Disorder Dependence of the Ferromagnetic Quantum Phase Transition

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(Received 29 June 2014; published 12 November 2014)

We quantitatively discuss the influence of quenched disorder on the ferromagnetic quantum phase transition in metals, using a theory that describes the coupling of the magnetization to gapless fermionic excitations. In clean systems, the transition is first order below a tricritical temperature $T_{\rm tc}$. Quenched disorder is predicted to suppress $T_{\rm tc}$ until it vanishes for residual resistivities ρ_0 on the order of several $\mu\Omega\,$cm for typical quantum ferromagnets. We discuss experiments that allow us to distinguish the mechanism considered from other possible realizations of a first-order transition.

DOI: 10.1103/PhysRevLett.113.207201 PACS numbers: 75.20.En, 05.30.Rt, 64.70.Tg, 75.30.Kz

There is substantial experimental evidence for the quantum ferromagnetic transition in clean metals to be generically of first order. Examples of systems that were expected to display a quantum critical point, but instead display a first-order transition if the Curie temperature is suppressed, are MnSi [1,2], $ZrZn_2$ [3], UGe_2 [4–6], and URhGe [7]. All of these are low-temperature ferromagnets (although the magnetic moment in some of them is not small) with Curie temperatures T_c between $\approx$10 K (URhGe) and $\approx$50 K (UGe_2) and magnetic moments per formula unit of about 0.17, 0.4, and $1.5\mu_B$ for $ZrZn_2$, MnSi and URhGe, and UGe_2, respectively. T_c is tunable by hydrostatic pressure or, for URhGe, by an external magnetic field transverse to the easy axis. A tricritical point separates a line of second-order transitions above the tricritical temperature $T_{\rm tc}$ ($\approx$5, 10, 1, and 24 K in $ZrZn_2$, MnSi, URhGe, and UGe_2, respectively) from a line of first-order transitions below, and in all of these materials tricritical wings have been observed in an external magnetic field. The respective values of the critical field at the wing tips are $H_c \gtrsim 0.05$, $\approx$0.6, $\approx$1, and $\approx$10 T. The qualitative phase diagram is shown in the rightmost panel in Fig. 1. Evidence for a first-order quantum phase transition (QPT) at low temperatures has been found in many other systems, but the phase diagram has not been mapped out completely, or the tricritical point is not accessible (as in UCoAl [8]).

These observations are remarkable because of their universality. The only known instances in which the QPT to a homogeneous ferromagnet is not observed to be of first order are the quasi-one-dimensional material $YbNi_4P_2$ [9], where the physics is expected to be quite different from that of true bulk metals, and various disordered materials where the transition is tuned by chemical composition, e.g., $URu_{2-x}Re_xSi_2$ [10]. We will come back to the weakly disordered compounds Ni_xPd_{1-x} [11] and $(Cr_{1-x}Fe_x)_2B$ [12]. Also remarkable is the stark disagreement between experiment and early theories. The quantum ferromagnetic transition as described by Stoner's mean-field theory [13] is generically continuous. It was later considered as an example by Hertz in his seminal renormalization-group (RG) treatment of QPTs [14], which also predicted a continuous transition with mean-field critical behavior.

A theory that explains and, indeed, predicted the observed universality was developed in Refs. [15–17]. It relies on the coupling between the magnetization and soft or gapless fermionic excitations with a ballistic frequency-momentum relation that exist in any clean metal at $T = 0$. It leads to an equation of state of the form

$$h = rm - vm^3 \ln(1/m^2) + um^3, \tag{1}$$

where m is the magnetization in suitable units, h is the external field, r is the control parameter, and v and u are Landau parameters. The nonanalytic $m^3 \ln(1/m)$ term is the result of m coupling to the soft modes in $d = 3$; more generally its form is m^d. Crucially, $v > 0$, which leads to a first-order transition at some $r > 0$. This *universal* mechanism has been confirmed by a variety of other techniques [18–20]. $T > 0$ gives the soft modes a mass, which cuts off the $\ln m$ nonanalyticity and leads to a tricritical point (rightmost panel in Fig. 1). Quenched disorder has two effects. First, it also cuts off $\ln m$. Second, a coupling to diffusive soft modes leads to an $m^{d/2}$ nonanalyticity whose sign is opposite of that of the nonanalytic term in the clean case. For sufficiently strong disorder, in $d = 3$, one finds [21]

