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Nature of the quantum phase transition to a spin-nematic phase

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It is shown that the quantum phase transition in metallic non-s-wave ferromagnets, or spin nematics, is generically of first order. This is due to a coupling of the order parameter to soft electronic modes that play a role analogous to that of the electromagnetic vector potential in a superconductor, which leads to a fluctuation-induced first-order transition. A generalized mean-field theory for the p-wave case is constructed that explicitly shows this effect. Tricritical wings are predicted to appear in the phase diagram in a spatially varying magnetic field, but not in a homogeneous one.

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Analogies between certain liquid-crystal phases (smectic, cholesteric, nematic, columnar, blue) [1] and ordered states of electrons in solids provide a surprising connection between soft condensed matter and electronic systems. For instance, stripe phases in high-temperature superconductors are analogous to smectics [2, 3], helical magnets are analogous to cholesterics [4], and electronic analogs of nematics can be realized via Pomeranchuk instabilities of the Fermi surface [5]. Stripe and nematic order can occur in the spin channel as well as in the charge channel, and spin nematics provide magnetic analogs of non-s-wave superconductors that have been invoked to explain the enigmatic behavior of $\text{Sr}_3\text{Ru}_2\text{O}_7$ [6, 7] and the ‘hidden order’ in URu_2Si_2 [8].

For a theoretical description of phase transitions, Landau theory is a standard tool [9]. Once an order parameter (OP) ϕ has been identified one constructs all terms in the free energy that are consistent with the general symmetry properties of the system. Replacing the OP field by a constant yields the most general mean-field theory for the phase transition. Fluctuations of the OP can also be considered, which leads to the Landau-Ginzburg-Wilson (LGW) framework that is amenable to an analysis by renormalization-group methods [10]. Landau theory is applicable to both classical transitions that are driven by thermal fluctuations and tuned by changing the temperature T , and quantum transitions at zero temperature that are driven by quantum fluctuations and tuned by a non-thermal parameter such as external pressure or composition [11].

In order to experimentally check the proposals concerning liquid-crystal analogs in electronic systems it is important to predict as many qualitative features of this exotic order as possible. To this end a comprehensive analysis of the Landau theory for an electronic nematic state has been developed, and the quantum phase transition has been analyzed in analogy to Hertz’s theory of s-wave quantum ferromagnets [12], see Ref. 13 and references therein. The theory has been developed for both the spin and the charge channel; here we will focus on the spin channel and especially on the p-wave

case. The OP for a non-s-wave ferromagnet is of the form $\langle \bar{\psi}_a(x) \sigma_{ab}^i f(\partial_x) \psi_b(x) \rangle$, with $\sigma^{1,2,3}$ the Pauli matrices. $\psi = (\psi_\uparrow, \psi_\downarrow)$ is a fermionic spinor field, $\bar{\psi}$ is its adjoint, $x = (\mathbf{x}, \tau)$ comprises the real space position \mathbf{x} and the imaginary time variable τ , f is a tensor-valued monomial function of the gradient operator, and $\langle \dots \rangle$ denotes the quantum mechanical and thermodynamic average. In the p-wave case the function f is linear in the gradient and the OP field thus carries a spin index i and an orbital index α ($i = 1, 2, 3$, $\alpha = 1, 2, 3$). We will denote it by $N_{i,\alpha}(x)$ which in Landau becomes a number $N_{i,\alpha}$. The most general Landau free energy up to quartic order in $N_{i,\alpha}$ has the form [13]

$$F_L = t N_i^\alpha N_\alpha^i + u_1 (N_i^\alpha N_\alpha^i)^2 + u_2 N_i^\alpha N_\beta^i N_\alpha^j N_j^\beta, \quad (1)$$

