Metamagnetic Quantum Criticality in Metals

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We present a renormalization group treatment of *metamagnetic quantum criticality* in metals. We show that for clean systems the universality class is that of the overdamped, conserving (dynamical exponent $z = 3$) Ising type. We obtain detailed results for the field and temperature dependence of physical quantities including the differential susceptibility, resistivity, and specific heat. Our results are shown to be in quantitative agreement with data on $Sr_3Ru_2O_7$ except very near to the critical point itself.

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Quantum phase transitions in itinerant electron systems have been intensively investigated recently [1–3], because of the intrinsic interest of quantum criticality, the non-Fermi-liquid behavior near the critical point, and the possibility of novel ground states including non-s-wave superconductivity. An apparently controlled theory has been presented [2], but many of the experimental realizations show deviations from the predicted behavior [4]. It is presently controversial whether a straightforward modification (interplane frustration reducing the effective dimensionality, or a disorder induced crossover [5]) will solve the discrepancy, whether more fundamental modifications are required such as "spectator modes" [6], or whether the whole picture should be scrapped in favor of a new kind of criticality [7].

In this Letter we present the first renormalization group treatment of a new type of quantum criticality, namely, the metamagnetic quantum critical end point. Metallic metamagnetism was studied via mean field theory [8,9] and via the "SCR" method [10]. To date, however, the critical phenomena have not been investigated. The significance of our work is that we show that this new type of quantum critical behavior provides a clean test of the original [1,2] framework and the complicating factors added by other workers do not apply here. By a direct comparison of our theory with experiments [11], we show that $Sr_3Ru_2O_7$ is close to a quantum critical end point. Our theory explains a number of outstanding issues in this system: the finite temperature peak in the weak-field susceptibility [12] and the paramagnetic ground state in a metal that should, according to band structure calculations, be ferromagnetic [13]. One should further note that at the metamagnetic critical end point the material does not have a well-defined Fermi surface: the positions of the "spin-up" and "spin-down" Fermi surfaces undergo critical fluctuations leading to "non-Fermi-liquid" physics.

A metamagnetic transition is empirically defined as a rapid increase in magnetization at a particular value of applied magnetic field. Because there is no broken symmetry involved, one expects a first order transition from a low magnetization to a high magnetization state as an applied magnetic field H is swept through a (temperature dependent) critical value $H_{\rm mm}(T)$. The curve of first order transitions $H_{\rm mm}(T)$ terminates in a critical point (H^*, T^*). By appropriately tuning material parameters it is possible to reduce T^* to 0, yielding a *quantum-critical end point*. This situation is depicted in Fig. 1: (b) shows a typical metamagnetic line and the critical end point in the field-temperature plane and (a) shows a possible variation of the temperature of the critical end point with pressure. It has been argued [11,14] that at ambient pressure $Sr_3Ru_2O_7$ is naturally tuned to a quantum critical end point at moderate magnetic fields.

Quotes are placed about "spin-up" and "spin-down" because in many metamagnetic materials spin-orbit coupling is large and spin is not a good quantum number. However, for most purposes one may adopt a "pseudospin" notation [15] labeling the two Kramers-degenerate states in zero

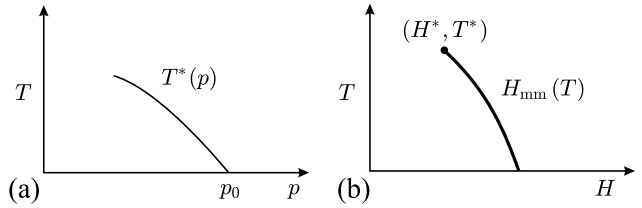

FIG. 1. (a) Schematic phase diagram, showing a variation of the end point of a line of metamagnetic first order phase transitions as the control parameter (e.g., pressure) is varied. (b) Schematic phase diagram in the H, T plane for $p < p_0$ showing a metamagnetic line and location of the end point.

field. The Kramer's degeneracy is broken by an applied field, leading to two Fermi surfaces and the theory carries through as in the non-spin-orbit case with one important exception noted below: if spin-orbit coupling is strong, impurity scattering may affect the dynamics differently.

