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Thomas Vojta
Missouri University of Science and Technology, vojtat@mst.edu

Rastko Sknepnek

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Quantum phase transition of itinerant helimagnets

Thomas Vojta[1,2] and Rastko Sknepnek[1]
[1]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany
[2]Theoretical Physics, University of Oxford, Oxford OX1 3NP, United Kingdom

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We investigate the quantum phase transition of itinerant electrons from a paramagnet to a state which displays long-period helical structures due to a Dzyaloshinskii instability of the ferromagnetic state. In particular, we study how the self-generated effective long-range interaction recently identified in itinerant quantum ferromagnets is cut off by the helical ordering. We find that for a sufficiently strong Dzyaloshinskii instability the helimagnetic quantum phase transition is of second order with mean-field exponents. In contrast, for a weak Dzyaloshinskii instability the transition is analogous to that in itinerant quantum ferromagnets, i.e., it is of first order, as has been observed in MnSi.

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Quantum phase transitions are phase transitions that occur at zero temperature as a function of some nonthermal control parameter like pressure, magnetic field, or chemical composition. While the usual finite-temperature phase transitions are driven by thermal fluctuations, zero-temperature quantum phase transitions are driven by quantum fluctuations which are a consequence of Heisenberg's uncertainty principle. Quantum phase transitions have attracted considerable attention in recent years, in particular since they are believed to be at the heart of some of the most exciting discoveries in modern condensed-matter physics, such as the localization problem, the quantum Hall effects, various magnetic phenomena, and high-temperature superconductivity.[1–5]

One of the most obvious examples of a quantum phase transition is the transition from a paramagnetic to a ferromagnetic metal that occurs as a function of the exchange coupling between the electron spins. In a pioneering paper this transition was studied by Hertz[6] who generalized Wilson's renormalization-group to quantum phase transitions. The finite-temperature properties were later discussed by Millis.[7] Building on these results the theory of the ferromagnetic quantum phase transition has recently been worked out in much detail. It was shown that in a zero-temperature correlated itinerant electron system additional noncritical soft modes couple to the order parameter. This effect produces a (self-generated) effective long-range interaction between the spin fluctuations, even if the microscopic exchange interaction is short ranged.[8] In a clean system the resulting ferromagnetic quantum phase transition is generically of first order.[9]

The experimentally best studied example of such a transition is probably provided by the pressure-tuned transition in MnSi.[10,11] MnSi belongs to the class of nearly or weakly ferromagnetic metals. These materials are characterized by strongly enhanced spin fluctuations. Thus their ground state is close to a ferromagnetic instability which makes them good candidates for actually reaching the ferromagnetic quantum phase transition experimentally. At ambient pressure MnSi is paramagnetic for temperatures larger than $T_c = 30$ K. Below T_c it orders magnetically. The phase-transition temperature can be reduced by applying pressure, and at about 14 kbar the magnetic phase vanishes altogether. Thus at 14 kbar MnSi undergoes a magnetic quantum phase transition. The properties of this transition are in semiquantitative agreement with the theoretical predictions,[9] in particular, the quantum phase transition is of first order while the thermal transition at higher temperatures is of second order.[12]

However, the magnetic order in MnSi is not exactly ferromagnetic but a long-wavelength (190-Å) helical spin spiral along the (111) direction of the crystal. The ordering wavelength depends only weakly on the temperature, but a homogeneous magnetic field of about 0.6 T suppresses the spiral and leads to ferromagnetic order. The helical structure is a consequence of the so-called Dzyaloshinskii mechanism,[13,14] an instability of the ferromagnetic state with respect to small "relativistic" spin-lattice or spin-spin interactions. The helical ordering in MnSi immediately leads to the question, to what extent the properties of the quantum phase transition in MnSi are generic for itinerant quantum ferromagnets or whether the agreement between the experiments and the ferromagnetic theory is accidental.

