Fluctuation-Driven Quantum Phase Transitions in Clean Itinerant Ferromagnets

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The quantum phase transition in clean itinerant ferromagnets is analyzed. It is shown that soft particle-hole modes invalidate Hertz's mean-field theory for $d \leq 3$. A renormalized mean-field theory predicts a fluctuation-induced first order transition for $1 < d \leq 3$, whose stability is analyzed by renormalization group techniques. Depending on microscopic parameter values, the first order transition can be stable, or be preempted by a fluctuation-induced second order transition. The critical behavior at the latter is determined. The results are in agreement with recent experiments.

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One of the most common and basic examples of a phase transition is the paramagnet-to-ferromagnet transition in metals, e.g., iron and nickel. These elements have high Curie temperatures, on the order of 1000 K. Examples of itinerant ferromagnets with much lower Curie temperatures, on the order of tens of degrees Kelvin, include MnSi [1], $ZrZn_2$ [1,2], and UGe_2 [3]. In the latter materials, the Curie temperature can be suppressed to zero by the application of hydrostatic pressure. This allows for an experimental investigation of the ferromagnetic quantum phase transition, which takes place at zero temperature as a function of a nonthermal control parameter, in this case, pressure. Another example is Ni_xPd_{1-x} [4], where the control parameter is the nickel concentration.

The ferromagnetic transition in metals was also the subject of the earliest theoretical studies of quantum phase transitions. In an important paper, Hertz [5] concluded that the critical behavior should be mean-field-like in all dimensions $d > 1$. This is because, in quantum statistical mechanics, statics and dynamics are coupled. As a result, the quantum phase transition in d dimensions is related to its classical counterpart in $d + z$ dimensions, with z the dynamical critical exponent. Since simple theories suggest $z = 3$ for clean itinerant ferromagnets, and since the classical Heisenberg ferromagnet has an upper critical dimension $d_c^+ = 4$, this argument suggests $d_c^+ = 1$ for the quantum transition.

It is now known, mostly through studies of the corresponding problem in the presence of quenched disorder, that the above argument is in general not correct. The basic physical reason is the existence of soft modes, particle-hole excitations in the case of itinerant ferromagnets, that couple to the order parameter and preclude the construction of a Hertz-type Landau-Ginzburg-Wilson (LGW) theory entirely in terms of the order parameter. These soft modes lead to time scales in addition to the critical one, and hence to multiple exponents z. This in turn leads to an instability of the mean-field fixed point that is not apparent in a power-counting analysis of the LGW theory. In the disordered case, the net result is an upper critical dimension $d_c^+ = 4$ (instead of $d_c^+ = 0$ in Hertz theory), with nonmean field (and nonpower law) critical behavior in the physically most interesting dimension $d = 3$ [6]. In the clean case, an analogous analysis of the stability of Hertz's fixed point shows that the upper critical dimension is $d_c^+ = 3$. In $d = 3$ a generalized Landau theory predicts a first order transition due to an $m^4 \ln m$ term in the Landau free energy, with m the magnetization [7]. For $1 < d < 3$ this theory also predicts a first order transition. Sufficiently high temperature or disorder lead to an analytic Landau free energy and render the transition second order.

This theoretical situation is at best in partial agreement with experiments. The existing theory predicts that the transition should always be of first order in sufficiently clean materials at sufficiently low temperatures [8]. If temperature or disorder drives it second order, then the predicted critical exponents are the classical Heisenberg exponents, or the strongly nonmean field exponents of Ref. [6], respectively. Experimentally, the transition in MnSi and UGe2 at low temperatures is indeed observed to be of first order [1,3], but in $ZrZn_2$ it is of second order even in very clean samples at very low temperatures [2], and the same is true in NiPd [4]. Furthermore, the critical behavior in NiPd was found to be mean-field-like to within the experimental accuracy, in good agreement with the predictions of Ref. [5]. This is suprising, given the above conclusion that Hertz theory cannot be correct in $d = 3$.