Our key assumption (which is the basis of the standard [1,2] theory of metallic quantum criticality) is that the electronic degrees of freedom may be integrated out leaving a model of an overdamped bosonic mode which may then be analyzed by renormalization group methods. For the case of the metamagnetic quantum end point, the tuning parameter (magnetic field) is conjugate to the order parameter allowing an unambiguous identification of the relevant fluctuations: longitudinal fluctuations $\psi(x,\tau) = [|m| - m_{\rm av}(H^*)]/m_0$ of the magnetization density m about its average value $m_{\rm av}$ at the critical field H^*, normalized to some typical magnetization density m_0 (for example, the high-field saturation magnetization). We define the critical field H^* by the requirement that at $T = 0$ the action has no static third order terms. We write $h = (H - H^*)/H^*$, introduce a cutoff length a (for example, the lattice constant), and define an energy scale E_c by the requirement that the coefficient of the static quartic term is $1/4$. The action in d space dimensions and imaginary time becomes

$$S_{\rm meta} = S_{\rm dyn} + \int \frac{d^d x}{a^d} E_c \, d\tau \times \left[\frac{1}{2} \xi_0^2 (\nabla\psi)^2 + \delta\psi^2 + \frac{1}{4}\psi^4 - h\psi + \ldots \right]. \quad (1)$$

Here δ (which may be varied, e.g., by changing pressure) tunes the system through the metamagnetic critical point and $S_{\rm dyn}$ (discussed below) expresses the order-parameter dynamics.

We have used a conventional gradient expansion for the static part of the action and assumed that the coefficients are simple numbers and that the parameters vary with temperature only as T^2, as usual in Fermi-liquid theory. For an $O(3)$ ferromagnetic quantum critical point this may not be the case [16,17], but in the presence of a symmetry breaking field, the T^2 and gradient expansions are believed [6] to apply.

The dynamic part $S_{\rm dyn}$ follows because the order parameter is essentially the difference in position of the spin-up and spin-down Fermi surfaces. Fluctuations at nonzero q correspond to locally increasing the number of spin-up electrons and decreasing the number of spin-down electrons. If spin is conserved such a fluctuation can relax only via propagation or diffusion of electrons within each spin manifold. In a clean spin-orbit-coupled system, pseudospin is conserved (at least for fields aligned along a crystal symmetry axis) and the same arguments apply. Therefore, in a clean system one expects (the term is most conveniently written in frequency-momentum space)

$$S_{\rm dyn} = \frac{T}{E_c} \sum_n \int \frac{a^d d^d q}{(2\pi)^d} \frac{|\omega_n|}{v|q|} |\psi(q,\omega_n)|^2 + \ldots, \quad (2)$$

corresponding to overdamped but conserved fluctuations, and yielding the dynamical exponent $z = 3$. Here v is a velocity, presumably of the order of the Fermi velocity and $\psi(q,\omega_n) = \int \frac{d^d x}{a^d} E_c \, d\tau \, e^{i\vec{q}\cdot\vec{x} - i\omega_n\tau} \psi(x,\tau)$. Note that we are concerned only with longitudinal fluctuations, so "precession" terms $\partial_\tau \vec{\psi} \cdot \nabla^2 \vec{\psi} \times \vec{\psi}$ are not important. Strong (pseudo)-spin-conserving scattering would lead to diffusion ($|\omega_n|/vq \to |\omega_n|/Dq^2$) changing z to 4. A momentum non-conserving spin orbit coupling (as from impurities in the presence of strong spin orbit scattering) would lead to relaxation (i.e., Eq. (2) with vq replaced by a momentum independent scattering rate) implying $z = 2$. An important scale is the characteristic energy $\omega_{\rm sf}$ of a spin fluctuation at momentum $q_c = 1/a$, $\omega_{\rm sf} = v\xi_0^2 q_c^3$. Typical $\omega_{\rm sf}$ values for transition metal magnets are of the order of 500 K; for heavy fermion systems they are at least an order of magnitude smaller [18].