with a summation convention implied. Depending on the relative values of the Landau parameters u_1 and u_2 there are two distinct phases, the α -phase and the β -phase [13]. They are characterized by $N_{i,\alpha} = n_\alpha \hat{N}_i$ for the α -phase, with \hat{N} a unit vector in spin space, and $N_{i,\alpha} = N \hat{e}_i^{(\alpha)}$ for the β -phase, with N a number and $\hat{e}^{(1,2,3)}$ three mutually orthogonal unit vectors. The Landau theory predicts a second-order transition into either phase at $t = 0$. The corresponding phase diagram is shown in Fig. 1. For the classical transition at $T > 0$ in 3-d fluctuations of the OP will modify the mean-field critical behavior predicted by Eq. (1). For the corresponding quantum phase transition the dynamical critical exponent stabilizes the Gaussian fixed point in 3-d and the LGW theory that generalizes Eq. (1) predicts the transition to be second order with mean-field critical behavior [13].

There are reasons to doubt the validity of the latter prediction. Despite its generality, Landau theory hinges on certain implicit assumptions. One is that an expansion of the free energy in powers of the OP is well behaved, i.e., that the coefficients in a Taylor expansion are finite. The analogous statement within an LGW framework is that the field theory is local. This assumption can be violated if there are soft modes other than the OP fluctuations that couple to the OP. In such a situation, the

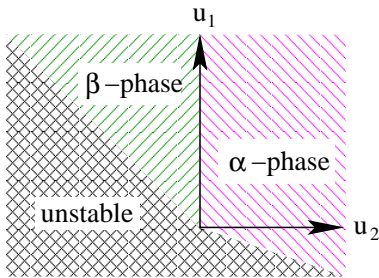


FIG. 1: Phase diagram for the Landau free energy given in Eq. (1). The α and β -phases are stable for $u_2 > 0$, $3u_1 > -u_2$, and $u_2 < 0$, $u_1 > -u_2$, respectively. The Landau theory predicts a second-order transition into either phase at $t = 0$.

construction of a Landau theory entirely in terms of the OP amounts to integrating out these soft modes, which may lead to a non-local theory. Technically, a nonzero OP can give the additional soft mode(s) a mass, which implies that the free energy as a function of the OP cannot be analytic at $\phi = 0$. The resulting changes to the phase transition depend on the properties of the original Landau theory and on the sign of the leading nonanalytic term. A classic example is the case of a type-I or weakly type-II BCS superconductor, where a simple Landau theory predicts a second-order or continuous transition. However, the coupling of the OP to the electromagnetic vector potential leads to an effective free energy that contains a term of cubic order in the OP, which leads to a first-order phase transition [14]. The same is true for the nematic-to-smectic-A transition in liquid crystals, with the nematic Goldstone modes playing a role analogous to that of the vector potential. This phenomenon is known as a fluctuation-induced first-order transition in condensed matter physics, and as the Coleman-Weinberg mechanism for mass generation in particle physics [15]. Another possibility is that the transition remains second order, but the coupling to the additional soft modes changes the universality class. This is believed to be the case deep in the type-II region [16, 17].

For the quantum phase transition from a Fermi liquid to an electronic nematic state there are soft modes in addition to the OP fluctuations, namely, particle-hole excitations that are soft at $T = 0$ and acquire a mass at nonzero T . The question is whether these soft modes couple to the OP in a way that invalidates simple Landau theory. In this Letter we show that they do for spin nematics (but not for charge nematics) and generically lead to a quantum phase transition that is fluctuation-induced first order. For simplicity, we will discuss the p-wave case in three dimensions (3-d) unless noted otherwise.

We will first state and discuss our results, and then sketch their derivation. In a generalized mean-field theory analogous to Ref. 14 that neglects order-parameter fluctuations, but keeps the fermionic degrees of freedom

and their coupling to the OP in a Gaussian approximation one finds, for a 3-d system, an equation of state whose qualitative features are represented by

$$h_N = tN + vN^3 \ln(N^2 + T^2) + uN^3 + o(N^3). \quad (2)$$

Here N is the number-valued OP for the α -phase (the result for the β -phase is structurally the same), $u = u_1 + u_2$, and h_N is the field conjugate to N (more on this below). $v > 0$ is a positive definite Landau coefficient that is given in terms of spin-triplet interaction amplitudes. $o(x)$ denotes terms smaller than x as $x \rightarrow 0$. The Landau parameters t and u are also (weakly) T -dependent, but we explicitly show only the T -dependence of the logarithmic term since it cuts off a nonanalytic dependence on N . For $1 < d < 3$ the corresponding nonanalyticity at $T = 0$ is given by N^d instead of $N^3 \ln N$.