In this Letter, we show that the nature of the clean ferromagnetic quantum phase transition is determined by physical effects that had not previously been recognized, and that taking these effects into account removes the above discrepancies between theory and experiment. We will use renormalization group (RG) techniques to show the following. (i) The first order transition can be

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understood as a fluctuation-induced first order transition. (ii) For certain microscopic parameter values the first order transition is unstable with respect to a fluctuation-induced second order transition. (iii) The upper critical dimension is $d_c^+ = 3$. (iv) In the second order case, the critical behavior in $d = 3$ is given by mean-field exponents with logarithmic corrections, and in $d < 3$ it can be controlled by means of a $3 - \epsilon$ expansion. We will present our results first, and then sketch their derivation and explain their physical origin.

If the bare value of the quartic coefficient in the Landau free energy is sufficiently small (in a sense to be specified below), one finds the first transition discussed in Ref. [7]. However, if the bare quartic coefficient is sufficiently large, the transition is of second order. In $d = 3$, the critical behavior is mean-field-like with logarithmic corrections to scaling. Specifically, the paramagnon propagator in the critical regime in the paramagnetic phase has the form

$$\mathcal{M}(k, \Omega_n) = 1/[t + a(k)\,k^2 + |\Omega_n|/k], \tag{1a}$$

where t is the dimensionless distance from criticality at zero temperature ($T = 0$), k is the wave number, and $\Omega_n = 2\pi T n$ is a bosonic Matsubara frequency. k and Ω_n have been made dimensionless by means of suitable microscopic scales. The leading behavior of the coefficient a for small k is

$$a(k \to 0) \propto (\ln 1/k)^{-1/26}. \tag{1b}$$

Such logarithmic corrections to power-law scaling can be conveniently expressed in terms of scale dependent critical exponents. For instance, with $b \sim 1/k$ a RG length scale factor [9], we can write $a(k)\,k^2 \propto k^{2-\eta}$, with a scale dependent critical exponent η given by

$$\eta = \frac{-1}{26}\ \ln\ln b/\ln b. \tag{2a}$$

The correlation length exponent ν, the susceptibility exponent γ, and the dynamical exponent z can be directly read off Eqs. (1a) and (1b). The order parameter exponents β and δ can be obtained from scaling arguments for the free energy. We find

$$\nu = 1/(2 - \eta), \qquad z = 3 - \eta,$$
$$\gamma = 1, \beta = 1/2, \qquad \delta = 3. \tag{2b}$$

These exponents are defined as usual, i.e., $\xi \sim t^{-\nu}$, $\Omega \sim T \sim \xi^{-z}$, $\mathcal{M} \sim t^{-\gamma}$, $m \sim t^{\beta}$, and $m \sim h^{1/\delta}$, with ξ the correlation length and h an external magnetic field. The result for η is valid to leading logarithmic accuracy; the values of γ, β, and δ, as well as the relations between η and ν and z, respectively, are exact. Finally, we define a specific heat exponent α by $C_V \propto T^{-\alpha}$ at criticality. (This is a generalization of the usual definition of α at thermal phase transitions.) We obtain the exact relation

$$\alpha = -1 - \eta/z - \ln\ln b/\ln b. \tag{2c}$$

In $d = 3 - \epsilon$, the second order transition can be treated in an ϵ expansion. We find

$$\eta = -\epsilon/26, \qquad \alpha = -1 + (\epsilon - \eta)/z. \tag{3}$$

The value for η is valid to one-loop order, the second equality is exact. The other exponents are still given by the exact Eqs. (2b) above.

These results predict that the transition in $3 - d$, to the extent that it is of second order, is characterized by mean-field exponents with logarithmic corrections. Within the accuracy of existing experiments, this is indistinguishable from Hertz's critical behavior. In addition to explaining why the transition is of first order in some materials, and of second order in others, our theory therefore provides an explanation for the fact that the observed critical behavior in the second order case is mean-field-like. We now sketch the derivation of the above results.