We analyze the theory by the usual one loop renormalization group equations [2] which, after mode elimination and rescaling, relate the theory with parameters δ, u, h to a new theory with parameters δ', u', h'. The behavior at $h = 0$ has been previously reported [2]; we focus here on the h dependence. The scaling equations are (we assume henceforth that $z = 3$)

$$\frac{\partial\delta}{\partial\lambda} = 2\delta + 3u(\lambda) f[T(\lambda)], \quad (3)$$

$$\frac{\partial u}{\partial\lambda} = (1 - d) u(\lambda). \quad (4)$$

The field h scales as $h(\lambda) = e^{[(d+5)/2]\lambda}$ and $T(\lambda) = Te^{3\lambda}$. The effect of eliminated modes on δ is contained in f which is calculated by expanding the theory about the value $\overline{\psi}(\delta h)$ which extremizes the static part of $S_{\rm meta}$ at the rescaled field, and then using the Gaussian approximation to the resulting action to evaluate the integral over eliminated modes. Operationally, this means that we calculate f assuming the scales of interest are larger than the running "mass" $r_{\rm eff} = \delta + 3u\overline{\psi}^2$ and then stop scaling at $r_{\rm eff} = 1$. Expressing momenta and frequencies in units of $q_c = 1/a$ and $\omega_{\rm sf}$, then $f = \Lambda \int' \frac{d^d u}{(2\pi)^d} \frac{dy}{\pi} \times \coth(\frac{y}{2t}) \frac{y/u}{(y/u)^2 + u^4}$ with $\Lambda = (\omega_{\rm sf}/E_c)(a/\xi_0)^2$ (the $'$ denotes summation over eliminated modes).

The solution of Eqs. (3) and (4) follows [2] and is discussed in detail elsewhere [19]. Because in all cases of physical interest the model is at or above its upper critical dimension, quantal fluctuations lead only to a finite renormalization of the $T = 0$ parameters of $S_{\rm meta}$ while thermal fluctuations are controlled by a "dangerous irrelevant operator," so the effects of quantal fluctuations may be absorbed into the $T = 0$ parameters and only thermal effects need be explicitly treated. We note, however, that the effects of quantal fluctuations are not small in general. Thus band theory predictions of parameters of the model (such as u) are *a priori* not a good estimate of the low energy properties. Further, their sign reduces the tendency to order predicted by band theory [13].

The results of the calculation may be summarized as follows. At $\delta = 0$ (i.e., parameters tuned so that the material is at the metamagnetic quantum critical point) as $T \to 0$ the differential susceptibility $\partial m/\partial h$ scales as $u^{1/3}h^{-2/3}$; as $T \to 0$ the specific heat coefficient $\gamma = C/T$ is proportional to $\ln h^{-1}$ in $d = 3$ and to $h^{-1/3}$ in $d = 2$ and the resistivity $\rho(T)$ has the leading T dependence $\rho(T) - \rho(T = 0) = AT^2$ with A varying as $h^{-1/3}$ in $d = 3$ and as $h^{-2/3}$ in $d = 2$. The crossover to the thermally dominated regime occurs at $T \sim h^{1/2}$ ($d = 3$) and $T \sim h^{2/3}$ ($d = 2$). If $\delta > 0$ then the scaling in h is cut off when $h^{2/3} \sim \delta$ and there is no phase transition in the h, t plane. If $\delta < 0$ then a first order transition occurs as h is varied at $T = 0$; a line of first order transitions extends upwards in the h, T plane and terminates at a critical end-point temperature $T^* \sim \delta^{z/(d+z-2)}$. Finally, we note that corrections to scaling may be numerically important, as is seen from the numerical results below.

The preceding considerations were generic. It is possible to proceed further in the particular case of $Sr_3Ru_2O_7$, because it seems (see below) that at ambient field this material is very near to a weakly first order ferromagnetic-paramagnetic quantum phase transition. The physics over a wide range of fields and temperatures should therefore be describable by a generalized Ginzburg-Landau action for a three-component order parameter ϕ (corresponding to long wavelength fluctuations of the magnetization):

$$S_0 = S_{\rm dyn} + \int \frac{d^d x}{a^d}\, d\tau \left\{ \frac{1}{2}\, \xi_0^2 [\nabla_b \phi_a(x,\tau)]^2 + \frac{r}{2}\, \phi_a^2(x,\tau) + \frac{1}{4}\, u_{ab} \phi_a^2 \phi_b^2 + \frac{1}{6}\, v_{abc} \phi_a^2 \phi_b^2 \phi_c^2 - g_{\rm eff} \mu_B \vec{h} \cdot \vec{\phi}(x,\tau) + \ldots \right\}. \tag{5}$$

