The quantum phase transition of itinerant helimagnets

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(December 21, 2021)

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.

I. INTRODUCTION

Quantum phase transitions are phase transitions that occur at zero temperature as a function of some non-thermal 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.

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 who generalized Wilson’s renormalization group to quantum phase transitions. The finite temperature properties were later discussed by Millis. 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 non-critical 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. In a clean system the resulting ferromagnetic quantum phase transition is generically of first order.

The experimentally best studied example of such a transition is probably provided by the pressure-tuned transition in MnSi. 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 semi-quantitative agreement with the theoretical predictions.

In particular, the quantum phase transition is of first order while the thermal transition at higher temperatures is of second order.

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, 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. We show that the self-generated long-range interaction between the spin fluctuations is cut-off by the helical ordering. Depending on the relative strengths of this interaction and the Dzyaloshinskii instability two different quantum phase transition scenarios are possible. For a sufficiently strong Dzyaloshinskii instability the quantum phase transition is of second order with mean-field exponents while for a weak Dzyaloshinskii instability the transition remains first order with the same properties as the quantum ferromagnetic transition. This is the case realized in MnSi.

The paper is organized as follows. In Sec. I we define the starting action and identify the helical ordering at...
mean-field level. In Sec. III we derive an order parameter field theory for the paramagnet–helimagnet quantum phase transition, analyze it by means of the renormalization group and discuss the resulting phase transition scenarios. We conclude in Sec. IV.

II. ITINERANT QUANTUM HELIMAGNETS

A. The model

Our starting point is the effective action for the spin degrees of freedom in a three-dimensional itinerant quantum ferromagnet. This action can be derived from a microscopic model of interacting electrons. In terms of the magnetization $\mathbf{M}$ the action reads

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

We have used a 4-vector notation with $x = (r, \tau)$ comprising a real space vector $\mathbf{r}$ and imaginary time $\tau$. Analogously, $\int dx = \int \! dr \, \int_0^{1/T} \! d\tau$, where $T$ is the temperature. The bare Gaussian vertex $\Gamma_0$ 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). In the appropriate limit of small momenta and frequencies the Fourier transform of $\Gamma_0$ is given by

$$
\Gamma_0(k, \omega) = t_0 + B_1 k^2 + C_3 k^2 \log(1/k) + C_\omega \frac{|\omega|}{k}. \quad (2)
$$

Here the third term represents the effective long-range interaction induced by the coupling between the magnetization and non-critical soft modes. Generically, it is repulsive, i.e. $C_3 < 0$, but rather weak, $|C_3| \ll B_1$ since it is caused by electronic correlations. Therefore it becomes important only at small momenta. The last term is the conventional Landau damping of the paramagnet. The coefficients $\chi^{(n)}$ of the higher order terms in eq. (2) are proportional to the higher spin density correlation functions of the reference system. Because of the same mode coupling effects that lead to the non-analytic $C_3$ term in the Gaussian action they are in general not finite in the limit of zero frequencies and wave numbers. For $p \to 0$ they behave like $\chi^{(n)} \sim v^{(n)}|p|^{4-n}$.

We now add a new term, the helical or Dzyaloshinskii term, to the effective action (2), which will cause an instability of the ferromagnetic state,

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

Physically, this term may be caused by relativistic interactions between spins of the form $\mathbf{S}_i \times \mathbf{S}_j$. In general, it will be small compared to the other Gaussian terms, with the possible exception of the long-range $C_3$ term.

B. Mean-field theory: The spiral ordering

In this subsection we analyze the action (3) at saddle point-level, i.e. we minimize it with respect to $\mathbf{M}(x)$. In the absence of the Dzyaloshinskii term the action is minimized by a homogeneous (in space and imaginary time) $\mathbf{M}(x)$. If the Dzyaloshinskii term is present, the action is minimized by a state which is periodic in space but homogeneous in time:

$$
\mathbf{M}(r, \tau) = \mathbf{A}_k e^{ik \cdot r} + \mathbf{A}_k^* e^{-ik \cdot r}. \quad (4)
$$

Here $\mathbf{A}_k = a_k + ib_k$ is a complex vector. Inserting this ansatz into the action (3) we obtain

$$
S^{\text{SP}}(k) = [t_0 + B_1 k^2 + C_3 k^2 \log(1/k)] |\mathbf{A}_k|^2 + iD k \cdot (\mathbf{A}_k \times \mathbf{A}_k^*) + O(|\mathbf{A}_k|^4). \quad (5)
$$

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

$$
S^{\text{SP}}(k) = [t_0 + B_1 k^2 + C_3 k^2 \log(1/k) - 2|D||k|] |\mathbf{A}_k|^2 + O(|\mathbf{A}_k|^4). \quad (6)
$$

The term in brackets is minimized by the ordering wave vector $\mathbf{K}$. Since in general $|D| \ll B_1$ the ordering wavevector 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. We will come back to these terms in the next subsection. In MnSi the spiral wavevector is known to be parallel to the (111) or equivalent crystal directions. In the following we will focus on this case, a generalization to other directions is straightforward.