In this paper we therefore study how the long-period helimagnetism caused by a Dzyaloshinskii instability influences the properties of the quantum phase transition of an itinerant magnet. Our starting point is the effective action for the spin degrees of freedom in a three-dimensional itinerant quantum magnet. This action can be derived from a microscopic model of interacting electrons.[8] In terms of the magnetization $\mathbf{M}$ the action reads

$$S_{\mathrm{FM}}[\mathbf{M}] = \frac{1}{2}\int dx dy \mathbf{M}(x)\Gamma_0(x-y)\mathbf{M}(y) - \sum_{n=3}^{\infty}\frac{(-1)^n}{n!}\int dx_1\cdots dx_n \chi^{(n)}(x_1,\ldots,x_n) \times \mathbf{M}(x_1)\cdots\mathbf{M}(x_n). \tag{1}$$

We have used a four-vector notation with $x=(\mathbf{r},\tau)$ comprising a real space vector $\mathbf{r}$ and imaginary time τ. Analogously, $\int dx = \int d\mathbf{r}\int_0^{1/T} d\tau$, where T is the temperature. The bare Gaussian vertex Γ_0 is proportional to $(1-J\chi^{(2)})$ where J is the spin-triplet (exchange) interaction amplitude and $\chi^{(2)}$ is the spin susceptibility of a reference system which is a Fermi liquid (precisely, it is the original electron system with the bare spin-triplet interaction taken out). For the purpose of this paper we can consider the Fourier transform $\Gamma_0(\mathbf{k},\omega)$ of the Gaussian vertex in the limit of long wavelengths and low frequencies, $|\mathbf{k}|\ll k_F$ and $\omega\ll\epsilon_F$, since we are interested in spiral states whose wavelength is large compared to the Fermi wavelength and in long-wavelength low-frequency fluctuations around such states. In this limit Γ_0 is given by[8]

$$\Gamma_0(\mathbf{k},\omega)=t_0+B_1k^2+C_3k^2\ln(1/k)+C_\omega\frac{|\omega|}{k}. \tag{2}$$

The third term in $\Gamma_0(\mathbf{k},\omega)$ merits particular attention. It represents an effective long-range interaction induced by the coupling between the magnetization and additional noncritical soft modes in a zero-temperature electronic system. Generically, this interaction is repulsive, i.e., $C_3<0$, but rather weak, $|C_3|\ll B_1$, since it is caused by electronic correlations. In the ordered phase the magnetization M cuts off the logarithmic singularity, and the term qualitatively takes the form $C_3M^4\ln(1/M)$ which leads to a first-order phase transition.[9] The nucleation length scale l_{Nucl} associated with this transition is given by the length at which the B_1 and C_3 terms in the Gaussian vertex (2) are equal and opposite, i.e., $\ln(l_{\mathrm{Nucl}})\sim B_1/|C_3|$. The coefficients $\chi^{(n)}$ of the higher-order terms in Eq. (1) are proportional to the higher spin-density correlation functions of the reference system. Because of the same mode-coupling effects that lead to the nonanalytic C_3 term in the Gaussian action they are in general not finite in the limit of zero frequencies and wave numbers. For $\mathbf{p}\to 0$ they behave like $\chi^{(n)}\sim v^{(n)}|\mathbf{p}|^{4-n}$.

We now add a new term, the helical or Dzyaloshinskii term,[13,14] to the effective action (1):

$$S[\mathbf{M}]=S_{\mathrm{FM}}[\mathbf{M}]+D\int dx\,\mathbf{M}(x)\cdot\mathrm{curl}\mathbf{M}(x). \tag{3}$$

This term will cause an instability of the ferromagnetic state. Physically, it may be caused by relativistic interactions between spins of the form $\mathbf{S}_i\times\mathbf{S}_j$. Therefore it will generically be small compared to the other Gaussian terms, with the possible exception of the long-range C_3 term. The Dzyaloshinskii term defines a new length scale l_{Spiral} which is the length at which the Dzyaloshinskii term and the conventional gradient (B_1) term in the action are of the same strength, $l_{\mathrm{Spiral}}\sim B_1/|D|$.

Clearly, the qualitative properties of the helimagnetic quantum phase transition crucially depend on the ratio of the two length scales l_{Spiral} and l_{Nucl}. Let us first discuss the two possible scenarios qualitatively: In the case $l_{\mathrm{Spiral}}\ll l_{\mathrm{Nucl}}$, i.e., for a strong Dzyaloshinskii instability or weak electronic correlations the growing magnetic correlation length first reaches l_{Spiral} when approaching the quantum phase transition. Therefore the system crosses over from ferromagnetic to helimagnetic behavior *before* the self-generated effective long-range interaction becomes sufficiently strong to induce a first-order transition. The dominant fluctuations close to the quantum phase transition are therefore of spiral character. In the opposite case, $l_{\mathrm{Spiral}}\gg l_{\mathrm{Nucl}}$, i.e., a weak Dzyaloshinskii instability or strong electronic correlations, the magnetic correlation length first reaches l_{Nucl}, and the system undergoes a first-order phase transition. In this case, the dominant fluctuations close to the quantum phase transition are of ferromagnetic nature even though the ordered state is a spiral. Therefore the properties of the transition are completely analogous to that of the ferromagnetic quantum phase transition.

