Metamagnetic Quantum Criticality

A. J. Millis,1 A. J. Schofield,2 G. G. Lonzarich,3 and S. A. Grigera4

1Center for Materials Theory, Department of Physics, Rutgers University, 136 Frelinghuysen Rd, Piscataway NJ 08854
2School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK.
3Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, UK
4School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife, KY16 9SS, UK

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A renormalization group treatment of metamagnetic quantum criticality in metals is presented. In clean systems the universality class is found to be of the overdamped, conserving (dynamical exponent z = 3) Ising type. Detailed results are obtained for the field and temperature dependence of physical quantities including the differential susceptibility, resistivity and specific heat near the transition. An application of the theory is made to Sr3Ru2O7, which appears to exhibit a metamagnetic critical end-point at a very low temperature and a field of order 5–7T.

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 \( H_{\text{c}}(T) \). The curve of first order transitions \( H_{\text{c}}(T) \) 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 critical end-point in the field-temperature plane and (a) shows a possible variation of the temperature of the critical end-point with pressure.

A number of ‘strongly correlated metals’, including UPt3, CeRh2Si2 and other heavy fermion compounds, as well as d-electron systems such as MnSi exhibit metamagnetic transitions with properties suggestive of proximity to a quantum critical point. Recent measurements strongly indicate that the bilayer ruthenate d-electron system Sr3Ru2O7 is, at ambient pressure and moderate applied field, tuned almost exactly to such a quantum-critical end-point.

Metamagnetism in metals has not been extensively studied. Mean-field treatments have recently appeared and some discussion was given in the context of a treatment of weak ferromagnets via the ‘SCR’ method, but the critical phenomena have not so far been investigated. Apart from the experimental relevance, the issue is of fundamental importance. In a metal at \( T = 0 \) a nonzero magnetization corresponds to a splitting of the “spin up” and “spin down” Fermi surfaces and a first-order metamagnetic transition corresponds to a jump in this splitting. At the metamagnetic quantum-critical end-point fluctuations of the magnetization, and therefore of the Fermi surface positions, become large: in a certain sense the material does not have a well defined Fermi surface and may therefore be thought of as a non-Fermi-liquid. In this paper we give what we believe is the first renormalization group theory of metamagnetic quantum criticality. We present general results, which may be applicable to a number of systems, and a detailed application to Sr3Ru2O7. We use the standard approach to metallic quantum criticality, which involves integrating out the electron degrees of freedom to obtain a model of overdamped bosonic excitations which are analysed by renormalization group methods.

Quotes are placed about “spin up” and “spin down” above 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 ‘pseudo-spin’ notation labeling the two Kramers-degenerate states in zero-field. The Kramers 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.

To treat the critical behavior we assume that the fluctuations in the relative Fermi surface positions may be represented by fluctuations of a magnetization variable \( m \). We write an action for longitudinal fluctuations \( \psi(x, \tau) = (|m| - m_{\text{av}}(H^*) ) / m_0 \) of the magnetization

FIG. 1: (a) Schematic phase diagram, showing variation of end-point of line of metamagnetic first order phase transitions as control parameter (e.g pressure) is varied. (b) Schematic phase diagram in \( H, T \) plane for \( p < p_0 \) showing metamagnetic line and location of end-point.
density $m$ about its average value $m_{\text{av}}$ 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

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

(1)

Here $\delta$ (which may be varied e.g. by changing pressure) tunes the system through the metamagnetic critical point. We define the critical field $H^*$ by the requirement that the coefficient of the static quartic term is $1/4$; the action in $d$ space dimensions and imaginary time becomes

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

(1)

We have assumed in writing the static part of $S_{\text{meta}}$ that the gradient expansion is the conventional one, that the coefficients are simple numbers and that the parameters vary with temperature only as $T^2$, as usual in Fermi-liquid theory. However, several recent papers have called these assumptions into question [14, 13]. In particular, Belitz, Kirkpatrick and Vojta [14] have presented perturbation-theory results indicating that the expansion of the static spin susceptibility of a conventional, non-critical clean Fermi-liquid about the $q = 0$ value contains terms of order $|q|$ (in $d = 2$). Such terms would violate the usual gradient expansion. Subsequently, a closely related $[T]$ temperature dependence of the susceptibility and other parameters was studied [13]. The available perturbative calculations [14] suggest that spin rotational invariance is required to obtain the anomalous momentum dependence, so that in the present situation the gradient expansion might be the conventional one. However, one might expect $\xi_0^2$ to be unusually large if $m_{\text{av}}(H^*)$ is small. A detailed investigation of the behavior near a metamagnetic point could therefore be a useful test of this still unsettled issue.

The dynamic part $S_{\text{dyn}}$ 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, pseudo-spin 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)

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

(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

$$\psi(q, \omega_n) = \int \frac{d^d x}{a^d} E_c d \tau e^{iq \cdot \vec{x} - i \omega_n \tau} \psi(x, \tau) .$$

Note that we are concerned only with longitudinal fluctuations, so ‘precession’ terms $\partial_x \psi \cdot \nabla^2 \psi \times \vec{\psi}$ are not important. Strong (pseudo)-spin-conserving scattering would lead to diffusion ($|\omega_n|/vq \rightarrow |\omega_n|/Dq^2$) 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 $\omega_{sf}$ of a spin fluctuation at momentum $q_c = 1/a$, $\omega_{sf} = v \xi_0^2 q_c^2$. Typical $\omega_{sf}$ values for transition metal magnets are of the order of 500K; for heavy fermion systems they are at least an order of magnitude smaller [13].