The lesson learned from the disordered quantum ferromagnetic problem [6] is the following: For a reliable analysis of the critical behavior it does not suffice to construct a LGW theory. Rather, in addition to the order parameter fluctuations, all other soft modes that couple to the latter must be kept explicitly and on equal footing. Accordingly, the effective action should consist of a part depending on the order parameter field $\mathbf{M}$, a part depending on the soft fermionic two-particle modes described by a field q, and a coupling between the two,

$$\mathcal{A}[\mathbf{M}, q] = \mathcal{A}_M + \mathcal{A}_q + \mathcal{A}_{M,q}. \tag{4}$$

$\mathcal{A}_M$ is a static LGW functional (the dynamics will be provided by $\mathcal{A}_{M,q}$),

$$\mathcal{A}_M = \int dx \mathbf{M}(x)\,[t - a\nabla^2]\,\mathbf{M}(x) + u \int dx \mathbf{M}^4(x). \tag{5}$$

Here $x \equiv (\mathbf{x}, \tau)$ comprises the real space position $\mathbf{x}$ and the imaginary time τ. $\int dx = \int d\mathbf{x} \int_0^\beta d\tau$ with $\beta = 1/k_B T$. a and u are constants.

The soft fermion field q originates from the composite fermion variables [10]

$$Q_{12} = \frac{i}{2}\begin{pmatrix} -\psi_{1\uparrow}\bar{\psi}_{2\uparrow} & -\psi_{1\uparrow}\bar{\psi}_{2\downarrow} & -\psi_{1\uparrow}\psi_{2\downarrow} & \psi_{1\uparrow}\psi_{2\uparrow} \\ -\psi_{1\downarrow}\bar{\psi}_{2\uparrow} & -\psi_{1\downarrow}\bar{\psi}_{2\downarrow} & -\psi_{1\downarrow}\psi_{2\downarrow} & \psi_{1\downarrow}\psi_{2\uparrow} \\ \bar{\psi}_{1\downarrow}\bar{\psi}_{2\uparrow} & \bar{\psi}_{1\downarrow}\bar{\psi}_{2\downarrow} & \bar{\psi}_{1\downarrow}\psi_{2\downarrow} & -\bar{\psi}_{1\downarrow}\psi_{2\uparrow} \\ -\bar{\psi}_{1\uparrow}\bar{\psi}_{2\uparrow} & -\bar{\psi}_{1\uparrow}\bar{\psi}_{2\downarrow} & -\bar{\psi}_{1\uparrow}\psi_{2\downarrow} & \bar{\psi}_{1\uparrow}\psi_{2\uparrow} \end{pmatrix}. \tag{6a}$$

Here the ψ and $\bar{\psi}$ are the Grassmann-valued fields that provide the basic description of the electrons, and all fields are understood to be taken at position $\mathbf{x}$. The indices 1, 2, etc., denote the dependence of the fields on fermionic Matsubara frequencies $\omega_{n_1} = 2\pi T(n_1 + 1/2)$, etc., and the arrows denote the spin projection. A convenient basis in the space of 4×4 matrices is given by $\tau_r \otimes s_i$ $(r, i = 0, 1, 2, 3)$, with $\tau_0 = s_0$ the 2×2 unit matrix, and $\tau_{1,2,3} = -s_{1,2,3} = -i\sigma_{1,2,3}$, with the σ_i the Pauli matrices. The matrix elements of Q are bilinear in the fermion fields, so Q-Q correlation functions describe two-fermion excitations. In a Fermi liquid, the Q fluctuations are massive and soft, respectively, depending on whether the two frequencies carried by the Q field have the same sign, or opposite signs. We thus separate the Q fluctuations into massless modes, q, and massive modes, P, by splitting the matrix Q into blocks in frequency space [10],

$$Q_{nm}(\mathbf{x}) = \Theta(nm)\,P_{nm}(\mathbf{x}) + \Theta(n)\Theta(-m)\,q_{nm}(\mathbf{x}) + \Theta(-n)\Theta(m)\,q^{\dagger}_{nm}(\mathbf{x}). \tag{6b}$$

In what follows, we will incorporate the frequency constraints expressed by the step functions into the fields P and q, respectively. That is, the frequency indices of q must always have opposite signs.