Equation (2) predicts several features that are qualitatively different from the Landau theory of Ref. 13. At $T = 0$, the term $N^3 \ln N$ is negative and larger than N^3 , which drives the transition first order below a tricritical temperature $T_{tc} = \exp(-u/2v)$. At $T = 0$ there is a first-order transition at $t = t_1 > 0$ that preempts the second-order transition predicted by Landau theory and leads to a discontinuous change of N from 0 to $N_1 = \exp[-(1+u/v)/2]$. For t_1 one finds $t_1 = vN_1^2/4$. In the presence of a conjugate field, tricritical wings appear in the parameter space spanned by T , h_N , and t , as is the case at any tricritical point [18]. As a result, we predict the phase diagram to have the same qualitative structure as the one observed for quantum ferromagnets [19, 20], see Fig. 2. There are surfaces (“wings”) of first-order transitions that are bounded by second-order transitions and end in a pair of quantum critical points in the $T = 0$ plane. The quantum critical exponents at these points are mean-field like. We choose as independent the static exponents β and δ , and the dynamical exponent z , i.e., the scale dimension $[T]_c$ of T at criticality. We find

$$\beta = 1/2 \quad , \quad \delta = 3 \quad , \quad z = 3. \quad (3)$$

These exponents are *exact*, since the conjugate field renders massive the fermionic soft modes that, in the absence of a field, lead to the first-order transition described above. β and δ govern the dependence of N on t and h_N , respectively and z determines the temperature scaling of, e.g., the specific heat. The T -dependence of the OP at criticality, however, is *not* given by z for the same reason as in the s-wave case [21, 22]. It is determined by a fluctuation scale $[T]_{\text{fluc}} = 9/(d+1)$ that yields the leading T -dependence for all $d < 5$. For $d = 3$ we find for the deviation δN of N from its value at the critical point

$$\delta N(t_c, h_N^c, T) \propto -T^{4/9}, \quad (4)$$

which also is exact. The continuous transitions at $T > 0$, on the other hand, will be modified by OP fluctuations.

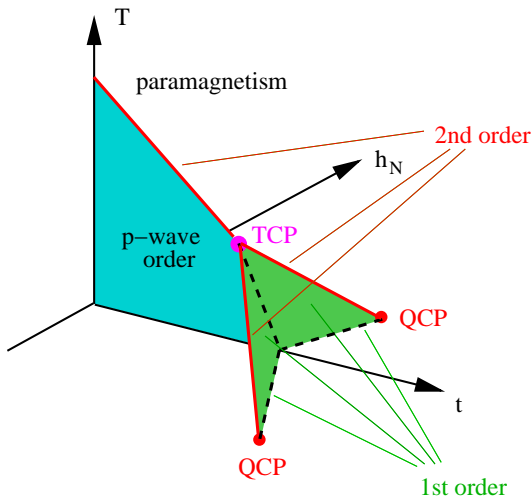


FIG. 2: Schematic phase diagram in the space spanned by T , h_N , and the non-thermal control parameter t . Shown are the region of p-wave order, the tricritical point (TCP), the two quantum critical points (QCP), and the various phase transition lines and surfaces. For $h_N = 0$ the transition is first order above the TCP and second order below. For $h_N \neq 0$ tricritical wings connect the TCP and the two QCPs.

In $d = 2$ there is no long-range order at $T > 0$. However, at $T = 0$ one still has a first-order quantum phase transition, with $N_1 = (3v/4u)^2$, $t_1 = u N_1^2/6$ [23].

