Quantum phase transitions of magnetic rotons

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Due to weak spin-orbit coupling, the magnetic excitations of itinerant ferromagnet become magnetic rotons, excitations with degenerate minima on a hypersphere at finite wavevector. Using self-consistent Hartree and renormalization group calculations, we study weak fluctuation-driven first-order quantum phase transitions, a quantum tricritical point controlled by anisotropy and non-Fermi liquid behavior associated with the large phase volume of magnetic rotons. We propose that magnetic rotons are essential for the description of the anomalous high-pressure behavior of the itinerant helical ferromagnet MnSi.

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The theory of classical, second-order phase transitions has been extended to quantum phase transitions, especially so in itinerant electron systems. Critical non-Fermi electron-liquid properties and new phases can emerge near the quantum critical point, and unconventional behavior of quantum criticality attracts a lot of current interest. Among different scenarios for unconventional behavior near the phase transition, a generic scenario associated with a large phase space of fluctuational modes has been little explored, even though it is well-known for classical phase transitions. A classical phase transition becomes fluctuation-driven first-order if soft fluctuational modes have a minimum at a nonzero wave vector $|q| = q_0$ on a hypersphere in $D$-dimensional space. In the presence of spin-orbit interaction such soft modes with large phase space appear naturally (see below) in the proximity of a continuous ferromagnetic transition and can be called magnetic rotons (in analogy with roton excitations of superfluid $He^3$). In this letter we present the theory of quantum phase transitions of magnetic rotons.

We show that the large phase volume of magnetic fluctuations with minima at $|q| = q_0$, independent on the direction of $q$, is responsible not only for the first-order nature of the transition and strong non-Fermi liquid damping of itinerant electrons, but also for a new tricritical point controlled by anisotropy. We combine the theory of quantum critical fluctuations, as developed in Refs., with the theory of weak “crystallization” via fluctuation-driven first-order transitions, as developed in Refs.. In addition, the resistivity of itinerant helical ferromagnet and the electron self-energy are calculated due to the scattering of electrons by roton fluctuations as well as the strong tendency towards glassy behavior. Finally, we argue that magnetic rotons form a starting model for the description of the anomalous high pressure behavior of the itinerant helical ferromagnet MnSi.

We introduce a collective magnetization $M(x, \tau)$ along the lines of Refs., valid for a crystal without inversion symmetry, like MnSi, and obtain the effective action $S[M] = S_{dyne}[M] + S_{stat}[M]$ which consists of a dynamic term (see below) as well as the static term

$$S_{stat}[M] = \int d^3x d\tau \left( \frac{\alpha}{2} |M| + u \frac{|M|^4}{4} \right)$$

$$+ \int d^3x d\tau \left( \gamma M \cdot \nabla \times M \right). \quad (1)$$

Here, $i = (x, y, z)$ and $\delta$ determines the proximity to the transition point. The last term is due to the Dzyaloshinskii-Moriya interaction, caused by spin-orbit interaction in non-centrosymmetric crystals. The constant $\gamma \ll \alpha/a$ is small due to the relativistic origin of the spin-orbit coupling. We assume analyticity of the Landau expansion, Eq., and $\alpha, u > 0$, while other scenarios were suggested. We have not included anisotropic terms like $\alpha' \sum_i (\partial_i M_i)^2$ and $u' \sum_i M_i^4$ allowed by crystal symmetry, but smaller by $(q_0a)^2 \ll 1$. Quantitative estimates demonstrate that the Dzyaloshinskii-Moriya interaction is indeed the dom-

FIG. 1: The lowest paramagnon mode of a helical magnet becomes, for weak anisotropy, a magnetic roton with minima for all $|q| = q_0 > 0$. The large phase space of magnetic roton fluctuations is responsible for the unconventional behavior.
inan effect due to spin orbit interaction in MnSi.

