there is always exactly one string of Green's functions $G_\sigma(k_j, \omega - \omega_1 - ...) = (\omega + \sigma h/2 - \omega_1 - ... - \epsilon_{k_j})^{-1}$ (carrying the external spin label) connecting beginning and end of the diagram. In those Green's functions a shift of magnetic energy σh is equivalent to a shift of ω . All other Green's functions belong to closed loops in which the spin index is summed over. The closed loop contributions are then necessarily functions of H^2. In the limit $H \to 0$ those H^2 corrections drop out. Hence in this limit the relation Eq. (6) holds. At non-zero field the H^2 corrections are not negligible (although they may be small of $O(H/\epsilon_F)^2$, where ϵ_F is the Fermi energy) and Eq. (6) does not hold in general. However, near the critical field h_c the derivative $\partial\Sigma_\sigma(k,0;h)/\partial h$ is critically enhanced. As suggested in Ref. 5, the vertex function corresponding to the derivative $\partial\Sigma_\sigma(k,0;h)/\partial h$ is enhanced $\propto 1/Z$, diverging at the QCP just like $\partial\Sigma(k,\omega;0)/\partial\omega$. Therefore, the relation Eq. (6) still holds, as far as the critical contributions are concerned, and, as explained in the previous subsection, we have

$$h = R_{nl} h_0 + h_{reg}. \tag{7}$$

In the following we shall drop the regular contribution h_{reg}, since it vanishes at the critical point faster than the first contribution, at least $\propto Z^2$.

The relation of the renormalized Zeeman splitting h to the magnetic field H is somewhat involved and in general may not be expressed as a simple functional relationship. Near the QCP of YRS, however, we may use the result[4] $Z^{-1} \propto (H - H_c)^{1/3} \propto h$, from which follows $T^*(H) \propto (H - H_c)^{2/3}$ as the asymptotic form of the T^* line. At the temperatures for which data are available, the behavior of the magnetic susceptibility, in particular, as a function of T, H is not well-represented by a simple scaling form. It is then more reliable to use directly the available experimental information on the specific heat coefficient $\gamma(T,H)$ (see Ref. 17), the differential spin susceptibility $\chi(T,H)$ (see Refs. 18–21), and the magnetization $M(T,H)$ (see Refs. 20, 22, and 23) to determine the quasiparticle Zeeman splitting $h(T,H)$. In this way one may derive a parameter-free representation of the Zeeman splitting. In Fig. 1 we show results for $h(T,H)$ versus magnetic field H at four selected temperatures $T = 18, 38, 65, 100$ mK, for which magnetoresistivity data,[24] Sec. IV below, are available. The $T = 18$K data is shown as the purple line while the other three temperatures give similar results, as shown. Also shown is the bare Zeeman splitting $h_0(H)$. One can see that h is substantially enhanced by the ferromagnetic molecular field. At these temperatures the asymptotic behavior $h \propto (H - H_c)^{1/3}$ mentioned above is not yet seen. It is masked by the relatively strong increase of the spin susceptibility towards lower fields (at these low temperatures critical antiferromagnetic spin fluctuations dominate and χ eventually reaches its asymptotic $T = 0$ limiting value).

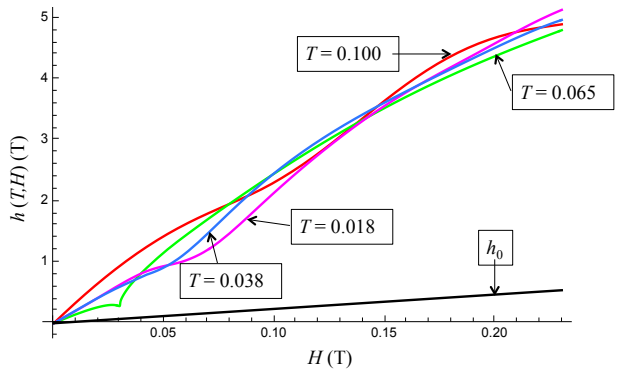

FIG. 1. Renormalized Zeeman splitting $h(T,H)$ at various T, in degrees K. The unrenormalized Zeeman splitting h_0 is also shown. The magnetic field unit is Tesla and the temperatures are in Kelvin.