These predictions are all analogous to the properties of quantum s-wave ferromagnets [19, 20, 24, 25]. A crucial difference that allows to distinguish the two cases is the nature of the conjugate field. In the s-wave case, it is the physical magnetic field. In the p-wave case (as well as for all higher angular momenta) a homogeneous magnetic field does not couple to the OP. However, a conjugate field h_N is induced by a non-homogeneous magnetic field. For instance, a magnetic field $\mathbf{h}(\mathbf{x})$ with components h_i in two independent directions induces a conjugate field

$$h_N^{i,\alpha}(\mathbf{x}) \propto \epsilon_{ijk} \frac{1}{V} \int d\mathbf{y} h_j(\mathbf{y}) \partial_\alpha h_k(\mathbf{x}) \quad (5)$$

with V the system volume and a prefactor proportional to the p-wave interaction amplitude. A homogeneous field h_N results if $h_k(\mathbf{x})$ is a linear function of position.

To summarize, our theory of low- T p-wave ferromagnets or magnetic nematics predicts a first-order transition at asymptotically low T that is separated from a second-order transition at higher T by a tricritical point (see, however, the third of our concluding remarks below). In this respect it behaves the same way as an ordinary s-wave ferromagnet. However, in contrast to the s-wave case a p-wave ferromagnet is unaffected by a homogeneous magnetic field, whereas in a properly designed inhomogeneous field it shows the same striking tricritical structure found in s-wave ferromagnets [19, 20, 25].

A derivation of these results hinges on an effective the-

ory of soft modes in clean electron systems that will be described in detail elsewhere [26]; here we just sketch some salient features. The building blocks are bilinear products $\bar{\psi}_{n_1}(\mathbf{x}) \psi_{n_2}(\mathbf{y})$ that can be constrained to bosonic, quaternion-valued, fields $Q_{n_1 n_2}(\mathbf{x}, \mathbf{y})$. Here n_1 and n_2 label fermionic Matsubara frequencies $\omega_n = 2\pi T(n + 1/2)$. This was pioneered by Wegner in the context of noninteracting electronic systems with quenched disorder [27, 28], generalized by Finkel'stein to interacting electrons [29, 30], and later elaborated on by the present authors [31]. These theories were all formulated in terms of local density matrix fields $Q_{n_1 n_2}(\mathbf{x}, \mathbf{x})$. Here we need to generalize to non-local phase-space variables $Q_{n_1 n_2}(\mathbf{x}, \mathbf{y})$. For a spherical Fermi surface we expand the Fourier transform of the Q in spherical harmonics Y_l^m ,

$$Q_{n_1 n_2}^{l,m}(\mathbf{k}) = \frac{\sqrt{4\pi}/V}{\sqrt{2l+1}} \sum_{\mathbf{p}} Y_l^m(\Omega_{\mathbf{p}}) Q_{n_1 n_2}(\mathbf{p} + \mathbf{k}/2, \mathbf{p} - \mathbf{k}/2), \quad (6)$$

with $\Omega_{\mathbf{p}}$ the solid angle for the wave vector \mathbf{p} . For our purposes we need an effective theory for soft modes in clean systems. This is a harder problem than the disordered one since in clean systems there are many more soft modes, namely, *all* moments of the phase-space excitations, not just the zeroth one. A Ward identity shows that all $Q_{n_1 n_2}^{l,m}(\mathbf{k})$ with $n_1 n_2 < 0$ are soft. They are the Goldstone modes of a symmetry between retarded and advanced degrees of freedom that is spontaneously broken if the Fermi energy lies within a band; we denote them by $q_{n_1 n_2}^{l,m}(\mathbf{k})$ [32]. The role of the q in the present theory is analogous to that of the vector potential in the case of the BCS transition in Ref. 14. The various angular momentum channels, $l = 0, 1, \dots$, couple and all q -correlation functions scale as the inverse of the wave number which in turn scales as a frequency. In a schematic notation, leaving out all constant prefactors,

$$\langle q_{n_1 n_2}^{l_1, m_1}(\mathbf{k}) q_{n_3 n_4}^{l_2, -m_1}(-\mathbf{k}) \rangle \propto \frac{\delta_{n_1 - n_2, n_3 - n_4}}{|\mathbf{k}| + \Omega_{n_1 - n_2}} \quad (7)$$