III. THE HELIMAGNETIC QUANTUM PHASE TRANSITION

A. Order parameter field theory

In the last subsection we found that the action is minimized by long-period spin spirals which in MnSi are parallel to the (111) direction. There
are four equivalent ordering wave vectors \( K_j \), \( K(1,1,1)/\sqrt{3} \), \( K(-1,1,1)/\sqrt{3} \), \( K(-1,-1,1)/\sqrt{3} \), and \( K(1,-1,-1)/\sqrt{3} \). For each wave vector \( K_j \) there are two equivalent directions in the plane orthogonal to \( K_j \).

Together this defines 8 equivalent spirals, i.e. the order parameter has eight components, \( \psi_j, \bar{\psi}_j \) (\( j = 1 \ldots 4 \)).

We now consider slow fluctuations of the order parameter by writing the magnetization as

\[
M(r, \tau) = \sum_{j=1}^{4} \left\{ \psi_j(r, \tau) \left[ A_{K_j} e^{iK_j \cdot r} + A^*_{K_j} e^{-iK_j \cdot r} \right] + \bar{\psi}_j(r, \tau) \left[ -iA_{K_j} e^{iK_j \cdot r} + iA^*_{K_j} e^{-iK_j \cdot r} \right] \right\},
\]

where \( A_{K_j} = a_{K_j} + ib_{K_j} \) with \( |a_{K_j}| = |b_{K_j}| = 1 \), \( a_{K_j} \perp b_{K_j} \), and \( K_j \) parallel or antiparallel to \( a_{K_j} \times b_{K_j} \), depending on the sign of \( D \). The order parameter fields \( \psi_j(r, \tau) \) and \( \bar{\psi}_j(r, \tau) \) 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. The leading terms in an expansion of the Landau-Ginzburg-Wilson free energy functional \( \Phi \) in powers of momenta and frequencies of the order parameter field are given by

\[
\Phi[\psi_j, \bar{\psi}_j] = \frac{1}{2} \sum_{q, \omega, j} \left[ |\psi_j(q, \omega)|^2 + |\bar{\psi}_j(q, \omega)|^2 \right] \times \\
\times \left[ t + B_1 q^2 + C_3 K^2 \log \left( \frac{1}{K} \right) + \bar{\psi}_j \right]
\]

\[
\times \left( \hat{B}_1 q^2 \log(1/K) + C_\omega \frac{|\omega|}{K} + O(q^3, \omega q^2) \right)
\]

\[
+ O(\psi^4, \bar{\psi}^4).
\]

As a consequence of the spiral magnetic ordering the non-analyticities in the Gaussian vertex (2) are cut-off at the ordering wave vector \( K \). For clarity we have written the resulting \( K \)-dependent terms explicitly in (8). In the following they will be absorbed into \( t \) and \( B_1 \), respectively. Analogously, in the frequency-dependent term \( K \) will be absorbed into \( C_\omega \). The spiral ordering cuts-off not only the non-analyticities in the Gaussian vertex but also the singularities in the higher-order terms. Therefore the coefficients of all higher-order terms in (8) are now finite in the limit \( q, \omega \to 0 \). Keeping only the most relevant terms (in the renormalization group sense) and suppressing unessential constants, the Landau-Ginzburg-Wilson functional \( \Phi \) can finally be written as

\[
\Phi[\psi_j, \bar{\psi}_j] = \frac{1}{2} \sum_{q, \omega, j} \left[ (t + q^2 + |\omega|) \left[ |\psi_j(q, \omega)|^2 + |\bar{\psi}_j(q, \omega)|^2 \right] \right] + u \int dx \left\{ \sum_j \left[ \psi_j^2(x) + \bar{\psi}_j^2(x) \right] \right\}^2
\]

Here the \( u \) term is the conventional isotropic 4th order term, while the \( \lambda \) term represents a cubic anisotropy connected with the discrete 4-fold degeneracy of the action with respect to the direction of the spiral wave vector \( K \). One might worry whether additional relevant contributions to (9) arise from the anisotropic terms in the action necessary to fix the directions of the spirals, as discussed after (8). 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 (9). An explicit calculation shows that they only renormalize the coefficients \( u \) and \( \lambda \).

\[\text{B. Renormalization group analysis}\]