$$h = rm + \frac{w}{(k_F\ell)^{3/2}} m^{3/2} + um^3, \tag{2}$$

with $w > 0$ another parameter, k_F the Fermi wave number, which sets the microscopic length scale, and ℓ the elastic

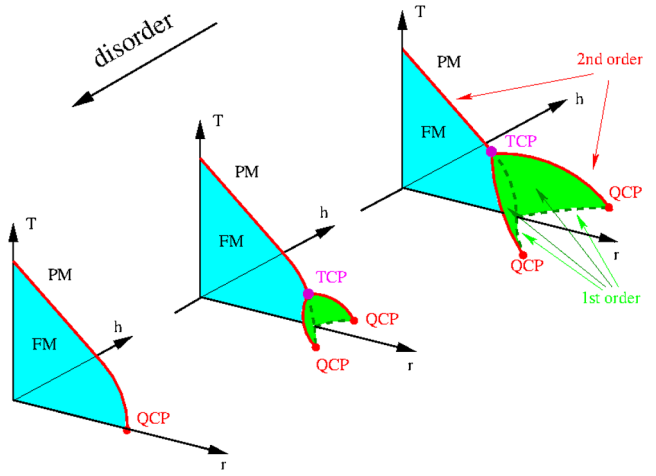

FIG. 1 (color online). Evolution of the phase diagram of a metallic quantum ferromagnet in the space spanned by temperature (T), magnetic field (h), and the control parameter (r) with increasing disorder. Shown are the ferromagnetic (FM) and paramagnetic (PM) phases in the $h = 0$ plane, lines of second-order transitions (solid red), the tricritical point (TCP), and surfaces of first-order transitions ("tricritical wings") that end in quantum critical points (QCP) in the $T = 0$ plane. With increasing disorder, the tricritical temperature decreases, the wings shrink, and above a critical disorder strength a QCP is realized in zero field.

mean-free path. This leads to a continuous transition with non-mean-field exponents (leftmost panel in Fig. 1). Equations (1) and (2) both represent renormalized Landau theories, which replace the fluctuating order-parameter field by its mean. Since the order-parameter fluctuations at the QPT are above their upper critical dimension ($d_c^+ = 1$ (0) for the clean (disordered) case [14]), this should not affect the nature of the QPT. Indeed, in the disordered case a RG study has shown that order-parameter fluctuations leave the power laws described by Eq. (2) intact, although they lead to non-power-law modifications of the leading scaling behavior [22,23].

While Eq. (1) is in qualitative agreement with all experiments on clean samples, there still are open questions. First, Eqs. (1) and (2) represent only the extremes of ultraclean and strongly disordered systems. Many experiments fall in between these two cases, e.g., Ni_xPd_{1-x}, which shows a second-order transition with mean-field exponents at $x = 0.027$ [11]. Second, the mechanism proposed in Ref. [15] is not the only possibility for a first-order transition; e.g., in classical compressible magnets the coupling between the magnetization and phonons can lead to a first-order transition [24]. This mechanism is not as universal as the one leading to Eq. (1), but the authors of Refs. [25–27] have argued that an adaptation to the quantum transition can explain the observations, at least in the case of the pressure-tuned quantum ferromagnets.