We analyse the theory by the usual one loop renormalization group equations [4] which, after mode elimination and rescaling, relates the theory with parameters $\delta, u, h$ to a new theory with parameters $\delta', u', h'$. The behavior at $h = 0$ has been previously reported [4]; we focus here on the $h$ dependence. The scaling equations are (we assume henceforth that $z = 3$)

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

(3)

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

(4)

The field $h$ scales as $h(\lambda) = \epsilon^{d-3} h$ and $T(\lambda) = T_0^{3} \lambda$.

The effect of eliminated modes on $\delta$ is contained in $f$ which is calculated by expanding the theory about the value $\bar{\psi}(\delta h)$ which extremizes the static part of $S_{\text{meta}}$ 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’ $r_{\text{eff}} = \delta + 3 u(\lambda)$ and then stop scaling at $r_{\text{eff}} = 1$. Expressing momenta and frequencies in units of $q_c = 1/a$ and $\omega_{sf}$ then $f = \Lambda \int \frac{d^d u}{(2\pi)^d} \frac{d^d v}{(2\pi)^d} \coth(\frac{\pi}{2} \frac{|u/a|}{|v/a| + u})$ with $\Lambda = (\omega_{sf}/E_c)(a/\xi_0)^2$ (the $'$ denotes summation over eliminated modes).

The solution of Eqs. 3 and 4 follows [13] and is discussed in detail elsewhere [10]. Because in all cases of physical interest the model is at or above its upper critical dimension, quantum fluctuations lead only to a finite renormalization of the $T = 0$ parameters of $S_{\text{meta}}$ while thermal fluctuations are controlled by a ‘dangerous irrelevant operator’. The mathematical consequence is that the solution of the scaling equations may be written so the effects of quantal fluctuations are 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, so that a priori one finds the parameters (such as $u$) of the theory
are not well estimated by band theory calculations.

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 $T^* \sim \delta^{2/(d+2-2)}$. Finally, we note that corrections to scaling may be numerically important, as will be seen from the numerical results below.

The proceeding considerations were generic. It is possible to proceed further in the particular case of Sr$_3$Ru$_2$O$_7$, 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 $\vec{\phi}$ (corresponding to long wavelength fluctuations of the magnetization)

$$S_0 = S_{\text{dyn}} + \int \frac{d^dx}{a_d} d\tau \left\{ \frac{1}{2} \xi_0^2 [\nabla_b \phi_a(x, \tau)]^2 + \frac{1}{2} \phi_0^2 (x, \tau) + \frac{1}{4} u_{ab} \phi_a^2 \phi_b^2 + \frac{1}{6} u_{abc} \phi_a^2 \phi_b^2 \phi_c^2 - g_{\text{eff}} \mu_B \vec{H} \cdot \vec{\phi}(x, \tau) + \ldots \right\}. \ (5)$$

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 in high-field magnetization and higher temperature $\chi$) require a breaking of rotational invariance in the mode coupling terms, but not in the quadratic one. We take $\phi$ to be a dimensionless magnetization variable measured in units of the putative saturation magnetization $2\mu_B / \text{Ru}$ (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 $r_{\text{eff}} = r + 3 u_{02} \gamma + 5 u_{00} \gamma$. A Heisenberg-XY or Heisenberg-Ising crossover occurs when then larger of $r_{\text{eff}}$ 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 [6], extending the important work of Yamada and collaborators [5], 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 as before, provided one interprets the parameters in Eq. (5) as renormalized parameters. If $9u^2/20v > r > 0$ 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 $m = \langle \phi \rangle$ and magnetic field $H^*$ are, for fields in the $c$-direction,

$$m_c = \frac{-3u_{\text{cc}}}{10v_{\text{cc}}}, \quad g_{\text{eff}} \mu_B H^* = \frac{-3u_{\text{cc}}}{10v_{\text{cc}}} 6u_{\text{cc}}^2 \frac{25v_{\text{cc}}}{10v_{\text{cc}}}. \ (6)$$

Fig. 1 of Ref. [6] shows that at low $T$ and low applied field the susceptibility is about $0.025 \mu_B / T$ implying $r \approx 160 \mu_B / T \approx 100K$. 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 $0.25 - 0.3 \mu_B / \text{Ru}$ implying $u_{\text{cc}} = 3000 - 4300K$ and $v_{\text{cc}} = 40,000 - 80,000K$ with the larger values corresponding to the smaller $m$. The consistency of these estimates may be verified by substitution into Eq. (5) use of $g_{\text{eff}} = 2$ yields an estimate of $5 - 6T$ for the metamagnetic field, in the range found experimentally. Expansion of Eq. (5) about the metamagnetic point yields Eq. (5) with $E_{\text{cc}} = -2u_{\text{cc}} = 6000 - 8000K$. 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 $\frac{\partial m}{\partial T}(\delta = 0, T = T_0) = \chi(H = 0, T = 0) = \chi_0$.

We now present the results of a numerical solution of the scaling equations. Fig. 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$_3$Ru$_2$O$_7$. The inset shows the temperature dependence of the differential susceptibility for different $h$. Note the non-monotonic temperature dependence for fields different from $h = 0$ if the control parameter is tuned to criticality. Fig. 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
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 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). (\(T_0\) defined in text.)

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, which should be amenable to detailed experimental tests. The universality class was identified, a form for the order parameter dynamics was obtained, and detailed results were presented for a range of physical quantities. Subsequent papers \[1\] will present details omitted here as well as results for three dimensional materials, and a comprehensive analysis of \(\text{Sr}_2\text{RuO}_4\) and \(\text{MnSi}\). The key assumption is that electronic degrees of freedom may be integrated out, and the fluctuating Fermi surface expressed in terms of an overdamped bosonic magnetization variable. Experimental tests of the theory will show whether this assumption, which underlies much recent work on quantum phase transitions in metals and indeed on non-Fermi-liquid physics, is justified.

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