Breakdown of Landau-Ginzburg-Wilson theory for certain quantum phase transitions

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The quantum ferromagnetic transition of itinerant electrons is considered. It is shown that the Landau-Ginzburg-Wilson theory described by Hertz and others breaks down due to a singular coupling between fluctuations of the conserved order parameter. This coupling induces an effective long-range interaction between the spins of the form $1/r^{2d-1}$. It leads to unusual scaling behavior at the quantum critical point in $1 < d \leq 3$ dimensions, which is determined exactly.

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One of the most obvious examples of a quantum phase transition is the ferromagnetic transition of itinerant electrons at zero temperature T as a function of the exchange coupling between the electron spins. Hertz [1] derived a Landau-Ginzburg-Wilson (LGW) functional for this case in analogy to Wilson's treatment of classical phase transitions, and analyzed it by means of renormalization group methods. He found that the critical behavior in dimensions $d = 3, 2$ is mean-field like, since the dynamical critical exponent z decreases the upper critical dimension d_c^+ compared to the classical case. In a quest for nontrivial critical behavior, Hertz studied a model with a magnetization confined to $d < 3$ dimensions, while the coefficients in the LGW functional are those of a 3-d Fermi gas. For this model he concluded that $d_c^+ = 1$, and performed a $1 - \epsilon$ expansion to calculate critical exponents in $d < 1$. Despite the artificial nature of his model, there is a general belief that the qualitative features of Hertz's analysis, in particular the fact that there is mean-field like critical behavior for all $d > 1$, apply to real itinerant quantum ferromagnets as well.

In this Letter we show that this belief is mistaken, since the LGW approach breaks down due to the presence of soft modes in addition to the order parameter fluctuations, viz. spin-triplet particle-hole excitations that are integrated out in the derivation of the LGW functional. These soft modes lead to singular vertices in the LGW functional, invalidating the LGW philosophy of deriving an effective local field theory in terms of the order parameter only [2]. In Hertz's original model this does not change the critical behavior in $d > 1$, but it invalidates his $1 - \epsilon$ expansion. More importantly, in a more realistic model the same effect leads to nontrivial critical behavior for $1 < d \leq 3$, which we determine exactly.

Our results for realistic quantum magnets can be summarized as follows. The magnetization, m, at $T = 0$ in a magnetic field H is given by the equation of state

$$t\,m + v\,m^d + u\,m^3 = H \quad , \tag{1}$$

where t is the dimensionless distance from the critical point, and u and v are finite numbers. From (1) one obtains the critical exponents β and δ, defined by $m \sim t^\beta$ and $m \sim H^{1/\delta}$, respectively, at $T = 0$. For β and δ, and for the correlation length exponent ν, the order parameter susceptibility exponent η, and the dynamical exponent z, we find

$$\beta = \nu = 1/(d-1), \quad \eta = 3 - d, \quad \delta = z = d, \qquad (1 < d < 3), \tag{2}$$

and $\beta = \nu = 1/2$, $\eta = 0$, $\delta = z = 3$ for $d > 3$. These exponents 'lock into' mean-field values at $d = 3$, but have nontrivial values for $d < 3$. In $d = 3$, there are logarithmic corrections to power-law scaling. Eq. (1) applies to $T = 0$. At finite temperature, we find homogeneity laws for m, and for the magnetic susceptibility, χ_m,

$$m(t,T,H) = b^{-\beta/\nu} m(tb^{1/\nu}, Tb^{\phi/\nu}, Hb^{\delta\beta/\nu}) \quad , \tag{3a}$$

$$\chi_m(t,T,H) = b^{\gamma/\nu} \chi_m(tb^{1/\nu}, Tb^{\phi/\nu}, Hb^{\delta\beta/\nu}) \quad , \tag{3b}$$

where b is an arbitrary scale factor. The exponent γ, defined by $\chi_m \sim t^{-\gamma}$ at $T = H = 0$ and the crossover exponent ϕ that describes the crossover from the quantum to the classical Heisenberg fixed point (FP) are given by

$$\gamma = \beta(\delta - 1) = 1 \quad , \quad \phi = \nu \quad , \tag{4}$$

for all $d > 1$. Notice that the temperature dependence of the magnetization is *not* given by the dynamical exponent. However, z controls the temperature dependence of the specific heat coefficient, $\gamma_V = c_V/T$, which has a scale dimension of zero for all d, and logarithmic corrections to scaling for all $d < 3$ [3],

$$\gamma_V(t, T, H) = \Theta(3-d)\, \ln b + \gamma_V(tb^{1/\nu}, Tb^z, Hb^{\delta\beta/\nu}) \quad . \tag{5}$$

Eqs. (1) - (5) represent the exact critical behavior of itinerant quantum Heisenberg ferromagnets for all $d > 1$ with the exception of $d = 3$, where additional logarithmic corrections to scaling appear. We are able to obtain the critical behavior exactly, yet it is not mean-field like. The exactness is due to the fact that we work above the upper critical dimension $d_c^+ = 1$. The nontrivial exponents are due to a singular coupling between the critical modes which leads, e.g., to the unusual term $\sim v$ in (1). Experimentally, we predict that for 3-d magnets with a very low T_c there is a crossover from essentially mean-field quantum behavior to classical Heisenberg behavior. In $d = 2$, where there is no classical transition, we predict that with decreasing T, long-range order will develop, and the quantum phase transition at $T = 0$ will display the nontrivial critical behavior shown above.