It is thus desirable to develop criteria that allow for a discrimination between the different theoretical ideas. In this Letter, we show that the disorder dependence of the phase diagram allows for such a discrimination. A phonon-based effect is not expected to qualitatively change by introducing disorder into the sample, in part because the electron-phonon interaction is only weakly affected by disorder [28]. The mechanism of Ref. [15], on the other hand, is crucially affected by disorder, since in the strong-disorder limit the equation of state changes to Eq. (2). As we will show, our theory predicts three distinct disorder regimes. In a weak-disorder regime the transition is first order, but T_{tc} is gradually suppressed until it vanishes at a critical value of the disorder. For common quantum ferromagnets, this is expected to happen for residual resistivities ρ_0 on the order of several $\mu\Omega\,\mathrm{cm}$. The resulting quantum critical point in an intermediate-disorder regime displays mean-field exponents consistent with Hertz theory in the observable critical region, although asymptotically close to the transition there will be a crossover to the non-mean-field critical behavior of Ref. [21]. With increasing disorder, the crossover moves away from the transition and becomes observable for values of ρ_0 on the order of tens of $\mu\Omega\,\mathrm{cm}$. Finally, in a strong-disorder regime with ρ_0 on the order of hundreds of $\mu\Omega\,\mathrm{cm}$ the non-mean-field critical behavior will be present in the entire critical region. However, for disorder that strong, other effects may come into play. Our predictions can be tested by introducing quenched disorder, e.g., by means of irradiation, into any of the materials that display a first-order QPT, and following the changes in the phase diagram with increasing disorder.

To achieve these goals, we have constructed an equation of state that interpolates between Eqs. (1) and (2) and generalizes them to finite temperatures. We first state and discuss this equation of state and then sketch its derivation. It takes the form

$$h = rm + \frac{w}{(k_F\ell)^{3/2}} m^{3/2} g(k_F\ell m, ct/m) - vm^3 \ln\left(\frac{1}{m^2/m_0^2 + (\sigma_0/k_F\ell + t)^2}\right) + um^3, \tag{3a}$$

which reduces to Eqs. (1) and (2) in the limits $k_F\ell \to \infty, 0$. We will refer to the second and third term on the right-hand side as the diffusive and ballistic nonanalyticity, respectively; m, h, and t are the dimensionless magnetization, magnetic field, and temperature, respectively, defined as follows. Let μ be the magnetization measured in μ_B per volume, H the external field, and T the temperature. Let n_e be the conduction electron density and T_F be the Fermi temperature (or more generally, the microscopic energy scale). Then, $m = 8\mu/\pi n_e$, $h = \mu_B H/k_B T_F$, and $t = 3\pi T/T_F$; v and w depend on a coupling constant γ_t that measures the strength of conduction-electron correlations, with $\gamma_t \ll 1$ and $\gamma_t = O(1)$ corresponding to weakly and strongly correlated systems, respectively. Another coupling constant $c = O(1)$ describes the coupling

between the magnetization and the conduction-electron spin density. In terms of γ_t and c one finds, for small γ_t, $v = c\gamma_t^4$ and $w = c\gamma_t$. $r \ll 1$ is the dimensionless control parameter for the transition, and $u = O(1)$ is a Landau parameter. m_0 and σ_0 set the scales for the magnetic moment and the disorder, respectively. They depend on the band structure and the correlation strength; from general arguments one expects $0.1 \lesssim \sigma_0 \leq 1$ and $m_0 \gtrsim 10$; see the discussion below. Finally,

$$g(y,z) = \frac{1}{g_0}\int_0^{1/y} dx \int_z^\infty d\omega \frac{\sqrt{x}\omega[2(x+\omega)^2+1]}{(x+\omega)^3[(x+\omega)^2+1]^2} \tag{3b}$$

with $g_0 = \pi/3\sqrt{2} \approx 0.74$ is normalized such that $g(0,0) = 1$. $g(y,0)$ is well approximated by