Spin-orbit coupling ($\gamma \neq 0$) splits the otherwise degenerate paramagnons into longitudinal and transverse modes (see the Fig.1). The energy of the lowest mode, $E(q) = \Delta_0 + (|q| - q_0)^2/2$, has minima for all $|q| = q_0$, i.e. it is a magnetic roton. The mode corresponds for $\gamma > 0$ to a right handed helical mode. The bare gap $\Delta_0 = \delta - \omega q_0^2/2$, which might be tuned by varying pressure or chemical composition, will be renormalized, $\Delta_0 \to \Delta$, due to interactions. If $\Delta$ is much smaller than $\omega q_0^2$, the energy difference between the roton and the other modes, those modes can be omitted for $k_B T < \omega q_0^2$.

The dynamic part of the action depends on the coupling between magnetic rotons and particle-hole excitations. If the roton gap $\Delta$ is inside the particle-hole “stripe” in $(\omega, q)$-space, the damping is linear in frequency $2$: $S_{\text{dyn}} = \int_q |\omega q_1| |M|^2$. Here $\int_q = T \sum_n \frac{d^2q}{(2\pi)^2}$ and $\Gamma \equiv \frac{E^2_q}{\omega}$ with fermion-roton coupling constant, $g$. Since in general, it is complicated (especially in ordered helical states) to describe the particle-hole excitations[17] and thus the spectrum and damping of rotons, we introduce, for simplicity, the variable dynamic exponent $z$ via $|\omega| \to E_F (\frac{|\omega|}{E_F})^{1/z}$. $z = 2$ corresponds to the over-damped case, while $z = 1$ to the undamped case. As we will show, distinct universality classes occur for different $z$-values, making it natural to allow $z$ to vary. In fact, $\varepsilon = 3 - z$ plays a role similar to the $D - 4$ expansion parameter in classical critical phenomena.

Considering solely fluctuations of the lowest mode we obtain the effective low energy action

$$S = \frac{1}{2} \int_q \chi^{-1}_{q} \varphi_q \varphi_{-q} + \int_{q_1,q_2,q_3} \frac{\lambda(q)}{4} \varphi_{q_1} \varphi_{q_2} \varphi_{q_3} \varphi_{q_4}$$

with $q_4 = -q_1 - q_2 - q_3$ and

$$\lambda^{-1}_{q}(r_0) = |\omega|^{2/z} + r_0 + (|q| - 1)^2$$

expressed in terms of dimensionless variables: $q \to q/\theta_0$ for momenta, $r_0 = \Delta_0/(\alpha q_0^2/2)$ for the roton gap, $\omega \to \omega (2E_F/\Gamma \theta_0^2)^{1/z}$ for frequencies and $\lambda \sim \omega q_0^{D+z-4}$ for the coupling constant. Notice that for $D = 3$ the coupling constant $\lambda \ll 1$ is small for $z > 1$, making a weak coupling expansion much better defined than in the classical limit[11]. The momentum dependence,

$$\lambda_{q_1,-q_1,q_2,-q_2} = \frac{4}{3} (3 + (q_1 \cdot q_2)^2)$$

results from the projection onto the roton mode. It is useful to introduce two coupling constants: $\lambda$ averaged over the angle between $q_1$ and $q_2$ (i.e. for generic angles) and $\lambda_{||}$ where all wave vectors are parallel[11]. For a momentum independent initial interaction, $\lambda_{||} = \frac{\pi}{2} \lambda = \lambda$. A weak momentum dependence of $u$ can change $\lambda/\lambda_{||}$ further. Many anomalies related to rotons stem from the fact that, at low energies, the integrals over momenta are essentially one-dimensional and that $\lambda_{||}$ renormalizes qualitatively different from $\lambda$.