III. THRESHOLD BEHAVIOR OF SPIN FLIP SCATTERING OF SINGLE QUASIPARTICLES: SELF ENERGY

Since the differential spin susceptibility χ and the magnetization M both approach a constant finite value at the QCP, and since the specific heat coefficient C/T as well as Z^{-1} diverge as $T^{-1/4}$ (in 3d - for 2d AFM fluctuations, see Ref. 5), h is seen to nearly vanish at the QCP (more precisely, $h/h_0 = 1-b$ at the QCP, which is a very small quantity). In one-loop approximation of the self energy the most important effect of Zeeman splitting is from the intermediate quasiparticle line (straddled by a fluctuation propagator). The effect on the AFM spin fluctuation propagator is small (h does not enter the Landau damping term in lowest order).

Let us then look at the self energy expression (due to coupling to magnetic energy fluctuations, as in Ref. 5):

$$\mathrm{Im}\Sigma_\sigma(k,\omega) \approx \lambda_E^2 \sum_{\sigma'} \int (d\mathbf{q}) \int_{-\infty}^{\infty} d\nu F(\nu,\omega) \times \mathrm{Im}\chi^E_{\sigma\sigma'}(\mathbf{q},\nu)\mathrm{Im}G_{\sigma'}(\mathbf{k}+\mathbf{q},\nu+\omega) \quad (8)$$

where $F(\nu,\omega) = f(\nu+\omega)+b(\nu)$ and $f(\omega) = 1/(e^{\omega/T}+1)$ and $b(\omega) = 1/(e^{\omega/T}-1)$. The energy fluctuation spectrum is given by (see Ref. 5):

$$\mathrm{Im}\chi^E(\mathbf{q},\omega) \propto \frac{\omega(|\omega|/Z^2)^{3/2}}{(q^2+\xi^{-2}+|\omega|/Z^2)^2} \quad (9)$$

The wavevector $\mathbf{q}$ and the inverse correlation length ξ^{-1} are in units of the Fermi wavenumber k_F and the fluctuation energy ω as well as all other energies (T,h) in units of the Fermi energy ϵ_F, of the heavy quasiparticle band of YRS, approximately 10 K. The decisive effect of the Zeeman splitting is on the result of the angular integration over $\mathbf{q}$ in Eq. (8).

$$\begin{aligned} &\int \frac{d\Omega_q}{4\pi} \mathrm{Im}G_{\sigma'}(\mathbf{k}+\mathbf{q},\omega) \\ &\approx \int \frac{d\Omega_q}{4\pi} Z\delta(\omega - \epsilon^*_{k\sigma'} - v_F^* q\cos\theta) \\ &= \frac{Z}{v_F^* q}\theta(v_F^* q - |\omega - \epsilon^*_{k\sigma'}|) \end{aligned} \quad (10)$$

where $v_F^* = Zv_F$ and v_F are the quasiparticle and bare Fermi velocities. We need $\mathrm{Im}\Sigma_\sigma(k,0)$ at the Fermi energy, *i.e.* $\epsilon^*_{k\sigma} = 0$ and $\epsilon^*_{k\sigma'} = h(\sigma'-\sigma)/2$. Also, $\omega \ll v_F^* q$, as may be seen from the structure of $\mathrm{Im}\,\chi^E(\mathbf{q},\omega)$, so that ω may be dropped in Eq. (10). We now see that the non-spinflip term $\sigma' = \sigma$ gives rise to half of the contribution we had previously (at $H=0$). The spin-flip term, however, has the additional constraint on the q-integration $v_F^* q > |h|$. The q-integral of the spin flip term in Eq. (8) may be approximated by $\Phi(\omega;\xi,T,h)$ defined as

$$\begin{aligned} \Phi(\omega;\xi,T,h) &= \int q^2 dq\, \mathrm{Im}\chi_E(q,\omega)\frac{1}{v_F q}\theta(v_F^* q - h) \\ &\approx Z^{-3}\int \frac{(qdq)\omega^{5/2}}{(q^2+|\omega|/Z^2)^2}\theta(q^2 - h^2/Z^2 v_F^2) \\ &\approx \frac{\omega|\omega|^{3/2}}{Z^3}\left[\frac{\theta(|\omega|-h^2)}{|\omega|/Z^2} + \frac{\theta(h^2 - Z^2 - |\omega|)}{h^2/Z^2}\right] \end{aligned} \quad (11)$$