$$g(y,0) \approx 1/[1 + y^{3/2}/(9g_0 + y/g_0)]. \tag{3c}$$

We now discuss typical values for the various parameters in Eq. (3a), initially for a clean system. With $k_F \approx 1$ Å^{-1}, and a formula unit volume of about 50 Å^3, we find a dimensionless saturation magnetization ranging from $m \approx 0.25$ for $ZrZn_2$ to $m \approx 2.3$ for UGe_2. Choosing $u = 0.85$, $\gamma_t = 0.5$ (fairly strong correlation), and $c = 1$, we have $v = 0.06$. The tricritical temperature is $T_{tc} = (T_F/3\pi)e^{-u/2v}$ [15]. With $T_F \approx 10^5$ K, we have $T_{tc} \approx 10$ K, which is the correct order of magnitude for $ZrZn_2$, MnSi, and UGe_2. A slightly lower value of $\gamma_t \approx 0.45$ yields $T_{tc} \approx 1$ K, as observed in URhGe. At the first-order transition at $T = 0$, the magnetization changes discontinuously from zero to $m_1 = m_0 e^{-(1+u/v)/2}$ [15]. For m_0 between 75 (for $ZrZn_2$) and 350 (for UGe_2), this yields $m_1 \approx 0.05$–0.25, which is a reasonable fraction of the saturation magnetization in these materials. The critical field at the tips of the tricritical wings is given by $h_c = (4/3)e^{-13/4}m_0^3 v e^{-3u/2v}$ [16]. With parameters as above, this yields values from $H_c \approx 0.1$ T to $H_c \approx 10$ T. This is again the correct order of magnitude compared with the experimental observations [2,3,5].

Now consider quenched disorder. A Drude formula for ρ_0 with $k_F \approx 1$ Å^{-1} yields $k_F\ell \approx 1000\ \mu\Omega\,\mathrm{cm}/\rho_0$. $k_F\ell$ thus ranges from $\gtrsim 10^4$ in a clean metal ($\rho_0 \approx 0.1\ \mu\Omega\,\mathrm{cm}$) to about 10 in a poor metal ($\rho_0 \approx 100\ \mu\Omega\,\mathrm{cm}$). This in turn implies that values of $k_F\ell m$ between roughly 2.5 and 2×10^4 are realizable, with m the saturation magnetization. With m the actual magnetization, the lower limit is accordingly lower, depending on the minimal magnetization m_1 at the first-order transition, if any. From Eq. (3c) we see that $k_F\ell m \approx 5$ is the demarcation between two different regimes, which falls well within this range.

All of the above, and everything that follows, are just rough order-of-magnitude estimates. With this in mind, we can distinguish the following regimes, classified according to the values of $k_F\ell$ (clean vs dirty samples) and m (weak vs strong magnetism). They follow from the observation that the diffusive and ballistic nonanalyticities, at $T = 0$, are operative (inoperative) for $k_F\ell m \lesssim 5$ ($\gtrsim 5$) and $k_F\ell m \gtrsim m_0\sigma_0$ ($k_F\ell m \lesssim m_0\sigma_0$), respectively.

Regime I (clean or strong).—Exhibits $k_F\ell m \gtrsim m_0\sigma_0$. The diffusive nonanalyticity is inoperative, the equation of state is given by Eq. (1), and the transition is first order with $m_1 = m_0 e^{-(1+u/v)/2} \leq m$. For consistency, we must have $k_F\ell m_1 \gtrsim m_0\sigma_0$. With u and v as above and $\sigma_0 \approx 1/5$, this yields $k_F\ell \gtrsim 300$, or $\rho_0 \approx$ several $\mu\Omega\,\mathrm{cm}$.

Regime IIa (intermediate).—Exhibits $5 \lesssim k_F\ell m \lesssim m_0\sigma_0$. In this transient regime both nonanalyticities are inoperative, and the transition appears continuous with mean-field exponents in a range of m values. However, as m decreases, the system eventually enters regime IIb or III.