We now sketch the derivation of these results. A more complete account of the technical details will be given elsewhere [4]. We consider a d-dimensional continuum model of interacting electrons, and pay particular attention to the particle-hole spin-triplet contribution [5] to the interaction term in the action, $S^t_{\rm int}$, whose (repulsive) coupling constant we denote by J. Writing only the latter explicitly, and denoting the spin density by $\mathbf{n}_s$, the action reads,

$$S = S_0 + S^t_{\rm int} = S_0 + (J/2)\int dx\ \mathbf{n}_s(x)\cdot\mathbf{n}_s(x) \quad , \tag{6}$$

where S_0 contains all contributions to the action other than $S^t_{\rm int}$. In particular, it contains the particle-hole spin-singlet and particle-particle interactions, which will be important for what follows. $\int dx = \int d\mathbf{x} \int_0^{1/T} d\tau$, and we use a 4-vector notation $x = (\mathbf{x}, \tau)$, with $\mathbf{x}$ a vector in real space, and τ imaginary time. Following Hertz, we perform a Hubbard-Stratonovich decoupling of $S^t_{\rm int}$ by introducing a classical vector field $\mathbf{M}(x)$ with components M^i that couples to $\mathbf{n}_s(x)$ and whose average is proportional to the magnetization, and we integrate out all fermionic degrees of freedom. We obtain the partition function Z in the form

$$Z = e^{-F_0/T}\int D[\mathbf{M}]\ \exp\bigl[-\Phi[\mathbf{M}]\bigr] \quad , \tag{7a}$$

where F_0 is the noncritical part of the free energy. The Landau-Ginzburg-Wilson (LGW) functional Φ reads

$$\Phi[\mathbf{M}] = \frac{1}{2}\int dx\, dy\ \frac{1}{J}\delta(x-y)\mathbf{M}(x)\cdot\mathbf{M}(y) + \sum_{n=2}^{\infty} a_n \int dx_1\ \ldots\ dx_n\ \chi^{(n)}_{i_1\ldots i_n}(x_1,\ldots,x_n)M^{i_1}(x_1)\ \ldots\ M^{i_n}(x_n)\ , \tag{7b}$$

where $a_n = (-1)^{n+1}/n!$. The coefficients $\chi^{(n)}$ in (7b) are connected n-point spin density correlation functions of a reference system with action S_0 [1]. The particle-hole spin-triplet interaction J is missing in the bare reference system, but a nonzero J is generated perturbatively by the particle-particle interaction contained in S_0. The reference system then has all of the characteristics of the full action S, except that it must not undergo a phase transition lest the separation of modes that is implicit in our singling out $S^t_{\rm int}$ for the decoupling procedure breaks down.

$\chi^{(2)}$ is the spin susceptibility of the reference system. Performing a Fourier transform from $x = (\mathbf{x}, \tau)$ to $q = (\mathbf{q}, \Omega)$ with wavevector $\mathbf{q}$ and Matsubara frequency Ω, we have for small $\mathbf{q}$ and Ω [6],

$$\chi^{(2)}(\mathbf{q}, \Omega) = \chi_0(\mathbf{q})[1 - |\Omega|/|\mathbf{q}|] \quad , \tag{8a}$$

where $\mathbf{q}$ and Ω are being measured in suitable units, and $\chi_0(\mathbf{q})$ is the static spin susceptibility of the reference system. We now use the fact that in a Fermi liquid at $T = 0$, χ_0 is a nonanalytic function of $\mathbf{q}$ of the form

$$\chi_0(\mathbf{q}\to 0) \sim {\rm const} - |\mathbf{q}|^{d-1} - \mathbf{q}^2 \quad . \tag{8b}$$

Here we have omitted all prefactors, since they are irrelevant for our purposes. This holds for $1 < d < 3$; in $d = 3$ the nonanalyticity is of the form $\mathbf{q}^2 \ln|\mathbf{q}|$ [7]. Using (8), and with $\int_q = \sum_{\mathbf{q}} T \sum_{i\Omega}$, the Gaussian part of Φ can be written,

$$\Phi^{(2)}[\mathbf{M}] = \int_q \mathbf{M}(q)\bigl[t_0 + c_n|\mathbf{q}|^{d-1} + c_a\mathbf{q}^2 + c_d|\Omega|/|\mathbf{q}|\bigr]\,\mathbf{M}(-q) \quad . \tag{9}$$

Here $t_0 = 1 - \Gamma_t\chi^{(2)}(\mathbf{q}\to 0, \omega_n = 0)$ is the bare distance from the critical point, and c_n, c_a and c_d are constants.