where $\theta(x)$ is the unit step function and we have taken $\xi \to \infty$, since we restrict ourselves to the critical region We use this result in Eq. (8) to obtain

$$\begin{aligned} \mathrm{Im}\Sigma^{cr}_\sigma(\omega) &\approx \lambda_E^2 \int_{-\infty}^{\infty} d\nu F(\nu,\omega)[\Phi(\nu;T,0) + \Phi(\nu;T,h)] \\ &\approx a_s T^{3/4}[K(0,\omega/T) + K(u/T,\omega/T)], \end{aligned} \quad (12)$$

where $u = h^2/\epsilon_F$ and we defined a function $K(z,y)$ describing the scaling behavior as the magnetic field and the energy ω is varied as follows:

$$K(z,y) = I(z,y)/I(0,0) \quad (13)$$

$$I(z,y) = I_{3/2}(z,y) + [I_{5/2}(0,y) - I_{5/2}(z,y)]/z \quad (14)$$

$$I_\mu(z,y) = \int_z^\infty dx F(x,y) x^\mu \quad (15)$$

where the thermal factor $F(x,y)$ is defined below Eq. (8). We also used $\lambda_E \propto Z^{-3}$ and we approximated Z by $Z(\omega=0;\xi\to\infty,T,H) = \mathrm{const.}(T/T_0)^{1/4}$. In Eq.(12), a_s is a phenomenological parameter which may be determined, *e.g.*from a fit to the specific heat coefficient as a function of T at the critical field.

The function $K(h^2/\epsilon_F T,0)$ drops monotonically with increasing h, in a step-like fashion. The step width scales with temperature T. This means that the spin flip term shows threshold behavior as a function of h at $h \approx (\epsilon_F T)^{1/2}$. As mentioned above, the dependence of h on magnetic field does not follow a simple functional

form, so that the T^* line has to be determined numerically.

In the following we will use the above result for the self energy to determine the contribution of qp spin-flip scattering to several of the quantities for which a threshold behavior as a function of H has been observed. In particular we will give a detailed comparison of the magnetoresistance and Hall coefficient data with our theoretical result.

IV. MAGNETORESISTIVITY

The magnetoresistivity $\rho(T,H)$ is determined by the quasiparticle scattering rate due to impurities $1/\tau^{imp}$ and that due to scattering off the critical fluctuations $1/\tau^* = Z(\omega)\mathrm{Im}\Sigma(\omega)$. At low enough temperature, impurity scattering dominates. We obtain $\rho(T,H)$ from the Kubo formula for the conductivity by expanding in the small quantity $\tau^{imp}/\tau^* \ll 1$ as follows (f is the Fermi function):

$$\rho(T,H)-\rho(0,H)) = \left[\sum_\sigma \int d\omega \frac{\partial f}{\partial \omega}\frac{N_0^*(\omega)v_F^{*2}(\omega)(\tau^{imp})^2}{\tau^*(\omega)}\right] \times \left[\sum_\sigma \int d\omega \frac{\partial f}{\partial \omega} N_0^*(\omega)v_F^{*2}(\omega)\tau_{imp}\right]^{-2} = a\sum_\sigma \int d\omega \frac{\partial f}{\partial \omega}\mathrm{Im}\Sigma_\sigma(k,\omega) \quad (16)$$

where the renormalized density of states $N_0^*(\omega) = N_0/Z$, the Fermi velocity $v_F^* = v_F Z$, and the qp relaxation rate $1/\tau^* = Z\mathrm{Im}\Sigma$, so that $N^*(\omega)v_F^{*2}(\omega) \propto Z(\omega)$, cancelling the factor of Z in $1/\tau^*$, the quasiparticle relaxation rate (and we neglect a contribution from vertex corrections, which may be assumed to change only the prefactor).[3–5] Using Eq. (12) for $\mathrm{Im}\Sigma$ and scaling out the overall T-dependence, we find