Regime IIb (intermediate).—Exhibits $k_F\ell m \lesssim 5$ and $k_F\ell \gtrsim (k_F\ell)^*$, with $(k_F\ell)^*$ defined below. The ballistic nonanalyticity is inoperative, the equation of state is given by Eq. (2), and the transition is second order with the asymptotic critical behavior characterized by the non-mean-field exponents of Ref. [21]. However, farther away from the transition, this behavior will cross over to ordinary mean-field behavior at a disorder-dependent value r^* of r. The crossover occurs when the last two terms in Eq. (2) are about equal. Having the crossover occur at $r = r^*$ thus requires a disorder given by $k_F\ell = k_F\ell^* = w^{2/3}/u^{1/6}|r^*|^{1/2}$. If we require $r^* = 0.01$ and choose $\gamma_t = 0.5$ and $u = 1$ as before, we have $k_F\ell^* \approx 6$, or $\rho_0^* \approx 150\ \mu\Omega\,\mathrm{cm}$. ρ_0^* is the disorder that separates regime IIb, where the transition is continuous with effectively mean-field exponents, from regime III. Note that ρ_0^* depends on the correlation strength via w; for $\gamma_t = 0.1$ (weak correlation) one has $\rho_0^* \approx 500\ \mu\Omega\,\mathrm{cm}$.

Regime III (dirty or weak).—Exhibits $k_F\ell m \lesssim 5$ and $k_F\ell \lesssim (k_F\ell)^*$. The equation of state is dominated by the diffusive nonanalyticity, and the transition is continuous with non-mean-field critical exponents in the entire critical region. This requires $\rho_0 > \rho_0^*$, with ρ_0^* ranging from approximately 100 $\mu\Omega\,\mathrm{cm}$ for strongly correlated materials to hundreds of $\mu\Omega\,\mathrm{cm}$ for weakly correlated ones.

At a nonzero temperature, we see from Eq. (3a) that a disorder resulting in $k_F\ell = \sigma_0 T_F/3\pi T_{tc}$ has the same effect as $T = T_{tc}$ in a clean system. That is, $\rho_0 \gtrsim 10^4 T_{tc}/\sigma_0 T_F \approx$ several $\mu\Omega\,\mathrm{cm}$ will suppress T_{tc} to zero, consistent with the above estimate for the destruction of the first-order transition at $T = 0$. The tricritical wings shrink, and eventually disappear, commensurate with the suppression of T_{tc}. This prediction for the evolution of the phase diagram is shown in Fig. 1.

We now have the following predictions for the effects of quenched disorder on typical strongly correlated quantum ferromagnets: Disorder decreases T_{tc} and suppresses it altogether for a residual resistivity ρ_0 on the order of several $\mu\Omega\,\mathrm{cm}$. For larger ρ_0, the QPT will be continuous and appear mean-field-like in a substantial disorder range,

$\rho_0 \lesssim 100\ \mu\Omega\,\mathrm{cm}$, with a crossover to non-mean-field behavior only extremely close to the transition. For even larger ρ_0 the critical behavior is characterized by the non-mean-field exponents of Refs. [21–23]. However, for disorder that strong quantum Griffiths effects are expected to be present and compete with the critical behavior [29]; to distinguish between the two, one needs to measure the critical behavior of the magnetization. We stress that these predictions are semiquantitative in nature. The important point is the existence of the three regimes; the disorder strengths that delineate them are expected to show substantial variations from material to material. We also note that quenched disorder can suppress a tricritical point in a purely classical model [30]. This mechanism is not dependent on the presence of conduction electrons and is expected to be characterized by different disorder scales than the one discussed here.

Some experimental evidence exists in favor of this scenario. For $ZrZn_2$, the QPT was initially found to be second order [31], but with increasing sample quality a first-order transition emerged [3]. For UGe_2, measured values of T_{tc} range from 24 [5] to 31 K [7], which is possibly related to the sample quality, and in URhGe higher T_{tc} values were found for cleaner samples [32]. All of these materials are strongly correlated as evidenced by their unusual electronic properties independent of the quantum magnetism. Finally, the observation of a quantum critical point with mean-field exponents in Ni_xPd_{1-x} [11] and possibly in $(Cr_{1-x}Fe_x)_2B$ [12], where the transition occurs at a small value of x, can be understood if one realizes that these systems are likely in the intermediate regime II. While these observations are encouraging, no systematic experimental study of the influence of quenched disorder on the phase diagram of quantum ferromagnets exists. Such an experiment would allow us to discriminate between the explanation of the first-order transition discussed above and alternative proposals that predict only a weak disorder dependence of T_{tc}.