After this qualitative discussion we now analyze the action (3) in more detail. In order to determine the character of the ordered state we begin with a saddle-point-level investigation of the Gaussian term of the action. In the presence of the Dzyaloshinskii term, the Gaussian action is minimized by a state $\mathbf{M}(x)$ which is periodic in space but homogeneous in imaginary time:

$$\mathbf{M}(\mathbf{r},\tau)=\mathbf{A}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}+\mathbf{A}^*_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}. \tag{4}$$

Here $\mathbf{A}_{\mathbf{k}}=\mathbf{a}_{\mathbf{k}}+i\mathbf{b}_{\mathbf{k}}$ is a complex vector. Inserting this ansatz into the action (3) we obtain

$$S^{\mathrm{SP}}(\mathbf{k})=[t_0+B_1k^2+C_3k^2\ln(1/k)]|\mathbf{A}_{\mathbf{k}}|^2 + iD\mathbf{k}\cdot(\mathbf{A}_{\mathbf{k}}\times\mathbf{A}^*_{\mathbf{k}})+O(|\mathbf{A}_{\mathbf{k}}|^4). \tag{5}$$

The Gaussian part of $S^{\mathrm{SP}}(\mathbf{k})$ is minimized for $|\mathbf{a}_{\mathbf{k}}|=|\mathbf{b}_{\mathbf{k}}|$ and $\mathbf{a}_{\mathbf{k}}\perp\mathbf{b}_{\mathbf{k}}$. The sign of D determines the handedness of the resulting spin spiral. For $D>0$ the minimum action is achieved for $\mathbf{k}$ antiparallel to $\mathbf{a}_{\mathbf{k}}\times\mathbf{b}_{\mathbf{k}}$, this is a right-handed spiral. In contrast, for $D<0$ the vector $\mathbf{k}$ must be parallel to $\mathbf{a}_{\mathbf{k}}\times\mathbf{b}_{\mathbf{k}}$, leading to a left-handed spiral. Taking all these conditions into account the saddle-point action reads

$$S^{\mathrm{SP}}(\mathbf{k})=[t_0+B_1k^2+C_3k^2\ln(1/k)-2|D|k]|\mathbf{A}_{\mathbf{k}}|^2 + O(|\mathbf{A}_{\mathbf{k}}|^4). \tag{6}$$

The term in brackets is minimized by the ordering wave vector $\mathbf{K}$. Since in general $|D|\ll B_1$ the ordering wave vector will be small. The direction of $\mathbf{K}$ cannot be determined from our rotational invariant Gaussian vertex (2). It will be fixed by additional (weak) anisotropic terms in the model. In MnSi the spiral wave vector is known to be parallel to the (111) or equivalent crystal directions.[10,11,15,16] In the following we will focus on this case; a generalization to other directions is straightforward. There are four equivalent ordering wave vectors $\mathbf{K}_j$, viz., $K(1,1,1)/\sqrt{3}$, $K(-1,-1,1)/\sqrt{3}$, $K(-1,1,-1)/\sqrt{3}$, and $K(1,-1,-1)/\sqrt{3}$. For each wave vector $\mathbf{K}_j$ there are two equivalent directions in the plane orthogonal to $\mathbf{K}_j$. Together this defines eight equivalent spirals, i.e., the order parameter has eight components, $\psi_j,\overline{\psi}_j$, $(j=1,\dots,4)$.[14] We now consider slow fluctuations of the order parameter by writing the magnetization as

$$\mathbf{M}(\mathbf{r},\tau)=\sum_{j=1}^{4}\{\psi_j(\mathbf{r},\tau)[\mathbf{A}_{\mathbf{K}_j}e^{i\mathbf{K}_j\cdot\mathbf{r}}+\mathbf{A}^*_{\mathbf{K}_j}e^{-i\mathbf{K}_j\cdot\mathbf{r}}] + \overline{\psi}_j(\mathbf{r},\tau)[-i\mathbf{A}_{\mathbf{K}_j}e^{i\mathbf{K}_j\cdot\mathbf{r}}+i\mathbf{A}^*_{\mathbf{K}_j}e^{-i\mathbf{K}_j\cdot\mathbf{r}}]\}, \tag{7}$$