$$\rho(T,H)-\rho(0,H) \approx a(m/e^2N_0)T^{3/4}L(u/T) \quad (17)$$

$$L(z) = \int_0^\infty dy \frac{K(0,y)+K(z,y)}{\cosh^2(y/2)}, \quad (18)$$

where a is a constant to be adjusted. In Sec. IIB, we found the renormalized Zeeman splitting h numerically from the available experimental data (see Fig. 1). It enters the functions $K(z,y)$, Eq. (13) which determine the magnetoresistivity. Substituting the found renormalized Zeeman splitting into the expression for the magnetoresistivity, we have evaluated Eq. (17) for four temperatures $T = 18, 38, 65$, and 100 mK for which data are available. In Fig. 2, we compare our results with the data for sample #1 of Friedemann et al.[24] Here, assuming an analytic dependence of the impurity scattering rate on the magnetic field, we approximated the magnetic field dependence of the background resistivity by $\rho(0,H)) = c_1 + c_2H^2$, assuming an analytic dependence of the impurity scattering rate on the magnetic field. The characteristic energy $u = h^2/\epsilon_F$, where $\epsilon_F \approx 10$K and h is obtained from Eq. (2), as shown in Fig. 1. The remaining unknown parameter set $\{a \approx 1\mu\Omega\mathrm{cm}, c_1 \approx 0.9\mu\Omega\mathrm{cm}, c_2 \approx 0.5\mu\Omega\mathrm{cm/T}^2\}$ was chosen to give the best fit to the data for all the temperatures chosen. As one can see, the experimental data are described quite well by the theory, with the single set of parameters. The width of the step ΔH is found to approximately scale with T .

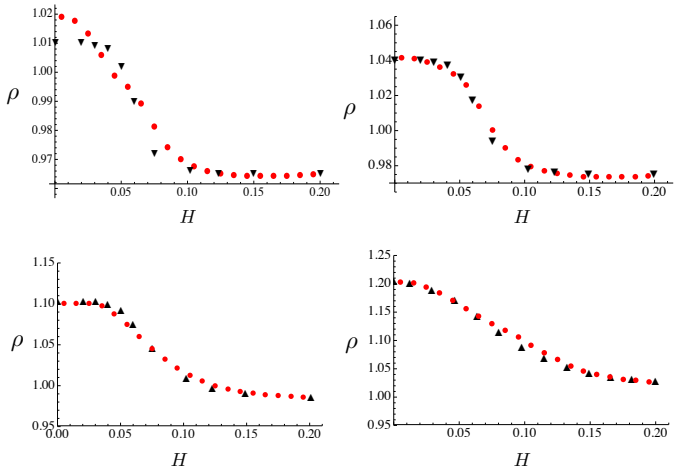

FIG. 2. Magnetoresistivity $\rho(T,H)$ at various T. Clockwise from upper left, $T = 18, 38, 65$ and 100 mK. H in Tesla and ρ in $\mu\Omega$-cm. Dots are theory, Eq. (17); triangles are from the data, Ref. 24

The agreement of our simplified model calculation with experiment is remarkable, considering that we have adopted a number of approximations, including the neglect of the H-dependence of Z (assuming that the magnetic field region considered here lies completely inside the critical regime, and neglect of the difference of effective masses of spin $(\uparrow,\downarrow)$-quasiparticles.

V. HALL COEFFICIENT R_H

Electronic structure calculations,[25] in particular within the "renormalized band theory," *i.e.* taking the Kondo resonance scattering at the Yb ions into account,[26] have revealed two relevant bands involved in transport, one of particle, the other of hole character. As a consequence, substantial compensation is observed in the Hall coefficient data, leading to small values of R_H and an enhanced sensitivity to disorder.[6,24,26] The Hall coefficient is given in terms of the partial Hall (σ^j_{xyz}) and longitudinal (σ^j_{xx}) conductivities of the two bands ($j = 1, 2$) as[26]

$$R_H(T,H) = \frac{\sum_{j=1,2}\sigma^j_{xyz}}{(\sum_{j=1,2}\sigma^j_{xx})^2} \quad (19)$$

