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## Ferromagnetic Quantum Critical Point in Noncentrosymmetric Systems

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Ferromagnetic quantum criticality in clean metals has proven elusive due to fermionic soft modes that drive the transition first order. We show that noncentrosymmetric metals with a strong spin-orbit interaction provide a promising class of materials for realizing a ferromagnetic quantum critical point in clean systems. The spin-orbit interaction renders massive the soft modes that interfere with quantum criticality in most materials, while the absence of spatial inversion symmetry precludes the existence of new classes of soft modes that could have the same effect.

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Ferromagnetism in metals has provided one of the earliest examples of a quantum phase transition. Stoner [1] developed an eponymous mean-field theory that describes both the classical and the quantum ferromagnetic (FM) transition. Hertz [2] later argued that, in the quantum case (i.e., for the transition at zero temperature driven by a nonthermal control parameter), Stoner theory is exact, as far as the critical behavior is concerned, for all spatial dimensions d > 1. The reason is that the coupling between the statics and the dynamics at zero temperature (T = 0)lowers the upper critical dimension, above which the fluctuations neglected by mean-field theory are irrelevant, from  $d_c^+ = 4$  in the classical case to  $d_c^+ = 1$  in the quantum case. Hertz's renormalization-group treatment, as refined by Millis [3], agreed with results obtained by different methods by Moriya [4]. Collectively, this became known as the Hertz-Millis-Moriya (HMM) theory of FM quantum criticality.

These theoretical predictions were not borne out experimentally. In stoichiometric systems with minimal amounts of quenched disorder, and the quantum phase transition (QPT) driven by pressure, the transition almost invariably becomes first order if the Curie temperature is sufficiently low, and this is true for local-moment ferromagnets as well as itinerant ones [5]. Notable exceptions are  $CeRh_6Ge_4$ [6,7] and UIr [8], which we will come back to. The reason for this failure of HMM theory is by now well known: A generic Fermi liquid with a negligible spin-orbit interaction (more on this later) contains soft or massless two-particle excitations that couple to, and are rendered massive by, an external magnetic field or a magnetization [9,10]. This coupling results in the free energy being a nonanalytic function of the magnetization, which in turn drives the FM OPT first order [11]. This mechanism is operative for localmoment ferromagnets as well as for itinerant ones, and also for canted ferromagnets and for ferrimagnets [12] as well as for magnetic nematics [13]; for a review, see Ref. [5]. It has recently been shown that it also is operative in Dirac metals, i.e., systems where a linear band crossing is caused by a strong spin-orbit coupling [14–16], if for unobvious reasons. A nonzero temperature gives the soft modes a mass and thus cuts off the first-order mechanism; this leads to a tricritical point in the phase diagram [11]. Similarly, an external magnetic field gives the soft modes a mass, which results in tricritical wings that emerge from the tricritical point in the temperature-pressure-field parameter space and end in quantum critical points (QCPs) at a nonzero field [17].

One way to avoid these conclusions and realize a FM QCP in zero field is to introduce quenched disorder, which has been predicted [11,18] and observed [19] to restore a QCP. However, the resulting critical behavior is not described by HMM theory but is substantially more complicated [20–22]. Experimental results are consistent with these predictions [23,24]. Another possibility is one-dimensional or quasi-one-dimensional materials; see Ref. [25] for a model of FM quantum criticality in such systems.

It would be very interesting if clean materials could be found in which the mechanism for a first-order transition is inoperative, so that a FM QCP in zero field can be realized in three-dimensional systems. In this Letter, we show that a promising class of materials involves systems with a strong spin-orbit coupling that are not centrosymmetric. Our central result is an equation of state that takes the form

$$h = rm - vm^3 \ln\left(\frac{1}{m^2 + \nu^2 + t^2}\right) + um^3.$$
(1)