The nature of the phase transition can be understood from an analysis of the roton gap $r$ and the interaction vertex $\lambda(q)$. A self-consistent equation for the gap within Hartree approximation, valid for small $\lambda$, can be obtained from the Dyson equation for the field propagator: $r = r_0 + \lambda \Sigma_H(r)$, with singular Hartree self-energy,

$$\Sigma_H(r) = \int_q \chi_{q}(r) = \frac{\lambda^{z-1} - r^{z-1}}{2\pi^2 (z-1)}$$

proportional to the local fluctuations of the magnetization, and physical roton gap, $r$. $\Lambda$ is the upper momentum cutoff. For $0 < z \leq 1$ the fluctuations of the local magnetization diverge as $r \to 0$, like for the classical ($T \neq 0K$) fluctuation-driven 1st-order transition explored by Brazovskii[11]. In contrast, $\Sigma_H(r \to 0)$ stays finite for $z > 1$, relevant for itinerant magnets, and no disordered state is allowed for $r_0 < -\lambda \Sigma_H(0)$. In the ordered state, the gap of magnetic rotons

$$r = r_0 + \lambda \Sigma_H(r) + 6\lambda |m_0|^2$$

is obtained by adding the Hartree energy due to an helical order parameter with amplitude $m_0$. $m_0$ is determined by the equation of state

$$m_0 r = 3\lambda_{||} \kappa m_0^3$$

with $\kappa = 2\lambda/\lambda_{||} - 1$. For $r_0$ smaller than the value $r_0^{\text{spinodal}} = -\lambda \Sigma_H(0) + c_3 \lambda (\lambda \kappa)^{3/2}$ and $z \leq 3$ three extrema of the energy exist if $\kappa > 0$. $c_3$ is of order unity. Decreasing $r_0$, the lowest energy solution jumps from $m_0 = 0$ in the disordered phase to $m_0 \neq 0$ in the ordered phase. The roton mass $r$ discontinuously jumps to a larger value in the ordered state. The regime of metastability, $r_0^{\text{spinodal}} + \lambda \Sigma_H(0)$, vanishes as $\kappa \to 0$. For $\kappa < 0$, $m_0 = 0$ is the only solution of the equation of state, but solutions exist for several ordering directions of $q_0$ (see below). For $1 < z \leq 3$, the phase transition remains 1st-order for $\kappa > 0$, despite the fact that the Hartree energy does not diverge as $r \to 0$. It is important to notice that for $r \to 0$ the $r$-dependent part of the self-energy remains the dominant one: $r(z-1)^2 \gg r_0 + \lambda \Sigma_H(0)$.

A direct way to demonstrate the 1st-order nature of phase transition is to analyze the renormalized interaction vertex $\lambda'$. The dominant renormalization of this interaction comes from the polarization “bubble” diagrams. The polarization “bubble” is defined as $\Pi(r) = \int_q \chi_q(r)^2$ and behaves as $\Pi(r) = -\frac{\delta \Sigma_H(r)}{\delta \gamma} \sim r^{(z-3)/2}$. It is necessary to account for a constructive interference between two channels of zero total momentum[11]. Still, the perturbation series is dominated by terms due to $\Pi(r)$ (for a proof see below). The summation of the leading terms gives: $\lambda'^r = \lambda_{||} \frac{1-\lambda M(r)}{1+\lambda M(r)}$. If $\Pi(r \to 0)$ diverges,
λ^r changes sign for κ > 0, implying a 1st-order transition. The renormalized vertex \( \langle \lambda^r \rangle = \frac{\lambda^r}{1+\text{AH}(r)} \) with generic angle between momenta behaves differently, and does not change sign. The case \( z > 3 \), corresponds to an ordinary 2nd-order phase transition above the upper critical dimension. In contrast, \( z \leq 1 \) corresponds to the dimensionality below the lower critical dimension for second order transitions. Therefore we have to distinguish between two classes of fluctuation-driven 1-order transitions characterized by diverging \( z \leq 1 \) “classical like” and non-diverging \( (1 < z \leq 3 \text{ “quantum”}) \) local fluctuations.

In the two-loop approximation, an important difference between an ordinary \( \phi^4 \)-theory and the roton field theory becomes evident. Diagrams not taken into account in the above renormalized vertices, \( \lambda^r \) and \( \lambda^l \), are small by a factor \( r(D-1)/2 \) which comes from the angle integration if the total momentum of the propagators inside the “bubble” is not zero. This implies in case of \( \lambda^l = \lambda^r \), where the 1st-order transition occurs if \( 1-\text{AH}(r) < 0 \), or \( r(D-1)/2 \approx \lambda \), that self-consistency of the Hartree solution is guaranteed by the condition \( \lambda^{(D-1)/(3-z)} \ll 1 \), much less stringent than for classical systems [11].