We now sketch the derivation of Eq. (3a). The relevant soft fermionic modes, as functions of wave vector $\boldsymbol{k}$ and bosonic Matsubara frequency Ω_n, are diffusive for disordered electrons and ballistic for clean ones [33,34],

$$\mathcal{D}_{\mathrm{diff}} = \frac{1}{\Omega_n + D\boldsymbol{k}^2}, \qquad \mathcal{D}_{\mathrm{ball}} = \frac{1}{\Omega_n + v_F|\boldsymbol{k}|} \tag{4a}$$

with $D = v_F^2\tau/3$ the diffusion coefficient, τ the elastic mean-free time, and v_F the Fermi velocity. The soft-mode propagator $\mathcal{D}$ can be modeled by $\mathcal{D}_{\mathrm{diff}}$ for $|\boldsymbol{k}| < 1/\ell$ and by $\mathcal{D}_{\mathrm{ball}}$ for $|\boldsymbol{k}| > 1/\ell$, with $\ell = v_F\tau$ the elastic mean-free path. The magnetization m couples to the soft fluctuations and cuts off the singularities that result from integrating over $\mathcal{D}$, which leads to nonanalytic dependences on m. Integrating out the soft modes yields a fluctuation correction to the free energy density f of the form [33]

$$\Delta f = \frac{2}{V}\sum_{\boldsymbol{k}} T\sum_{n=1}^{\infty} \ln N(\boldsymbol{k}, \Omega_n; m). \tag{5}$$

At $T = 0$ the sum over Ω_n turns into an integral over a continuous variable ω, and the effect of a nonzero temperature can be modeled by the replacement $\omega \to \omega + 2\pi T$. The fluctuation contribution to the equation of state is obtained by differentiating Δf with respect to m. We measure m in units of the conduction electron density n_e and the magnetic field h in units of $k_B T_F/\mu_B$. The Landau parameters r and u are then dimensionless. Up to factors of $O(1)$, the resulting equation of state takes the form of Eq. (3a) with $m_0 \approx 7/\gamma_t$ and $\sigma_0 = 1$. These two values are based on a nearly free-electron model for the conduction electrons. For real materials, m_0 is expected to be an independent parameter that depends on microscopic details. It sets the scale for the magnetic moment, which differs by a factor of 10 between, e.g., $ZrZn_2$ and UGe_2; σ_0 in general depends on the correlation strength and is ≤ 1. The reason is that in a strongly correlated material two electrons with opposite spins cannot simultaneously take advantage of a disorder-induced potential well, because of the strong repulsion between the electrons. This is consistent with the fact that, in the absence of symmetry-breaking fields, interactions cause the disorder to get renormalized downward [35,36]. Correlations will thus effectively weaken the effects of the disorder; values of σ_0 between 1 (no correlation) and 0.1 (strong correlation) are reasonable based on the RG flow equations of Ref. [35]. Finally, the soft-mode effects are stronger the lower the dimension; in $d = 2$, the $m^3 \ln(1/m)$ term in Eq. (3a) turns into an m^2 term. For the diffusive modes, $d = 2$ is the lower critical dimension, and the effects of quenched disorder become strong and very complex [36].

We thank Greg Stewart, Andrew Huxley, and Nihat Berker for discussions. This work was supported by the NSF under Grants No. DMR-1401410 and No. DMR-1401449. Part of this work was performed at the Aspen Center for Physics and supported by the NSF under Grant No. PHYS-1066293.

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