where

$$\sigma^j_{xyz} = \sum_{\mathbf{k}} \tau^{*2}_{\mathbf{k},j} u^*_{\mathbf{k},xy,j} \left(\frac{\partial f}{\partial \epsilon^*_{\mathbf{k}j}} \right) \quad (20)$$

$$\sigma^j_{xx} = \sum_{\mathbf{k}} \tau^*_{\mathbf{k},j} v^{*2}_{\mathbf{k},x,j} \left(-\frac{\partial f}{\partial \epsilon^*_{\mathbf{k}j}} \right) \quad (21)$$

Here $u^*_{\mathbf{k},xy,j} = [v^*_{\mathbf{k},x,j} v^*_{\mathbf{k},x,j} M^{*-1}_{yx,j} - v^{*2}_{\mathbf{k},x,j} M^{*-1}_{yy,j}]$, and $v^*_{\mathbf{k},x,j}$ and $M^{*-1}_{yx,j}$ are the x-component of the quasiparticle velocity and the yx-component of the inverse quasiparticle mass tensor of the j-th band (as earlier, the asterix indicates the quasiparticle renormalization). As in the case of the magnetoconductivity, we use the fact that the inelastic scattering from critical fluctuations gives only a small contribution to the scattering rate, thus allowing expansion in the small parameter $\tau^{imp}_{\mathbf{k}j}/\tau^*_{\mathbf{k}j}$:

$$\begin{aligned} \Delta\sigma^j_{xyz}(T,H) &= 2\sum_{\mathbf{k}} \frac{(\tau^{*imp}_{\mathbf{k},j})^3}{\tau^{*inel}_{\mathbf{k}j}} u^*_{\mathbf{k},xy,j} \left(\frac{\partial f}{\partial \epsilon^*_{\mathbf{k}j}} \right) \\ &\propto (N_0 v_F^2/m)(\tau^{imp}_j)^3 u_j \\ &\times \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) \mathrm{Im}\Sigma_j(\omega) \end{aligned} \quad (22)$$

where $\Delta\sigma^j_{xyz}(T,H) = \sigma^j_{xyz}(T,H) - \sigma^j_{xyz}(0,H)$. Here, we have used $u^*_{\mathbf{k},xy,j}(\partial f/\partial \epsilon^*_{\mathbf{k}j}) \to u_j (v_F^2/m) Z_j^2(\omega)(\partial f/\partial\omega)$, and have accounted for band structure effects in an average way by the dimensionless factor $u_j \lesseqgtr 0$. We recall that the impurity relaxation rate in the case of unitary scattering (which we assume to be dominant) is renormalized as $1/\tau^{*imp}_{\mathbf{k}_F,j} \propto Z(\omega)/\tau^{imp}_{\mathbf{k}_F,j}$. In the critical regime, using the results obtained for $Z(\omega)$ and $\mathrm{Im}\Sigma(\omega)$ for YRS in the regime dominated by three-dimensional antiferromagnetic fluctuations[5] we may scale out the temperature dependence by using $Z_j(\omega) \propto |\omega|^{1/4}$ and $\mathrm{Im}\Sigma_j(\omega) \approx \gamma_j |\omega|^{3/4}$, $\gamma_j > 0$. As mentioned above, both data and theory suggest that the Hall coefficient $R_H(0,H)$ at $T = 0$, and therefore $\sigma_{xyz}(0,H) = \sum_j \sigma^j_{xyz}(0,H)$, are rather small, as particle and hole contributions almost compensate. The temperature- dependent contribution may be approximated as

$$R_H(T,H) = [\rho(T,H)]^2 [\sigma_{xyz}(0,H) + \sigma'_{xyz}(T,H)], \quad (23)$$

where, using Eq. (22),

$$\begin{aligned} \sigma'(T,H) &= \sum_j \Delta\sigma^j_{xyz}(0,H) \\ &= a'_H \frac{n(\tau^{imp})^3 b}{m^2} T^{3/4} L(u/T). \end{aligned} \quad (24)$$