Here repeated indices are summed, the ellipsis denotes higher order terms, and the notations are as above, except that we have added a sixth order term and here the parameters r, u_{ab}, v_{abc} have dimension of energy. The data (isotropic susceptibility as $T \to 0$ but some angle dependence at higher fields and temperatures) require a breaking of rotational invariance in the mode-coupling terms, but not in the quadratic one. We take ϕ to be a dimensionless magnetization variable measured in units of the putative saturation magnetization $2\mu_B$/Ru (the important electrons are d electrons, of which there are four in the t_{2g} orbitals, leaving two holes, and the g factor should be close to 2). Scaling is as described previously, except the sixth order term renormalizes the fourth order one and in the presence of a field the mass (coefficient of the quadratic part of the fluctuations) becomes anisotropic, with the component corresponding to fluctuations along the field becoming $r_{\rm eff} = r + 3u\overline{\phi}^2 + 5v\overline{\phi}^4$. A Heisenberg-$XY$ or Heisenberg-Ising crossover occurs when the larger of $r_{\rm eff}$ or r passes through unity and scaling stops when the smaller of the two becomes of order unity. In the Heisenberg regime extra precession terms in the dynamics may be important. A detailed analysis of the behavior of this model will be presented elsewhere [19], extending the important work of Yamada and collaborators [10], who showed that such an analysis was possible but did not consider the precession terms or anisotropic scaling and also used a simplified version of the SCR theory instead of the renormalization group method. At $T = 0$, one may use mean field theory provided one interprets the parameters in Eq. (5) as renormalized parameters. If $9u^2/20v > r > 3u^2/16v$ and $u < 0$ (for simplicity we do not write the directional subscripts here) the model has a $T = 0$ metamagnetic transition. The point $r = 9u^2/20v$ corresponds to the quantum critical end point. At the quantum-critical end point the magnetization $m = \langle \dot{\phi} \rangle$ and magnetic field H^* are, for fields in the c direction,

$$m_c^* = \sqrt{\frac{-3u_{cc}}{10v_{ccc}}}, \qquad g_{\rm eff}\mu_B H_c^* = \sqrt{\frac{-3u_{cc}}{10v_{ccc}}}\, \frac{6u_{cc}^2}{ccc}. \tag{6}$$

Figure 1 of Ref. [11] shows that at low T and low applied field the susceptibility is about $0.025\mu_B/T$ implying $r \approx 160\mu_B - T \approx 100$ K. This small value implies a very large enhancement of the susceptibility over the band value, as noted previously, and implies that the material is near a paramagnetic-ferromagnetic transition. For fields directed along the c axis the observed metamagnetic transition occurs at a magnetization of about 0.25–$0.3\mu_B$/Ru implying $u_{cc} = 3000$–4300 K and $v_{ccc} = 40\,000$–$80\,000$ K with the larger values corresponding to the smaller m. The consistency of these estimates may be verified by substitution into Eq. (6); use of $g_{\rm eff} = 2$ yields an

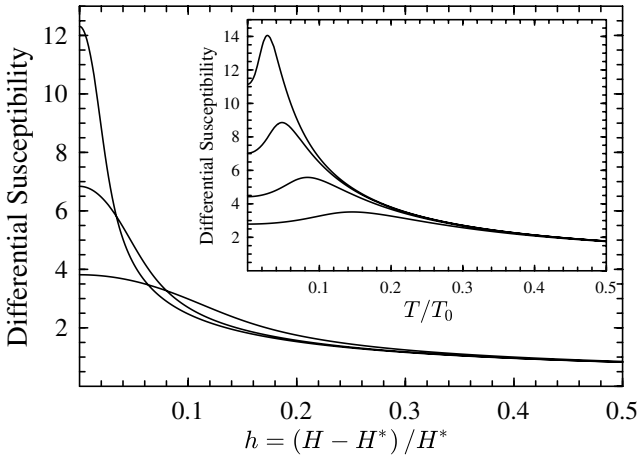

FIG. 2. Differential susceptibility, $\chi_0^{-1}(\partial m/\partial h)$, as a function of applied field H at temperatures $T/T_0 = 0.05, 0.1, 0.2$, for a two dimensional metamagnetic critical point. Inset: Dependence of $\chi_0^{-1}(\partial m/\partial h)$ on temperature T at $h = 0.01, 0.02, 0.04, 0.08$. (Normalizations are discussed in text.)