In the case \( \lambda^l = 2\lambda^r (\kappa = 0) \) the system is right between a regime with a fluctuation induced first order transition and a regime where the equation of state gives \( m_0 = 0 \), suggesting the existence of a new critical end point or a tricritical point. Insight into the roton model can then be gained by using a renormalization group approach, following Ref. [11][18]. As suggested by our earlier calculation, the two coupling constants, \( \Lambda \) and \( \lambda^l \), renormalize qualitatively different. We obtain the flow equations:

\[
\frac{d\lambda^l}{dl} = \varepsilon\lambda - \lambda^2 f\left(Te^{z_l}, r(l)\right)
\]

\[
\frac{d\lambda^r}{dl} = \varepsilon\lambda^r - 2\lambda^r f\left(Te^{z_r}, r(l)\right)
\]

(7)

and together with a corresponding flow equation for \( r(l) \).

Here \( f\left(T, r\right) = 3 \int_q \lambda^2 (r) \) with shell integration over momenta \( \Lambda/e^\varepsilon < |q - q_0| < \Lambda \). In agreement with the previous paragraph, our calculation is controlled if \( \varepsilon = 3 - z \) is small. The zero temperature flow is shown in Fig.2a and is characterized by an unstable fixed point \( \lambda^r = 2\lambda^r \propto \varepsilon \). The flow away from this fixed point is towards \( \lambda^l \rightarrow \pm \infty \) and \( \lambda^r \rightarrow \lambda^r \). The fixed point can only be reached by tuning \( r \) and the ratio \( \lambda^l \), i.e. it is a tricritical point or a critical end point, see also Fig.2b.

The flow towards \( \lambda^l \rightarrow \pm \infty \) corresponds to a fluctuation induced first order transition [21]. If \( \lambda^l \) (changes sign at the same scale where scaling stops \( r(l) = 1 \) we obtain the bare roton gap at the spinodal, \( r_0, \text{spinodal} \), identical to the result obtained within the Hartee approach.

Close to the fixed point we can perform a scaling analysis. The free energy of rotons to first order in \( \varepsilon \) is

\[
F\left(\tilde{\rho}, \tilde{\lambda}^l, T, h\right) = b^{-1+z} F\left(\tilde{\rho}^{1/\nu}, \tilde{\lambda}^l, T b^\nu, h b^{\mu}\right)
\]

(8)

where \( \nu^{-1} = 2 - \frac{3+\varepsilon}{2} \). \( b \) is a scaling parameter and \( \tilde{\rho} \) and \( \tilde{\lambda}^l \) are the deviations of \( r \) and \( \lambda^l \) from their fixed point values, respectively. \( h \) is a field conjugate to the order parameter with \( y_h = \frac{\Lambda^r}{2} \). Scaling arguments yield for the correlation length \( \xi\left(\tilde{\rho}\right) \approx \tilde{\rho}^{-\nu}\), \( \xi\left(\tilde{\rho}\right) \approx \tilde{\rho}^{-\nu}\), and \( \xi\left(T\right) \approx T^{-\frac{1}{\nu}}\), depending on how one approaches the critical point. Varying temperature at the fixed point gives \( C \sim T^2 \) for the singular contribution to the specific heat and \( T_1^{-1} \sim T^{-\frac{1}{2}} \) for the NMR spin lattice relaxation rate. The discontinuity of the order parameter at the first order transition vanishes like \( m \sim \tilde{\rho}^{\frac{2}{1+z}} \) as one approaches the fixed point. All these results require \( z > 2 \) such that an additional \( \nu \phi^6 \) interaction is irrelevant.