with $\Omega_n = 2\pi T n$ a bosonic Matsubara frequency. This structure holds for both noninteracting and interacting electron systems, which reflects the fact that the system in the absence of magnetic order is a Fermi liquid. By integrating out the massive degrees of freedom in a conserving approximation one can construct an effective soft-mode theory in terms of the q only that is analogous to, albeit more complex than, the generalized nonlinear sigma-model for disordered interacting electrons [29, 31]. The generalized mean-field theory discussed above can be derived analogously to the corresponding theory for the s-wave case [24, 33]. The leading coupling between the static, homogeneous OP N and the fermionic soft modes q takes the form $N \text{Tr} [q(\mathbf{k}) q^\dagger(\mathbf{k})]$ where Tr traces over the angular momentum, frequency, and spin degrees of freedom. To leading order in N and q one finds a

fermionic part of the action with the schematic structure

$$\mathcal{A}_q \propto \text{Tr}[(|\mathbf{k}| + \Omega + N) q(\mathbf{k}) q^\dagger(\mathbf{k})]. \quad (8)$$

Upon integrating out q one obtains a contribution to the equation of state that is schematically given by

$$I(N, T) \propto \frac{1}{V} \sum_{\mathbf{k}} T \sum_{n=1}^{\infty} \frac{N k^2 \Omega_n^2}{(k^2 + \Omega_n^2)^2 (k + \Omega_n)^2 + N^2 k^2 \Omega_n^2} \quad (9)$$

with a positive prefactor. $I(N, T)$ appears in the equation of state in addition to the standard Landau terms.

Asymptotic analysis reveals that the singularity at $N = 0$, $T = 0$ takes the form

$$I(N, T = 0) \propto N \begin{cases} \text{const.} - N^{(d-1)} & (1 < d < 3), \\ \text{const.} + N^2 \ln N & (d = 3), \end{cases} \quad (10a)$$

$$I(N, T)/N|_{N \rightarrow 0} \propto \text{const.} + T^{d-1} \quad (1 < d \leq 3). \quad (10b)$$

For $d = 3$, and neglecting the analytic T -dependence of the term linear in N , the v -term Eq. (2) adequately represents the coupling of the soft fermionic modes to the OP (note the absence of a $T^2 \ln T$ term in $d = 3$).

We close with four remarks. First, the coupling of $O(Nqq^\dagger)$ that generates the singular dependence on N is missing from the Hertz-type theory of Ref. 13. It amounts to taking into account fermionic loops in deriving the LGW theory, whereas Hertz theory treats the fermions in a tree approximation. Second, our results do *not* carry over to charge nematics. In that case the OP does not give the q a mass and the Hertz-type LGW theory [13] is valid, consistent with a general argument first given in Ref. 34. Third, the generalized mean-field theory still contains several approximations. The Gaussian approximation for the q is of no qualitative consequence; Fermi-liquid theory ensures that the exact propagators have the same scaling properties as Eq. (7). Higher-order coupling terms between N and the q are irrelevant in a renormalization-group sense and keeping only Eq. (8) suffices. This leaves the mean-field approximation for the OP. This becomes exact in a well-defined limit. $N \neq 0$ gives the q -propagator a mass, see Eq. (8), which defines a length scale $\lambda \propto 1/N$. Together with the magnetic correlation length ξ this defines a Ginzburg parameter $\kappa = \lambda/\xi$. For $\kappa \rightarrow 0$ (extreme type-I case) OP fluctuations are negligible and low- T transition inevitably is first order. For $\kappa > 0$, and especially for $\kappa \gg 1$ (type-II limit), the role of OP fluctuations must be examined. This is a difficult problem that has been studied for classical transitions [16, 17], and to some extent for the quantum s-wave ferromagnetic one [33], but more work is needed on magnetic transitions in this limit. Fourth, all of our conclusions also hold for spin nematics in higher angular momentum channels, only the realization of the conjugate field changes.

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