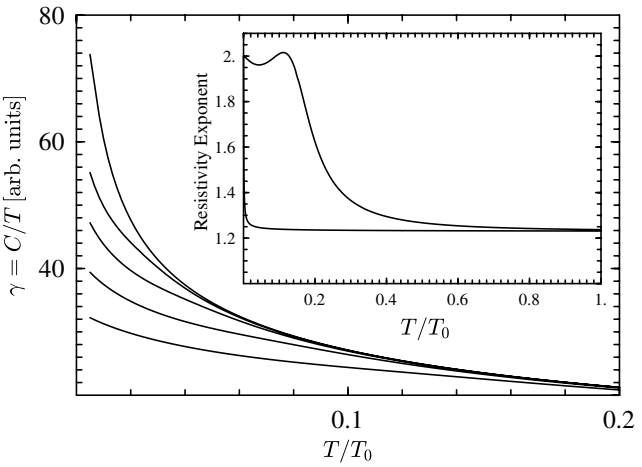

FIG. 3. Dependence of specific heat coefficient C/T on temperature T for $h = 0.01, 0.1, 0.2, 0.4$ calculated for a two dimensional metamagnetic critical point. Inset: Dependence of resistivity exponent $\partial \ln\rho/\partial \ln T$ on T for $h/H^* = 0$ (lower curve) and 0.1 (upper curve). (T_0 is defined in text.)

estimate of 5–6 T for the metamagnetic field, in the range found experimentally. Expansion of Eq. (5) about the metamagnetic point yields Eq. (1) with $E_c = -2u_{cc} =$ 6000–8000 K. The dimensionless critical field $g\mu_B H^*/u \sim 0.001$ so we should be concerned with variations which are small relative to this, i.e., with $h \approx 10^{-4}$. At present rather less information about the spin fluctuation frequencies is available; we therefore normalize our results to the temperature T_0 at which the differential susceptibility at the critical field is equal to the zero-field zero temperature susceptibility; i.e., $\frac{\partial m}{\partial h}(\delta = 0, T = T_0) = \chi(H = 0, T = 0) = \chi_0$.

We now present the results of a numerical solution of the scaling equations. Figure 2 shows the h dependence of the differential susceptibility for several values of T, obtained in the two dimensional case using parameters reasonable for $Sr_3Ru_2O_7$. The inset shows the temperature dependence of the differential susceptibility for different h. Note the nonmonotonic temperature dependence for fields different from $h = 0$ explains the previously mysterious peak seen in the experiments on $Sr_3Ru_2O_7$ and other materials [12].

Figure 3 shows the specific heat coefficient $\gamma = C/T$; in this quantity the crossover is much less sharp, in part because a 2D nearly critical Fermi liquid has a specific heat coefficient $\gamma \sim A + BT$ with both A and B divergent as the critical point is approached. This is an example of the corrections to scaling mentioned earlier. The inset shows the resistivity exponent $\alpha = -\partial \ln\rho/\partial \ln T$ plotted against temperature for $h = 0$ and $h = 0.1$. The high-T resistivity exponent is not precisely 4/3 because of the logarithmic corrections alluded to earlier. The crossover to the expected low-T T^2 behavior is very sharp.

In conclusion, we have presented a theory of metamagnetic quantum criticality in metals. We have identified the universality class and the form of the order parameter dynamics, and we presented detailed results for a range of physical quantities. Our theory accounts for the unusual temperature dependence of $\chi(T, H = 0)$, the paramagnetic ground state, and the main features of behavior seen in $Sr_3Ru_2O_7$ as the metamagnetic critical point is approached, providing strong support to the assumptions made in Refs. [1,2] and much other work on non-Fermi-liquid physics. Subsequent papers [19] will present details omitted here and a quantitive application to three dimensional materials and will also determine whether the anomalous behavior observed very close to the critical point in $Sr_3Ru_2O_7$ [14] (which is not consistent with our results for a metamagnetic critical point at $T = 0$) is consistent with a metamagnetic end point at a T slightly greater than 0 or whether fundamentally new physics is required.

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