Finally, we discuss the flow \( \lambda^l \rightarrow \infty \), which occurs when the bare values obey \( \tilde{\lambda} = 2\lambda^l \). From the equation of state follows that \( m_0 = 0 \) is the only allowed solution. However, for \( z > 1 \), the renormalized roton gap vanishes for \( r \rightarrow -\lambda \mu \zeta(0) \). If \( r \) becomes arbitrarily small there will be a crossover scale where the ignored anisotropy terms, no matter how small, dominate the low energy physics. States on the hypersphere are not degenerate anymore, and only isolated points of low energy excitations become relevant. The universality class is then the quantum version of the theory analyzed in Ref. [21] (see Ref. [17]). For \( D = 3 \) and \( z = 2 \) a mean field second order transition to a state with fixed direction of the helix occurs.
A crucial difference of the two ordered states reached on either side of the tricritical point is that the helix direction in the second order case is determined by anisotropies and therefore fixed, whereas it is arbitrary in case of the first order transition. In view of MnSi, we propose that this fixed point is the quantum critical end point \(15\) of the observed \((p, T) = (12\text{ kbar}, 12\text{ K})\) tricritical point \(7\) and might be reachable if one varies another thermodynamic variable like chemical composition.

The equation of state was obtained under the assumption of a single ordering direction of \(q_0\). However, following Ref.\(10, 22\) one can study more complex choices, like a sum over helix configuration with varying direction of \(q_0\). In case of large number of distinct directions (i.e. an amorphous superposition of helix domains) the equation of state changes and we obtain, just like in the classical case, that these amorphous configurations occur first, at least in form of metastable solutions. This is consistent with the recent results of Ref.\(24\) who showed within a replica mean field approach to a similar model that the low temperature state might not be perfectly ordered but rather be characterized by a distribution of defects of the perfectly ordered state with glassy properties. Thus in the regime of the 1\textsuperscript{st}-order transition the system becomes sensitive with respect to the smallest amounts of random field disorder and forms a self-organized glass.

If the low energy physics is dominated by the quantum tricritical point for \(\alpha q_0^2/2 \gg kT \gg \Delta = \alpha q_0^2 r/2\), we can also study the effects on fermions scattered by magnetic rotons. Since the phase volume of magnetic rotons is large, the non-Fermi-liquid properties are even more dramatic than close to a 2\textsuperscript{nd}-order quantum phase transitions\(2, 23\). Using a local contact coupling with coupling constant \(g\), we find the frequency dependence of the self-energy of fermions\(27\)

\[
\Sigma(k_F, \omega) \propto \frac{g_0 q_0^2 T^{1/2}}{k_F^2} \left( \frac{\omega}{E_F} \right)^{\frac{1}{2}} \tag{9}
\]

(up to a numerical factor), whereas the momentum dependence of the self energy and the corrections to the fermion-roton vertex are nonsingular. The absence of singular vertices and the existence of a small coupling constant are the key reasons why the the non-Fermi-liquid nature of the fermions does not cause feedback onto the collective roton mode, see also Ref.\(26\). Note, Eq. \(9\) was previously obtained in Ref.\(9\) for \(z = 2\). Using the variational approach to the Boltzmann equation or alternatively a quantum transport theory gives for the resistivity the result \(\rho \propto T^{\frac{z-1}{z}}\), where

\[
\rho \propto \int d^Dkd^Dk' T_{k,k'} (1 - \cos \theta_{k,k'}) \tag{10}
\]

is determined by the angle \(\theta_{k,k'}\) between \(k\) and \(k'\) and the scattering matrix \(T_{k,k'}\), determined by \(\text{Im} \chi_{q,\omega}\) (see Ref.\(17\)). Away from the quantum tricritical point, this behavior is only expected at higher temperatures, \(kT \gg \Delta\).