The massive modes can be formally integrated out to obtain an effective action for the soft modes, q_{nm}. The Gaussian part of the fermionic action has the form

$$\mathcal{A}_q = \frac{-1}{G}\int d\mathbf{x}\,d\mathbf{y}\sum_{1,2,3,4}\mathrm{tr}\,[q_{12}(\mathbf{x})\,\Gamma^{(2)}_{12,34}(\mathbf{x}-\mathbf{y})\,q^{\dagger}_{34}(\mathbf{y})], \tag{7a}$$

where tr traces over the matrix degrees of freedom of Eq. (6a). As we see from Eq. (6a), the q propagator describes particle-hole excitations, which in a clean electron system have a ballistic dispersion relation, i.e., the frequency scales linearly with the wave number. The vertex function $\Gamma^{(2)}$ in momentum space therefore has the form

$$\Gamma^{(2)}_{12,34}(k) = \delta_{13}\,\delta_{24}\,(k + GH|\Omega_{1-2}|). \tag{7b}$$

G and H are model dependent coefficients. A spin-singlet interaction amplitude can be included in the model, but will not be of qualitative importance for our purposes.

The coupling term $\mathcal{A}_{M,q}$ originates from the linear coupling between $\mathbf{M}$ and the electron spin density, which can be expressed in terms of Q by means of Eq. (6a). It is obvious that integrating out the massive field P will result in terms that couple $\mathbf{M}$ with all powers of q, $\mathcal{A}_{M,q} = \mathcal{A}_{M-q} + \mathcal{A}_{M-q^2} + \ldots$. Let us define a matrix magnetization field $B(\mathbf{x})$ by

$$B_{12}(\mathbf{x}) = \sum_{i,r}(\tau_r \otimes s_i)\,(-)^{r+1}\,{}^i_rB(\mathbf{x}), \tag{8a}$$

with components

$${}^r_iB_{12}(\mathbf{x}) = \sum_n \delta_{n,n_1-n_2}[M^i_n(\mathbf{x}) + (-)^{r+1}M^i_{-n}(\mathbf{x})], \tag{8b}$$

The first term in that series can then be written

$$A_{M-q} = c_1T^{1/2}\int d\mathbf{x}\,\mathrm{tr}\,[B(\mathbf{x})\,q(\mathbf{x})]. \tag{9a}$$

The second one has the overall form

$$\mathcal{A}_{M-q^2} \approx c_2T^{1/2}\int d\mathbf{x}\,\mathrm{tr}\,[B(\mathbf{x})\,q(\mathbf{x})\,q^{\dagger}(\mathbf{x})]. \tag{9b}$$

Its detailed structure will be derived elsewhere [11]. c_1 and c_2 are model dependent coupling constants.

The Gaussian field theory defined by the terms bilinear in $\mathbf{M}$ or B and q is easily diagonalized in terms of the paramagnon propagator

$$\mathcal{M}(k,\Omega_n) = 1\Big/\left[t + ak^2 + \frac{(4Gc_1^2/\pi)|\Omega_n|}{k + GH|\Omega_n|}\right], \tag{10a}$$

and the fermion propagator

$$\mathcal{D}(k,\Omega_n) = 1/(k + GH|\Omega_n|). \tag{10b}$$

We now subject the entire action to a RG analysis [12]. We employ a differential momentum-shell RG and integrate over all frequencies. With b the RG length rescaling factor, we rescale wave numbers and the fields via

$$k \to bk, \tag{11a}$$

$$\mathbf{M}_n(\mathbf{x}) \to b^{(d-2+\eta)/2}\mathbf{M}_n(\mathbf{x}), \tag{11b}$$

$$q_{nm}(\mathbf{x}) \to b^{(d-2+\tilde{\eta})/2}q_{nm}(\mathbf{x}). \tag{11c}$$

Here $\mathbf{M}_n(\mathbf{x})$ is the temporal Fourier transform of $\mathbf{M}(x)$, and η and $\tilde{\eta}$ are exponents that characterize the spatial correlations of the order parameter and the fermion fields, respectively. The rescaling of imaginary time, frequency, or temperature is less straightforward. We need to acknowledge the fact that there are two different time scales in the problem, namely, one that is associated with the critical order parameter fluctuations, and one that is associated with the soft fermionic fluctuations. Accordingly, we must allow for two different dynamical exponents, z and $\tilde{z}$, and imaginary time and temperature may get rescaled via either one of two possibilities,

$$\tau \to b^{-z}\tau, \qquad T \to b^{z}T, \tag{11d}$$

$$\tau \to b^{-\tilde{z}}\tau, \qquad T \to b^{\tilde{z}}T. \tag{11e}$$

How these various exponents should be chosen is discussed below.