We now analyze the Landau-Ginzburg-Wilson free energy functional (9) by conventional renormalization group methods for quantum phase transitions. We first carry out a tree-level analysis. 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 \([\psi] = [\bar{\psi}] = (d + z - 2)/2 = 3/2 \) \((d \) 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 (9) is identical to that derived by Hertz 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 \( \lambda \). They turn out to be \([u] = [\lambda] = d + z - 4 = 4 - d - z \). 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 helimagnetic quantum-critical point, if any, is characterized by the usual mean-field exponents and a dynamic exponent of \( z = 2 \).
C. Phase transition scenarios

In the last two subsections we have seen that in the long-distance and long-time limit the order parameter field theory takes the form of an itinerant quantum antiferromagnet, leading to a continuous transition with mean-field exponents. However, in order to discuss all possible scenarios for the helimagnetic quantum phase transition it is necessary to keep track of the physics at finite length scales. To do this it is useful to go back to the action (\(\mathcal{S}\)) in terms of the spin variables. In addition to the magnetic correlation length \(\xi\) the system is characterized by two non-trivial length scales, viz. the length scale of the spiral, \(\ell_{\text{Spiral}} = |K|^{-1}\), and the nucleation length scale \(\ell_{\text{Nucl}}\) associated with the first-order transition in itinerant quantum ferromagnets. It is given by the length at which the \(B_1\) and \(C_3\) terms in the Gaussian vertex (\(\mathcal{S}\)) are equal and opposite, i.e. \(\log \ell_{\text{Nucl}} = B_1/C_3\).

The qualitative properties of the helimagnetic quantum phase transition are determined by the relation between these two length scales. Let us first consider the case \(\ell_{\text{Spiral}} \ll \ell_{\text{Nucl}}\), i.e. a strong Dzyaloshinskii instability or weak electronic correlations. When approaching the transition the growing magnetic correlation length first reaches \(\ell_{\text{Spiral}}\). The system crosses over from a ferromagnet to a helimagnet before the self-generated effective long-range interaction becomes sufficiently strong to induce a first-order transition. In this case the asymptotic action is given by (\(\mathcal{S}\)). The helimagnetic quantum phase transition is therefore a continuous transition with mean-field critical exponents.

In the opposite case, \(\ell_{\text{Spiral}} \gg \ell_{\text{Nucl}}\), i.e. a weak Dzyaloshinskii instability or strong electronic correlations, the magnetic correlation length reaches \(\ell_{\text{Nucl}}\), before the Dzyaloshinskii term becomes strong enough to induce spiral ordering. The system undergoes a first-order phase transition which is completely analogous to the ferromagnetic transition. Here, the correlation length remains finite (of the order of \(\ell_{\text{Nucl}}\)), and the long-wavelength free energy functional (\(\mathcal{S}\)) does not describe the transition.

In order to describe the crossover between the two scenarios we derive a mean-field free energy for the helimagnetic quantum phase transition. A mean-field theory is sufficient to obtain the leading behavior in both scenarios: for the continuous transition this was shown in Subsec. 3 and for the first-order scenario in Ref. 3. In the ordered phase the non-analyticity in the long-range interaction in the Gaussian vertex (\(\mathcal{S}\)) is cut off by both a finite order parameter \(\psi\) and by the spiral wave vector \(K\).

Taking both cutoffs into account we obtain

\[
F = t \psi^2 - C_3 \psi^4 \ln(\psi^2 + K^2) + \tilde{u} \psi^4 + O(\psi^6) \ .
\]

For small \(K\) and large \(C_3\) this free energy displays a first order transition, in the opposite case a continuous transition. There is a quantum tricritical point at \(|K| = \exp(-\tilde{u}/2|C_3|)\) which separates the two regimes. The mean-field theory (\(\mathcal{S}\)) also correctly describes the quantum tricritical behavior at this point which is conventional.

IV. CONCLUSIONS

In this final section of the paper we relate our findings to the experiments on the quantum phase transition in the prototypical itinerant helimagnet, MnSi. In Subsection III C, we found that the properties of the helimagnetic quantum phase transition crucially depend on the ratio of two length scales, viz. the wave length \(\ell_{\text{Spiral}}\) of the spiral and the nucleation length \(\ell_{\text{Nucl}}\) associated with the first-order transition in the corresponding itinerant quantum ferromagnet. In MnSi the wave length 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 wave length, and Subsection III C 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.

We gratefully acknowledge helpful discussions with S. Bekhechi, D. Belitz, T.R. Kirkpatrick and R. Narayanan. This work was supported in part by the DFG under grant No. Vo659/2 and by the NSF under grant No. DMR–98–70597. Part of this work was performed at the Aspen Center for Physics.
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16 Technically, the spiral wave vector plays the same role as a finite temperature in protecting the singularity (see Ref. 9) but the physics is different. At a finite temperature the interaction range becomes finite since the temperature gives the fermionic particle-hole excitations a mass. In the case of helical ordering, however, the order parameter fluctuations beyond the spiral length scale cease to couple to the soft particle-hole excitations at $k = 0$. 