$L(z)$ was defined in Eq. (18). Here the dimensionless quantity $b \propto (b_1\gamma_1 + b_2\gamma_2)$, with $b_1 > 0$ (particles) and $b_2 < 0$ (holes) describes the extent of compensation. We note that in the extreme limit of low temperature, when the inelastic component of σ^j_{xx} may be neglected, such that the denominator of Eq. (19) may be replaced by $[\rho(0,H)]^{-2} \propto (\tau^{imp})^2$, two powers of τ^{imp} in Eq.(22) are cancelled and the T-dependent contribution to R_H scales with disorder strength as $\Delta R_H = R_H(T,H) - R_H(0,H) \propto \tau^{imp}$.

For the numerical evaluation of Eq.(23), we used again a parameterization of the impurity scattering contribution of the form $\sigma_{xyz}(0,H) = c_{H1} + c_{H2}H^2$ and defined $a_H = a'_H n(\tau^{imp})^3 u/m^2$. In Fig. 3, we show a comparison of the calculated R_H curves with experimental data,[24] again choosing a single set of parameters $\{c_{H1} \approx 1.7$, $c_{H2} = 1.5$, $a_H \approx 0.5\}$ and the magnetoresistivity as determined above in Sec. IV. We conclude that the theory accounts well for the observed behavior.

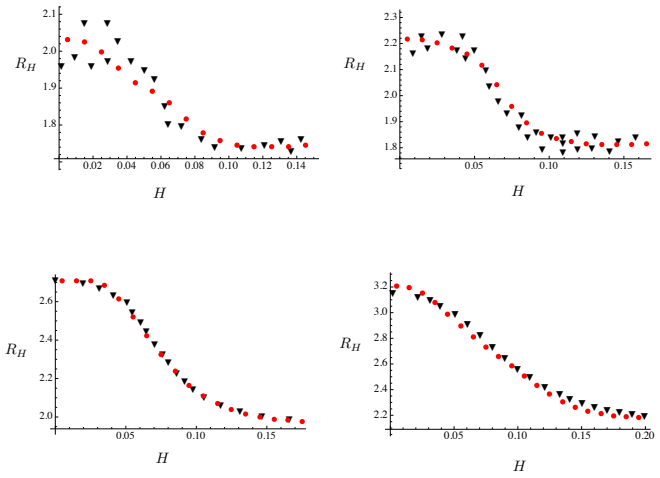

FIG. 3. Hall constant R_H at various T. Clockwise from upper left, $T = 18, 38, 65$ and 100 mK. H in Tesla and R_H in $10^{-10}\mathrm{m}^3/\mathrm{C}$. Dots are theory, Eq. (22); triangles are from the data, Ref. 24.

VI. SPECIFIC HEAT

The spin-flip contribution to the self energy of critical quasiparticles will also affect thermodynamic properties. For example, the specific heat coefficient will be proportional to $1/Z$. We now show how the specific heat coefficient acquires a step-like variation as a function of magnetic field at fixed temperature. Using the analyticity properties of Σ, we have approximately

$$\mathrm{Re}\Sigma_\sigma(\omega) \approx (|\omega|/Z^2)^{7/2}[1/|\omega| + 1/[|\omega| + h^2/\epsilon_F] \quad (25)$$

Since $Z^{-1}(T) = 1 - \partial\Sigma/\partial\omega|_{\omega\to T}$, we get the self-consistent equation for $Z(T)$ as

$$Z^{-1} = 1 + Z^{-7}|T|^{3/2}[1 + T/(T + h^2/\epsilon_F)] \quad (26)$$

The strong coupling solution of this equation is

$$Z(T,H) \propto |T|^{1/4}[1+T/(T+h^2/\epsilon_F)]^{1/6} \qquad (27)$$

such that the specific heat coefficient would be

$$\gamma \propto T^{-1/4}[1+T/(T+h^2/\epsilon_F)]^{-1/6} \qquad (28)$$

This expression for the specific heat coefficient also describes step-like behavior as the magnetic field is lowered through the T^*-line. The size of the step is of order 10%, but this time the step is reversed. We do not attempt a detailed comparison with experiment here because the transition to the antiferromagnetic phase at temperatures $T < 70$mK gives rise to a peaked contribution masking the step-like feature obtained above.