For the same physical reasons for which the nonanalyticity occurs in (8b), the coefficients $\chi^{(n)}$ in (7b) are in general not finite at zero frequencies and wavenumbers. Let us focus in $\chi^{(4)}$, which will be the most interesting one for our purposes. Again, standard perturbation theory shows that it is given schematically by [4]

$$\chi^{(4)} \sim \text{const} + v \int_k \left[|\mathbf{k}| + |\omega_n|\right]^{-4} \sim u + v|\mathbf{p}|^{d-3} \ . \tag{10}$$

Here we have cut off the singularity by means of a wavenumber $|\mathbf{p}|$, and u and v are finite numbers. More generally, the coefficient of $|\mathbf{M}|^n$ in Φ for $|\mathbf{p}| \to 0$ behaves like $\chi^{(n)} = v^{(n)}|\mathbf{p}|^{d+1-n}$. This implies that Φ contains a nonanalyticity which in our expansion takes the form of a power series in $|\mathbf{M}|^2/|\mathbf{p}|^2$.

The functional Φ can be analyzed by using standard techniques [8]. We look for a FP where c_d and either c_n (for $1 < d < 3$), or c_a (for $d > 3$) are not renormalized. This fixes the critical exponents η and z. Choosing the scale dimension of a length L to be $[L] = -1$, standard power counting [8] then yields the scale dimension of $v^{(n)}$ to be $[v^{(n)}] = -(n-2)(d-1)/2$. All non-Gaussian terms are thus irrelevant for $d > 1$, and they all become marginal in $d = 1$ and relevant for $d < 1$. Several features of the critical behavior follow immediately. The critical exponents η and z are fixed by the choice of our FP, and ν and γ as given in (2) and (4) are obtained by considering the $\mathbf{q}$-dependence of the Gaussian vertex (9). We determine the equation of state by taking the term of order $|\mathbf{M}|^4$ in Φ into account. $\chi^{(4)}$ is dangerously irrelevant with respect to the magnetization. We have shown [4] that for scaling purposes the cutoff $|\mathbf{p}|$ in (10) can be replaced by m. From this and (9) we obtain the effective equation of state as given in (1).

These results completely specify the critical behavior at $T = 0$. Their most interesting aspect is the nontrivial exponent values found for $1 < d < 3$, which can nevertheless be determined exactly. The reason for this is the $|\mathbf{q}|^{d-1}$-term in the Gaussian action (9). It reflects the fact that in an interacting electron system, static correlations between spins do not fall off exponentially with distance, but only algebraically like $r^{-(2d-1)}$. This slow decay leads to a long-range interaction in the effective action which falls off like $1/r^{2d-1}$, see (9). The critical behavior of *classical* Heisenberg magnets with such a long-range interaction has been studied before [9].

We now turn to the T-dependence of the specific heat, c_V. We expand the free energy functional (7b) about the expectation value, m, of $\mathbf{M}$ to second order, and then perform the Gaussian integral to obtain the partition function. The free energy is obtained as the sum of a mean-field contribution given by $\Phi[m]$, and a fluctuation contribution given by the Gaussian integral. The latter yields the leading nonanalytic term in the free energy. We find [4] that effectively H and T have the same scale dimension, viz. $d(=z)$, and that at $t = 0$ there is a logarithmic T-dependence of γ_V for *all* $1 < d < 3$. If we put the t-dependence back in, we obtain that the scale dependence of γ_V is given by (5).

For the magnetization the leading T-dependence is given by the mean-field contribution to the free energy. We calculate the temperature corrections to the equation of state (1) and find that for $m >> T$ (in suitable units) m^d in (1) will be replaced by $m^d[1 + \text{const} \times T/m + \ldots]$, while for $m << T$, t is replaced by $t + T^{1/\nu}$. The effective scale dimension of T in m is therefore 1 (*not* z), and we obtain for m and χ_m the homogeneity laws given by (3). Thus, the relevant operator T in (3) reflects the crossover from the quantum to the classical FP rather than dynamical scaling. Accordingly, we have written the T-dependence in (3) in terms of a crossover exponent ϕ which is given by (4).