Here m,  $\nu$ , and h are the dimensionless magnetization, spinorbit coupling, and magnetic field, respectively, in atomic units. They are formally defined as follows. Let  $\mu$  be the magnetization measured in units of  $\mu_B$  per volume and  $E_{ex}$ the exchange splitting due to that magnetization, let *H* be the external magnetic field, let  $E_{so}$  be the splitting of the conduction band near the Fermi energy induced by the spin-orbit coupling, let  $n_e$  be the conduction-electron density, and let  $T_F$  be the Fermi temperature. Then h = $\mu_B H/k_B T_F$ ,  $m = \mu/n_e \approx E_{ex}/k_B T_F$ , and  $\nu = E_{so}/k_B T_F$ .  $t = T/T_0$  is the dimensionless temperature, with  $T_0$  being a temperature scale that depends on microscopic details such as the band structure and the correlation strength. *r* is the control parameter, and u > 0 and v > 0 are Landau parameters. *u* is generically of order unity. *v* is a measure of the strength of correlations in the system; for very strong correlations,  $v \leq 0.1$ .

We first discuss Eq. (1) in the context of the general FM QPT problem and give plausibility arguments for its functional form, then we discuss its implications, and finally we sketch its derivation.

To make Eq. (1) plausible, consider the case of a vanishing spin-orbit coupling,  $\nu = 0$ . Then we recover an equation of state that has been discussed before [5,11]. The nonanalytic dependence of the free energy, and hence the equation of state, on the order parameter m at T = 0 is the result of ballistic soft modes that have been integrated out in order to express the free energy entirely in terms of the order parameter. The nonanalytic term dominates the quartic term in the free energy (or the cubic term in the equation of state), and its sign is negative, which leads to a first-order transition at  $r = r_1 = v e^{-(1+u/v)}$ , where the magnetization changes discontinuously from zero to  $m_1 =$  $e^{-(1+u/v)/2}$  [11]. A nonvanishing temperature gives the soft modes a mass, so T > 0 cuts off the singularity. As a result, there is a tricritical point at a temperature  $T_{\rm tc} = T_0 e^{-u/2v}$ [11]. In a magnetic field, tricritical wings emerge from the tricritical point that end in wing tips at T = 0 and h = $h_c = (4/3)ve^{-3u/2v-13/4}$  [17].

A spin-orbit interaction splits the conduction band and gives the soft modes a mass. However, in centrosymmetric systems a chiral degree of freedom leads to new soft modes that have the same effect as the original ones. Such metals were called Dirac metals in Refs. [14–16] in order to distinguish them from the ordinary, or Landau, metals with a negligible spin-orbit interaction. The net result is an equation of state that is again given by Eq. (1) with  $\nu = 0$ . This changes if spatial inversion symmetry is broken. The spin-orbit interaction still gives the soft modes a mass, but there is no chiral degree of freedom that leads to a new class of soft modes. One then obtains Eq. (1); the resulting phase diagram is shown in Fig. 1.

We now give a semiquantitative discussion of Eq. (1), with the goal of identifying promising candidate materials that might realize a FM QCP in clean systems. The critical value  $\nu_c$  of the dimensionless spin-orbit energy, above which the first-order transition is suppressed, is obviously the same as the dimensionless tricritical temperature  $t_{tc}^0$  for



FIG. 1. Phase diagram in the space spanned by *t*, *r*, and  $\nu$  based on Eq. (1). Shown are a flat surface of second-order transitions at r = 0 (solid blue area), a curved surface of first-order transitions (meshed green area), and a line of tricritical points delineating the two (red curve). In a given material,  $\nu$  will be fixed. For a given  $\nu$ , *r* will be a complicated function of pressure and temperature.

 $\nu = 0$ :  $\nu_c = e^{-u/2v}$ . The tricritical temperature  $T_{\rm tc}^0$  for centrosymmetric materials, where  $\nu$  is absent in the equation of state, is typically on the order of 10 K [5], albeit with a large spread that ranges from 1 K in URhGe to over 100 K in CoS<sub>2</sub>. For the critical spin-orbit energy, we thus have  $E_{\rm so}^c = k_B T_0 \nu_c = (T_F/T_0) k_B T_{\rm tc}^0$ . The temperature scale  $T_0$  was estimated in Ref. [18], which concluded that  $T_F/T_0$  is typically on the order of 1000 (as low as 750 in ZrZn<sub>2</sub> and as high as 3500 in UGe<sub>2</sub>). This implies that typically  $E_{\rm so}^c \approx 1$  eV, with a spread of a factor of up to 10 in either direction. If we assume  $T_F \approx 10^5$  K for a good metal, this implies  $E_{\rm so}^c/k_B T_F \approx 0.1$ . It is illustrative to compare this with values of  $m_1$  for  $\nu = 0$ , which typically fall into the range  $m_1 \approx 0.05$ –0.25 [5,18].