VII. SCATTERING OF QUASIPARTICLES BY SPIN RESONANCE BOSONS

ESR experiments on YRS have shown a well-defined spin resonance[13,14] in a wide region of the phase diagram extending from fields as high as 8T down to the critical field (see, for example, Fig. 1 in Ref. 12). Inelastic neutron scattering experiments[15] have shown the existence of the ESR resonance at small but non-zero momentum. Extending our earlier results[11,12] to non-zero q, we are led to the spin-fluctuation spectrum

$$\begin{aligned} \mathrm{Im}\chi(q,\omega) &= \mathrm{Im}\left[\chi_0 \frac{-\omega_r - aq^2 + i\gamma}{\omega - \omega_r - aq^2 + i\gamma}\right] \\ &= \chi_0 \frac{\omega\gamma}{(\omega-\omega_r-aq^2)^2+\gamma^2} \\ &\approx \chi_0\, \omega\delta(\omega-\omega_r-aq^2) \end{aligned} \qquad (29)$$

where ω_r is the spin-resonance frequency as calculated by us, see Eq. (2) of Ref. 12, χ_0 is the static susceptibility and γ is the line width, see Eq. (4) and following, of Ref. 12. The resonance frequency ω_r is everywhere non-zero; it does not vanish at the QCP, but gets renormalized to about 2/3 its high field limiting value in the critical regime.[12,27] The coefficient a has some T-dependence that we neglect. Since the resonance linewidth is found to be much less than the resonance frequency, we may take it to be infinitesimally small. The imaginary part of the electron self energy caused by scattering on the spin resonance is then given by

$$\begin{aligned} \mathrm{Im}\Sigma(\omega) = \lambda^2 \int_{-\infty}^{\infty} d\nu F(\nu,\omega)\chi_0\nu \int d\mathbf{q} \\ \times \mathrm{Im}G(\nu+\omega, \mathbf{k}+\mathbf{q})\delta(\nu-\omega_r-aq^2), \end{aligned} \qquad (30)$$

Where F is the thermal factor of Eq. (8). Again using the angular integral

$$\int \frac{d\Omega_q}{(2\pi)^3} \mathrm{Im}G(\nu+\omega,\mathbf{k}+\mathbf{q}) \propto \frac{1}{v_F q}, \qquad (31)$$

we find

$$\begin{aligned} \mathrm{Im}\Sigma(\omega) &\propto \lambda^2\chi_0 \int_{-\infty}^{\infty} d\nu F(\nu,\omega)\nu \int dq^2 \delta(\nu-\omega_r-aq^2) \\ &\propto \lambda^2\chi_0 \int_{\omega_r}^{\infty} d\nu F(\nu,\omega)\nu \\ &\propto \lambda^2\chi_0 T^2 I_1(\frac{\omega_r}{T},\frac{\omega}{T}) \end{aligned} \qquad (32)$$

where $I_1(z,y)$ has been defined in Eq. (15). The vertex correction λ and the static spin susceptibility are both temperature dependent. Below, we approximate χ_0 in the relevant regime $0.3K < T < 2K$ and $0 < H < 4T$ by $\chi_0(T) \propto \ln(10/T)$, which describes the data reasonably well. The corresponding contribution to the magnetoresistivity will have soft threshold behavior at $T_2^*(H) \approx \omega_r$.

VIII. T*-LINE IN THE PHASE DIAGRAM OF YRS

We are now ready to collect our results on the location of the T^* line in the $T-H$ phase diagram of YRS. These are determined in two ways, with identical results: i) from the position of the midpoint of the step feature in the magnetoresistance, Hall coefficient and other quantities, and ii) from the solutions of the implicit equations $\pi T^* \approx u(T^*,H)$ in the low temperature regime (spin-flip scattering) $T \lesssim 0.3K$ and $T^* \approx \omega_r(T^*,H)$ at higher T (scattering from spin resonance). The collected T^* points from our calculations are shown in Fig. 4 together with the T^* line published in numerous papers by the Dresden group.[6,7,24] The agreement is seen to be very good. As shown above, the step heights of the features associated with T_1^* and T_2^* vary with temperature as $T^{3/4}$ and T^2, respectively, which explains why the T_1^* feature is less important at higher T, and vice versa.