where $\mathbf{A}_{\mathbf{K}_j}=\mathbf{a}_{\mathbf{K}_j}+i\mathbf{b}_{\mathbf{K}_j}$ with $|\mathbf{a}_{\mathbf{K}_j}|=|\mathbf{b}_{\mathbf{K}_j}|=1$, $\mathbf{a}_{\mathbf{K}_j}\perp\mathbf{b}_{\mathbf{K}_j}$, and $\mathbf{K}_j$ parallel or antiparallel to $\mathbf{a}_{\mathbf{K}_j}\times\mathbf{b}_{\mathbf{K}_j}$ depending on the sign of D. The order-parameter fields $\psi_j(\mathbf{r},\tau)$ and $\overline{\psi_j}(\mathbf{r},\tau)$ are slowly varying in space and imaginary time, in particular, they are only slowly varying over the wavelength of the spiral. Inserting the order-parameter representation (7) into the action (3) leads to the desired order-parameter field theory for the itinerant quantum helimagnet.

In the nonmagnetic phase the leading terms in an expansion of the Landau-Ginzburg-Wilson free-energy functional Φ in powers of momenta and frequencies of the order-parameter field are given by

$$\Phi[\psi_j,\overline{\psi_j}]=\frac{1}{2}\sum_{\mathbf{q},\omega,j}[|\psi_j(\mathbf{q},\omega)|^2+|\overline{\psi_j}(\mathbf{q},\omega)|^2]\times\left[t+B_1q^2+C_3K^2\ln\left(\frac{1}{K}\right)+\tilde{B}_1q^2\ln(1/K)+C_\omega\frac{|\omega|}{K}+O(q^3,\omega q^2)\right]+O(\psi^4,\overline{\psi}^4). \tag{8}$$

As a consequence of the spiral magnetic ordering the nonanalyticities in the Gaussian vertex (2) are cut off at the ordering wave vector $\mathbf{K}$. For clarity we have written the resulting K-dependent terms explicitly in Eq. (8). In the rest of the paper they will be absorbed into renormalizations of the parameters t, B_1, and C_ω. The spiral ordering cuts off not only the nonanalyticities in the Gaussian vertex but also the singularities in the higher-order terms. In contrast to the ferromagnetic case (1) the coefficients of all higher-order terms in Eq. (8) are finite in the limit $\mathbf{q},\omega\to 0$.

We now analyze the order-parameter field theory (8) at mean-field level. As discussed after Eq. (2), in the magnetic phase the long-range interaction (the logarithmic term) will be cut off not only by K but also by $|\psi|$.[9] Qualitatively, the resulting term takes the form $-C_3\psi^4\ln(\psi^2+K^2)$. Consequently, the mean-field free energy in the magnetic phase reads

$$F\sim t\psi^2-C_3\psi^4\ln(\psi^2+K^2)+\tilde{u}\psi^4+O(\psi^6). \tag{9}$$

At mean-field level the order of the transition is determined by the sign of the coefficient u of the ψ^4 term. Expanding the logarithm in Eq. (9) we find $u=\tilde{u}-2C_3\ln K$. Thus for large K and small C_3 the mean-field free energy displays a continuous transition with conventional mean-field critical exponents (this is the first scenario mentioned above), in the opposite case a first-order transition analogous to that in itinerant ferromagnets[9] (the second scenario discussed above). There is a quantum tricritical point at $|K|=\exp(-\tilde{u}/2|C_3|)$ which separates the two regimes. The tricritical behavior is also conventional mean-field-like.

What remains to be done is to check the stability of the mean-field theory (9) with respect to quantum fluctuations. In the case of the first-order scenario this was done in Ref. 9. To do the same for the continuous-transition scenario we keep only the most relevant terms (in the renormalization-group sense) in Eq. (8) and suppress unessential constants. The resulting Landau-Ginzburg-Wilson functional Φ can be written as

$$\Phi[\psi_j,\overline{\psi_j}]=\frac{1}{2}\sum_{\mathbf{q},\omega,j}(t+q^2+|\omega|)[|\psi_j(\mathbf{q},\omega)|^2+|\overline{\psi_j}(\mathbf{q},\omega)|^2]+u\int dx\left\{\sum_j[\psi_j^2(x)+\overline{\psi}_j^2(x)]\right\}^2+\lambda\int dx\sum_j[\psi_j^2(x)+\overline{\psi}_j^2(x)]^2. \tag{10}$$