Considering the two entries in Table I with a first-order QPT for which  $E_{so}$  is known, MnSi and URhAl, it is plausible that  $E_{so}$  is not large enough to suppress the firstorder mechanism. For the two entries with a QCP, UIr and  $CeRh_6Ge_4$ , the spin-orbit splitting  $E_{so}$  is not known. For a list of  $E_{so}$  values in noncentrosymmetric materials that are not ferromagnetic, see Ref. [26]; they range from 0.004 to 0.2 eV. For interpreting these values, it is important to keep in mind that  $E_{so}$  should be compared to the Fermi energy. For instance, in BiTeBr,  $E_{so} \approx k_B T_F$  [27].  $E_{so} \approx 0.2$  eV has been reported for CePt<sub>3</sub>Si [28], which also is not ferromagnetic. If the spin-orbit coupling in CeRh<sub>6</sub>Ge<sub>4</sub> were of similar strength, then it would be in the lower range of values that can plausibly be expected to be responsible for the observed QCP. In UIr, one would expect an even higher value, which may well be the reason for the observed QCP.

System	Space group <sup>c</sup>	Order of QPT <sup>d</sup>	$T_C/{ m K}^{ m a}$	$T_{\rm tc}/{ m K}$	$E_{\rm so}/{\rm eV}$	Disorder <sup>b</sup> $(\rho_0/\mu\Omega \text{ cm})$	Comments
MnSi	P2 <sub>1</sub> 3 (198)	First	29.5	≈10	≈0.3 [29]	0.33	Weak helimagnet
$U_3P_4$	I43d (220)	First	138	32		4	ç
UCoAl	P62m (189)	First	0	> 11		24	
URhAl	P62m (189)	First	≈30	≈11	≈1 [30]	≈65	
SmNiC <sub>2</sub>	Amm2 (38)	First	$\approx 4$	>17 (?)		2	
UIr	<i>P</i> 2 <sub>1</sub> (4)	Second	46-1			0.4 [31]	Multiple FM phases; second order above 0.8 K
CeRh <sub>6</sub> Ge <sub>4</sub>	<i>P</i> 6 <i>m</i> 2 (187)	Second				1.5	QCP with non-Fermi liquid transport behavior [6,7]
$Sm_2Fe_{12}P_7$	P6 (174)		6.3 [32]			6 [32]	NPT
CePt <sub>3</sub> B	P4mm (99)		6 [33]				NPT; AFM phase between 7.8 and 6 K
CePdSi <sub>3</sub>	I4mm (107)		2.78 [34]				NPT; multiple magnetic phases
UPtAl	<i>P</i> 62 <i>m</i> (189)	•••	42.5 [35]		≈1 [36]		$T_C$ increases with pressure; no QPT observed
CeNiC <sub>2</sub>	Amm2 (38)		≈2 [37]			≈10 [37]	Transition to AFM under pressure

TABLE I. Noncentrosymmetric pressure-tuned quantum ferromagnets.  $T_C$ , Curie temperature;  $T_{tc}$ , tricritical temperature;  $E_{so}$ , spinorbit splitting of conduction band;  $\rho_0$ , residual resistivity; three center dots, not available; empty cell, not applicable; NPT, no pressure tuning to date; AFM, antiferromagnet. References are given only for properties not referenced in Ref. [5].

At ambient pressure for systems with a first-order QPT; range as a function of pressure for systems with a second-order QPT. <sup>b</sup>For the highest-quality samples.

<sup>c</sup>International short symbol (number index) [38]. <sup>d</sup>At the lowest  $T_C$  value achieved.

Of the third group of materials listed in Table I, the first three are potential candidates for a pressure-induced QCP, but the values of  $E_{so}$  are not known. More generally, we conclude that promising candidates for a FM QCP are noncentrosymmetric materials with a large ( $\approx 1 \text{ eV}$  or larger) spin-orbit splitting  $E_{so}$  of the conduction band near the Fermi energy.