Magnetic rotons - magnetic excitations with a minima on a hyper-sphere - were recently directly observed in a weak itinerant helical ferromagnet MnSi by elastic neutron scattering\(8\). In agreement between theory and experiment the magnetic phase transition is weakly 1\textsuperscript{st}-order type in the range of pressures close to critical pressure and 2\textsuperscript{nd}-order type away from critical pressure. The resistivity in the disordered high-temperature phase shows \(\sqrt{T}\)-behavior\(27\), which is consistent with our result using \(z = 2\) for the dynamic exponent due to conventional Landau damping.

In summary, we have shown that helicoidal magnets with weak anisotropy of the helix direction display a rich spectrum of interesting properties. We showed that the system is governed by a quantum tricritical point with accompanied non-Fermi liquid behavior of the electrons. We propose that the (dis)ordered state is likely characterized by an amorphous superposition of domains with different helix directions.

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\[\text{References}\]

[1] S. Sachdev, Quantum Phase Transitions (Cambridge Univ. Press 1999).
[2] J. A. Hertz, Phys.Rev. B 14, 1164 (1976).
[3] A. J. Millis, Phys.Rev. B 48, 7183 (1993).
[4] J. Custers, et al., Nature 424, 524 (2003).
[5] Q. Si, et al., Nature 413, 804 (2001); P. Coleman and C. Pepin, Physics B 312, 383 (2002).
[6] T. Senthil, M. Vojta, S. Sachdev, cond-mat/0305193
[7] C. Pfleiderer, S.R. Julian, and G.G. Lonzarich, Nature 414, 427 (2001).
[8] C.Pfleiderer, D. Reznik, L.Pintschovious, H.v. Lohneysen, M. Garst, A. Rosch, Nature 427, 227 (2004).
[9] A. Dyugaev, Sov. Phys. JETP, 43, 1247 (1976); ibid 56, 567 (1982).
[10] S.A.Brazovskii, Sov.Phys. JETP 41, 85 (1975).
[11] P.C.Hohenberg, J.B.Swift, Phys.Rev. E52, 1828 (1995).
[12] M. Kataoka, O. Nakanishi, Journal of the Phys.Soc. of Japan 50, 3888 (1981).
[13] H. Yamada and K. Terao, Phys. Rev. B 59, 9342 (1999).
[14] S. Misawa, Journal of Phys.Soc. of Japan 68, 32 (1999); D. Belitz, T. R. Kirkpatrick and T. Vojta, Phys. Rev. Lett. 82, 4707 (1999).
[15] T. Vojta and R. Sreenepke, Phys. Rev. B 64, 052404 (2001). Whether Refs.\[13, 14\], which did not include spin-orbit coupling, Ref.\[15\] or our theory distinctly explain
the behavior of MnSi requires further experimental and theoretical investigation.

[16] M. L. Plumer, J. Phys. C 17, 4663 (1984).
[17] T. Moriya, Spin Fluctuations in Itinerant Electron Magnetism, Springer-Verlag (1985).
[18] R. Shankar, Rev. Mod. Phys. 66, 129 (1994).
[19] A. J. Millis, A. J. Schofield, G. G. Lonzarich, and S. A. Grigera, Phys. Rev. Lett. 88, 217204 (2002).
[20] D. J. Amit, Field theory, the renormalization group and critical phenomena, World Scientific (1984).
[21] P. Bak and M. Hogh Jensen, J. Phys. C 13, L881 (1980).
[22] S. A. Brazovskii, I. E. Dzyaloshinskii and A. R. Muratov, Sov. Phys. JETP, 66 625 (1987).
[23] G.G. Lonzarich, in The Electron, edited by M. Springford (Cambridge University Press, Cambridge, 1996).
[24] H. Westfahl Jr., J. Schmalian and P. G. Wolynes, Phys. Rev. B 68, (2003).
[25] T. Holstein, R.E. Norton, and P. Pincus, Phys.Rev. B 8, 2649 (1973).
[26] Ar. Abanov, A. V. Chubukov and J. Schmalian, Adv. in Physics 52, 119 (2003).
[27] F.P. Mena, D. Van Der Marel, A. Damascelli, M. Fath, A. A.Menovsky, J. A. Mydosh, Phys. Rev, B 67, 241101 (2003).