Here the u term is the conventional isotropic fourth-order term, while the λ term represents a cubic anisotropy connected with the discrete fourfold degeneracy of the action with respect to the direction of the spiral wave vector $\mathbf{K}$. One might worry whether additional relevant contributions to Eq. (10) arise from the anisotropic terms in the action necessary to fix the directions of the spirals, as discussed after Eq. (6). However, once the rotational symmetry is broken by the discrete set of spiral directions additional anisotropic terms in the action do not produce new contributions to Eq. (10). An explicit calculation shows that they only renormalize the coefficients u and λ.

We proceed by analyzing the Landau-Ginzburg-Wilson free-energy functional (10) by conventional renormalization-group methods for quantum phase transitions.[6] At tree level the Gaussian fixed point is defined by the requirement that the coefficients of the q^2 and $|\omega|$ terms in the Gaussian vertex do not change under renormalization. Therefore the dynamical exponent is $z=2$. The other critical exponents which can be read off the Gaussian vertex take their mean-field values: $\nu=1/2$, $\gamma=1$, and $\eta=0$. Defining the scale dimension of a length to be $[L]=-1$, we find the scale dimension of the fields at the Gaussian fixed point to be $[\psi]=[\overline{\psi}]=(d+z-2)/2=3/2$ (d is the spatial dimensionality).

The properties of the Gaussian fixed point in our model are identical to those of a conventional itinerant antiferromagnet. This is not surprising since the structure of the Gaussian vertex of the Landau-Ginzburg-Wilson functional (10) is identical to that derived by Hertz[6] for itinerant antiferromagnets. The only difference is the number of order-parameter components.

In order to check the stability of the Gaussian fixed point we calculate the scale dimensions of the coefficients of the quartic terms, u and λ. They turn out to be $[u]=[\lambda]=d+z-4[\psi]=4-d-z$. In our case, $d=3$, $z=2$ this means $[u]=[\lambda]=-1$. The quartic terms are irrelevant at the Gaussian fixed point which is therefore stable. This is again analogous to a conventional itinerant quantum antiferromagnet, the more complicated order-parameter component structure does not play any role at the Gaussian fixed point. Consequently, the mean-field theory (9) of the helimagnetic quantum phase transition is indeed stable, and the quantum-critical point, if any, is characterized by the usual mean-field exponents and a dynamic exponent of $z=2$.

In the final section of the paper we relate our findings to the experiments on the quantum phase transition in the prototypical itinerant helimagnet, MnSi.[10,11] Our study has revealed that the properties of the helimagnetic quantum phase transition crucially depend on the ratio of two length scales, viz., the wavelength $l_{\rm Spiral}$ of the spiral and the nucleation length $l_{\rm Nucl}$ associated with the first-order transition in the corresponding itinerant quantum ferromagnet. In MnSi the wavelength of the spiral is rather large, approximately 190 Å. In contrast, the experimental data for the magnetic susceptibility suggest that the nucleation length of the first-order transition is small (of the order of the microscopic scales). This can be seen from the fact that no susceptibility increase is observed close to the quantum phase transition, instead the susceptibility close to the transition is approximately a step function. (If the first-order transition would occur at some large length scale the susceptibility should increase when approaching the transition until the magnetic correlation length reaches this scale.)

Therefore the nucleation length scale is much shorter than the spiral wavelength, and our theory predicts a first-order transition, in agreement with the experiments. According to our theory the properties of the quantum phase transition in MnSi are identical to that of the quantum *ferromagnetic* transition and MnSi is indeed a prototypical example for this transition.

In summary, we have studied the quantum phase transition of itinerant electrons from a paramagnet to a state which displays long-period helical structures due to a Dzyaloshinskii instability of the ferromagnetic state. We found that depending on the relative strengths of the helical (Dzyaloshinskii) term and the correlation-induced self-generated long-range interaction two different phase transition scenarios are possible. If the self-generated long-range interaction is stronger than the helical term the transition is of first order with the same properties as the quantum ferromagnetic transition. This is the situation encountered in MnSi. In contrast, if the helical term is stronger the transition is a continuous one with mean-field critical exponents and a dynamical exponent of $z=2$. The two regimes are separated by a quantum tricritical point.

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