Within this framework, Hertz's theory corresponds to a fixed point where $\tilde{\eta} = \tilde{z} = 1$, which makes G and H marginal, and $\eta = 0$, $z = 3$, which makes a and c_1 marginal. Power-counting then shows that c_2 is irrelevant for $d > 1$ if the time scale is given by the exponent z, but marginal for $d = 3$ and relevant for $d < 3$ if it is given by $\tilde{z}$. It is easy to find explicit diagrams, starting at one-loop order, where the latter is the case [11]. This establishes that the upper critical dimension, above which Hertz's fixed point is stable, is $d_c^+ = 3$.

To deal with the situation in $d \leq 3$ we go to one-loop order. Perturbation theory, combined with power counting, shows that in $d = 3$ there are no logarithmic corrections to c_1, c_2, G, and t. Motivated by the disordered case

[6], we will be looking for a fixed point where G and c_1 are marginal, which implies $\tilde{\eta} = 1$ and $z + \eta = 3$. As mentioned above, c_2 can have two different scale dimensions, depending on which time scale enters. We require c_2 with the fermionic time scale, corresponding to $\tilde{z}$, to be marginal, which yields $\tilde{z} + \eta = 1$. This leaves η as the only independent scale dimension. The critical time scale makes c_2 irrelevant with scale dimension -1. For the remaining coupling constants to one-loop order we find the flow equations

$$da/d\ln b = -\eta\, a - A_a/H, \tag{12a}$$

$$du/d\ln b = -(2 + \eta)u - A_u c_2^2/H, \tag{12b}$$

$$dH/d\ln b = \eta\, H + A_H/(a + t). \tag{12c}$$

Here c_2 is the irrelevant version of c_2, with flow equation

$$dc_2/d\ln b = -c_2. \tag{12d}$$

$A_u > 0$ is a model dependent positive coefficient. An explicit calculation yields for the other two coefficients, $A_H = 27A_a = 3Gc_2^2/\pi^3$, with c_2 the marginal incarnation of this coupling constant. The ratio $A_H/A_a = 27$ is what determines the critical exponents.

Solving the flow equations, Eqs. (12a)–(12d), at $t = 0$ shows that u becomes negative at a finite scale provided that its bare value satisfies $u^{(0)} < A_u[c_2^{(0)}]^2/A_a$. This results in a fluctuation-driven first order phase transition. Indeed, the generalized mean-field theory for this transition maps onto the one for the superconducting transition at $T > 0$, which is the canonical example of a fluctuation-driven first order transition [13]. However, if the opposite inequality holds, then u remains positive at all scales and the transition is continuous. Notice that within strict perturbation theory the second term on the right-hand side of Eq. (12b) is constant, so the transition is always of first order. This is the RG version of the theory given in Ref. [7]. We note that for sufficiently large t, perturbation theory is valid. If the first order transition predicted by perturbation theory occurs at sufficiently large t, it therefore is unaffected by the fluctuation effects. In order for the generalized mean-field theory of Ref. [7] to be controlled, the magnetization discontinuity must in addition be small.

As we see, fluctuations can qualitatively change the prediction of perturbation theory and drive the transition second order. The mechanism for this is very similar to the fluctuation-driven second order transition in classical Potts models [14]. The point is that the renormalization of a negative loop correction to the u-flow equation can make this term go to zero for large scales sufficiently fast to keep u positive, even if a scale independent loop correction would lead to a negative u. In the case of a second order transition, the critical exponents η, ν, and γ can be obtained by solving Eqs. (12a)–(12d) and substituting the result for $a(\ln b)$ in the paramagnon propagator, Eq. (10a). In $d = 3$ this procedure is tricky since it leads to scale dependent exponents; technical details will be reported elseswhere [11]. The results are given in Eqs. (2a)–(2c). In $d = 3 - \epsilon$ the procedure is straightforward and leads to η as given in Eqs. (3), and to Eqs. (2b). α is most easily obtained from the Gaussian free energy by replacing the Gaussian paramagnon propagator by the critical one. Differentiation with respect to T yields the specific heat. β and δ are most easily obtained from scaling arguments [11], taking into account that u is a dangerous irrelevant operator for the magnetization [12].

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