We now sketch the derivation of Eq. (1); see the Supplemental Material [39] for more details. In the absence of spatial inversion symmetry, a single-particle Hamiltonian that captures the dominant effects of the spinorbit interaction can be written [40]

$$H_0 = \xi_k \sigma_0 + v_{so} \boldsymbol{\sigma} \cdot \boldsymbol{\Omega}(\boldsymbol{k}) - \boldsymbol{h} \cdot \boldsymbol{\sigma}.$$
(2)

Here  $\xi_k = \epsilon_k - \mu$ , where  $\epsilon_k$  is the single-particle energymomentum relation and  $\mu$  the chemical potential, **h** is an external magnetic field,  $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$  denotes the Pauli matrices with  $\sigma_0$  as the 2 × 2 unit matrix, and  $v_{so}$  is a coupling constant that represents the strength of the spinorbit interaction. Invariance under time reversal (which flips the signs of both  $\sigma$  and k) in the absence of a magnetic field requires  $\Omega(-k) = -\Omega(k)$ . This implies that the spinorbit term is not invariant under spatial inversion (which flips the sign of k only).

The explicit form of  $\Omega(k)$  depends on the space group; well-known examples are the Dresselhaus spin-orbit coupling for the zinc blende structure, which is cubic in k [41], and the Rashba-Sheka coupling for the wurtzite structure, which is linear in k [42]. For definiteness, we will use the same form as in Refs. [14-16]-namely,

$$\mathbf{\Omega}(k) = k. \tag{3}$$

The coupling constant  $v_{so}$  is then dimensionally a velocity. The broken inversion symmetry is the crucial difference between the current discussion and the Dirac metals considered in Refs. [14–16]. Spatial inversion symmetry requires the existence of an additional, chiral, pseudospin degree of freedom that is odd under parity. The presence or absence of this degree of freedom qualitatively changes the soft-mode spectrum of the electron system, as we will now discuss.

The inverse Green's function for the Hamiltonian  $H_0$  in Eq. (2) is  $G_k^{-1} = i\omega_m \sigma_0 - H_0$ , with  $\omega_m$  being a fermionic Matsubara frequency and  $k = (i\omega_n, \mathbf{k})$ . In terms of quasiparticle resonances

$$F_k^{\beta} = 1/(i\omega_n - \xi_k - \beta |vk - h|)$$
(4a)

and spin matrices

$$M_{\beta}(\hat{\boldsymbol{e}}) = (\sigma_0 + \beta \boldsymbol{\sigma} \cdot \hat{\boldsymbol{e}}), \qquad (4b)$$

with  $\hat{e}$  being an arbitrary unit vector, we find that

$$G_k = \frac{1}{2} \sum_{\beta=\pm} F_k^{\beta} M_{\beta} \left( \frac{v_{so} \boldsymbol{k} - \boldsymbol{h}}{|v_{so} \boldsymbol{k} - \boldsymbol{h}|} \right).$$
(4c)

For a vanishing spin-orbit interaction, the index  $\beta$  turns into minus the spin-projection index, and the spin-orbit interaction in zero field has an effect similar to that of a field in the absence of a spin-orbit interaction. In particular,  $v_{so} \neq 0$ splits the doubly degenerate band. Now consider wavevector convolutions of the Green's function,

$$\varphi^{\beta_1\beta_2}(\boldsymbol{q}, i\Omega_n) = \frac{1}{V} \sum_{\boldsymbol{k}} F_k^{\beta_1} F_{\boldsymbol{k}-\boldsymbol{q}}^{\beta_2}$$
$$= \int \frac{d\Omega_{\boldsymbol{k}}}{4\pi} \frac{2\pi i N_F \operatorname{sgn}(\omega_m) \Theta(-\omega_m(\omega_m - \Omega_n))}{i\Omega_n - v_F \hat{\boldsymbol{k}} \cdot \boldsymbol{q} + (\beta_2 - \beta_1) |v_{\operatorname{so}} k_F \hat{\boldsymbol{k}} - \boldsymbol{h}|}.$$
(5)