Next we briefly discuss Hertz's original model, which differs from the one discussed above in two ways. First, the reference ensemble consists of noninteracting electrons. Second, the coefficients $\chi^{(n)}$ are taken to be the correlation functions of a 3-d fermion system. $\chi^{(2)}$ is then simply the Lindhard function, so (8) gets replaced by,

$$\chi^{(2)}(\mathbf{q}, \Omega) = 1 - \mathbf{q}^2 - |\Omega|/|\mathbf{q}| + \ldots \quad . \tag{11}$$

Due to the missing interaction in the reference ensenble, $\chi^{(2)}(\mathbf{q}, 0)$ is now analytic at $|\mathbf{q}| = 0$. The resulting quadratic term in (7b) allows for a Gaussian FP with mean-field static exponents and a dynamical exponent $z = 3$ [1]. Whether this FP is stable depends on the higher $\chi^{(n)}$. Hertz considered only the limit $\mathbf{q} = \Omega = 0$, where all of these terms are finite numbers and irrelevant for $d > 1$. The quartic term is marginal in $d = 1$ and relevant for $d < 1$ [1].

The striking difference between the finite coefficients in Hertz's model and the diverging ones in the realistic model above is due to the latter containing interactions in the reference ensemble. The interactions lead to frequency mixing, and hence to soft particle-hole excitations contributing to the $\chi^{(n)}$ even in the limit of zero external frequency. A similar effect is achieved for noninteracting electrons by considering correlation functions at nonvanishing external frequency. Therefore we include the higher order terms in an expansion of the $\chi^{(n)}$ in powers of Ω and analyze the arising LGW functional by the same power counting arguments as above. The details of this calculation will be presented elsewhere [4]. We find that all non-Gaussian terms are still irrelevant for $d \geq 2$ and the critical behavior is mean-field like. In $d = 1$, however, the $\chi^{(n)}$ change their functional form so that an infinite number of operators is relevant (*not* marginal) with respect to the Gaussian FP in $d = 1$ and below. Therefore the upper critical dimension is *not* one, but rather the 1-d sytem is *below* its upper critical dimension, and will show critical behavior that is substantially different from mean-field behavior.

We conclude with a few remarks. First, the vertices in the LGW functional discussed here are singular only if the order parameter is conserved, and only at zero temperature, which means that the phenomenon is confined to the quantum magnetic transition. Second, our conclusion, although derived for the special example of itinerant quantum ferromagnetism, is rather general: We expect the LGW formalism to break down whenever there are soft modes other than the critical order parameter fluctuations that couple to the order parameter. The general rule is that *all* of the soft modes should be retained on equal footing in the effective theory. If any of them are integrated out, the resulting penalty are ill-behaved coefficients in the LGW functional. This has been shown recently for *disordered* electrons [10]. The present results indicate that the underlying principle is very general. Indeed, it also applies to classical phase transitions with additional soft modes. However, there are many modes that are soft at $T = 0$ but acquire a mass at finite temperature, making quantum phase transitions more likely candidates. Finally, we mention that Sachdev [11] has noted that something must be wrong with Hertz's theory in $d < 1$, since it violates an exact exponent equality for quantum phase transitions with conserved order parameters. He suspected Hertz's omission of the cubic term in the LGW functional to be at fault. Our analysis provides instead the explanation given above, namely the presence of *infinitely* many relevant operators due to the soft particle-hole excitations.

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[1] J. A. Hertz, Phys. Rev. B **14**, 1165 (1976).

[2] We use the term 'LGW theory' in the narrow sense, in which it is usually used in the literature, of an effective field theory in terms of the order parameter field only.

[3] F. J. Wegner, Phys. Rev. B **5**, 4529 (1972), has shown how 'resonance' conditions between critical exponents lead to logarithmic corrections to scaling. Their appearance for a whole range of dimensionalities in (5) is a consequence of the exact relation $z = d$.

[4] T. Vojta, D. Belitz, R. Narayanan, and T.R. Kirkpatrick, unpublished.

[5] See, e.g., A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York 1975), Sec.5.

[6] We are considering $\chi^{(2)}$ in the limit $\mathbf{q} \to 0$, $|\Omega| << |\mathbf{q}|$, since for a conserved order parameter, Ω must be taken to zero *before* $\mathbf{q}$ in order to reach criticality.

[7] The physical origin of this nonanalyticity are mode-coupling effects analogous to those that generate a term $|\mathbf{q}|^{d-2}$ in disordered Fermi systems [10]. We have ascertained the presence of the effect in clean systems by calculating χ_0 perturbatively to second order in the interaction. To that order, the sign of the $|\mathbf{q}|^{d-1}$ term in Eq. (8b) is positive, but higher order terms will presumably lead to a negative sign for realistic values of the interaction, thus allowing for a ferromagnetic ground state. Here we discuss only the latter case. A more complete discussion, including the physical situation for weak interactions, will be given elsewhere [4].

[8] See, e.g., S. K. Ma, *Modern Theory of Critical Phenomena*, (Benjamin, Reading, MA 1976).

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