IX. CONCLUSION

We have addressed the crossover behavior in transport and thermodynamic quantities that occurs across the line $T^*(H)$ in the small (T,H) region of the phase diagram of YRS. We propose that the T^* line marks the onset of spin-flip scattering processes. We show in detail how these processes are switched on provided the temperature, and therefore the thermal energy is sufficiently high to allow additional scattering processes of at least two different types: (1) quasiparticle spin-flip scattering off the quantum fluctuations associated with the QCP of YRS. This involves excitation over the Zeeman gap, which we show to nearly vanish at the QCP; and (2) scattering off spin resonance bosons, relevant at higher magnetic fields. While the second contribution is noncritical and therefore affects only the transport quantities, the first involves quantum critical excitations and is therefore operative in both the transport and the thermodynamic quantities. We have demonstrated that the

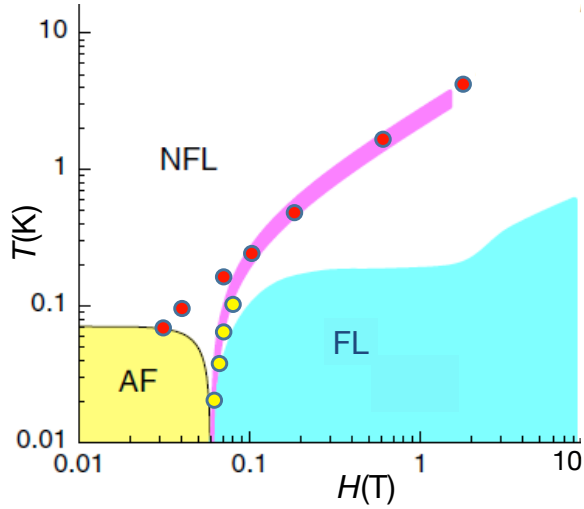

FIG. 4. Experimental phase diagram of YRS.[28] In the FL region (blue) the resistivity is $\propto T^2$. NFL denotes the non-Fermi liquid region where the resistivity varies with T as T^α with $\alpha \leq 1$. The purple region is where several experimental probes exhibit a crossover behavior, called the T^*-line. The dots are the theoretical positions of the onset of spin-flip scattering - from quantum fluctuations (yellow) and at higher (T, H), from the spin resonance (red). The red dots at $H < 0.1T$ are calculated using unpublished data[27]

observed magnetoresistivity and the Hall coefficient may be quantitatively explained by our model calculation.

In our calculation of the magnetotransport properties, we have made extensive use, as input, of experimental data on specific heat, susceptibility and magnetization. This enables us to conclude that in the experimentally relevant temperature regime the rapid drop of the Zeeman splitting h as the magnetic field is lowered to below the critical field at fixed temperature is not so much controlled by the decrease of the quasiparticle weight $Z(H, T)$, but it is governed by the H - dependence of the differential susceptibility and of the magnetization. Therefore the T^*-line is not necessarily tied to the critical field (although at lower temperature it presumably is). This is to say that if the QCP is shifted to higher or lower values of magnetic field by doping the pure compound appropriately, this does not necessarily mean that the $T^*(H)$ as obtained above will follow the shift of the QCP. Rather, it may stay approximately at the unshifted position. This may be easily checked as soon as sufficient data on specific heat, magnetization and susceptibility become available. The part of the T^*-line at higher temperature, which according to our calculation is controlled by the scattering off the spin resonance excitations will stay unchanged upon doping as long as the resonance frequency is not affected by doping.

We emphasize that our description of the $T^*(H)$-line derives from the magnetic field induced changes (1) of the fermionic spectrum as expressed by the Zeeman splitting, and (2) of the bosonic spectrum through the tuning parameter. The T^*-features result from incorporating spin-flip scattering from critical fluctuations and scattering from the spin resonance mode into the transport and thermodynamic responses. Within this picture, which successfully accounts for the observed crossover phenomena, there are no additional effects that would further change the spectra from those at $H = 0$.

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