Here  $\Omega_n$  is a bosonic Matsubara frequency,  $q = (i\Omega_n, q)$ ,  $d\Omega_k$  is the angular integration measure with respect to k, and the second line represents the leading contribution to the integral in the limit  $q, \Omega_n, h \to 0$ . These are the relevant ballistic soft modes. We have derived them for noninteracting electrons, but interactions cannot change their nature for reasons discussed in Refs. [14–16]. An inspection of Eq. (5) reveals the following. Convolutions of quasiparticle resonances F with different signs of the frequency (i.e., of retarded and advanced degrees of freedom) are soft as q,  $\Omega_n \to 0$  if  $\beta_1 = \beta_2$ . However, a magnetic field does not cut off this singularity. These modes therefore cannot contribute to a nonanalytic dependence of the free energy on the magnetic field or the magnetization. For  $\beta_1 \neq \beta_2$ , on the other hand, the spin-orbit interaction gives the ballistic modes a mass even for h = 0. For  $v_{so} \neq 0$ , there thus are no soft modes in a noncentrosymmetric system that can lead to a nonanalytic free energy, and this is the source of the parameter  $\nu$  in Eq. (1) that cuts off the nonanalyticity. This conclusion does not hinge on the particular form of the spin-orbit interaction given in Eq. (3); any spin-orbit interaction will split the band and give the soft modes a mass, so the equation of state will have the same form.

This scenario for restoring a FM QCP in zero field is qualitatively different from the case of a gapless Dirac metal discussed in Ref. [16], where the relevant soft modes exist but do not couple to the order parameter. The class of candidate materials for this scenario is much smaller than for the one discussed here since it requires a special lattice symmetry. The current mechanism is also very different from the effects of quenched disorder in the absence of a spin-orbit interaction: Disorder provides a mass under the logarithm in Eq. (1) just as  $\nu$  does, but it also leads to new soft modes that are diffusive in nature and provide an additional nonanalytic contribution to the equation of state.

In summary, we have shown that noncentrosymmetric systems with a large spin-orbit coupling provide a platform for the realization of a FM QCP in clean systems in zero field, a goal that had eluded all experimental efforts for a long time. Two materials in which this may already have been observed are UIr and CeRh<sub>6</sub>Ge<sub>4</sub>, but more detailed

studies of the quantum critical behavior are needed to support this suggestion.

We conclude with a few comments about likely features of the resulting critical theory for a noncentrosymmetric metal with a strong spin-orbit interaction. As mentioned after Eq. (4), the effects of  $v_{so}$  are similar to those of a magnetic field for  $v_{so} = 0$ . As a result, the Gaussian vertex for the 3 component of the magnetization has two eigenvalues with the structure of Hertz theory for a ferromagnet, with a dynamical exponent z = 3, while the remaining eigenvalue has the structure of Hertz theory for an antiferromagnet, with z = 2, and the latter will lead to corrections to the leading scaling behavior that results from the former. For instance, for the scaling of the critical temperature with the control parameter  $r = p - p_c$  for a pressure-tuned transition, one expects  $T_c \propto (-r)^{\tau}$  with an effective exponent  $\tau$  that is smaller than the standard HMM value  $\tau = 3/4$ . This is consistent with a recent experiment that found  $\tau = 3/5$  in CeRh<sub>6</sub>Ge<sub>4</sub> [6], but a more detailed investigation is needed. More generally, it is not clear whether the QCP whose existence we have discussed, and which Eq. (1) provides a mean-field description for, is in the HMM universality class for some systems, or for any systems. In particular, for Kondo lattice systems such as  $CeRh_6Ge_4$  [6,7], questions arise about the interplay between the Kondo effect and quantum criticality. This topic has been discussed predominantly for antiferromagnets [43], but various proposals have been debated for ferromagnets as well [7,25,44]. If HMM theory is not applicable, then the electrical resistivity in particular may not be governed by Mathon's  $T^{5/3}$  law [45] but may reflect a different "strange metal" behavior [7]. Also, FM analogs of the effects discussed for antiferromagnets in Ref. [46] might affect the critical behavior. These questions, as well as the interplay of the spin-orbit interaction with quenched disorder, are open problems.

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