Effect of Antisymmetric Interactions on Critical Phenomena: A System with Helical Ground State*

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A classical Heisenberg Hamiltonian, to which is added single-ion anisotropy and *antisymmetric* Dzialoshinsky-Moriya interactions is studied with use of Wilson theory. The phase diagram is obtained; it consists of ferromagnetic, spiral, and ferromagnetic-spiral regions, with critical exponents that are Ising-like, xy-like, and Heisenberg-like, respectively. These results lead to the conclusion that breaking of exchange symmetry does not change the nature of the phase transition. Crossover behavior is also discussed.

Consider a system composed of three-dimensional classical spins situated on a d-dimensional "hypercubical" lattice and described by the model Hamiltonian $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3$. Here

$$\mathcal{H}_1 \equiv -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = -J \sum_{\langle ij \rangle} (S_{ix}S_{jx} + S_{iy}S_{jy} + S_{iz}S_{jz}), \tag{1a}$$

where spins $\vec{S}_i \equiv (S_{ix}, S_{iy}, S_{iz})$ and $\vec{S}_j$ interact only if lattice sites i, j are nearest neighbors, and the energy of a pair of parallel spins is $-J$. The second term in the Hamiltonian is the single-ion anisotropy term, presumably due to interactions such as crystal fields:

$$\mathcal{H}_2 = -\tfrac{1}{2} D \sum_{i=1}^{N} S_{iz}^2. \tag{1b}$$

The third term is a Dzialoshinski-Moriya interaction,[1]

$$\mathcal{H}_3 = A_3 {\sum_{\langle ij \rangle}}' (S_{ix}S_{jy} - S_{jx}S_{iy}), \tag{1c}$$

where the prime on the summation means that it is restricted to nearest-neighbor pairs of spins that are on adjacent "hyperplanes" (this means $\vec{r}_j - \vec{r}_i = \hat{z}$, where $\hat{z}$ is a nearest-neighbor vector in the z *lattice* direction). Although the most general Dzialoshinski-Moriya interaction is $\vec{A} \cdot \vec{S}_i \times \vec{S}_j$, we have set $\vec{A} \equiv A_3\hat{z}$ in (1c) without loss of generality.

The impetus for this study is as follows:

(1) There are many magnetic materials[2] that display complex helical spin configurations in their ordered states, although there exists little analysis beyond mean-field theory. The Hamiltonian $\mathcal{H}$ is capable of describing systems with helical ordering [cf. Fig. 1].

(2) The antisymmetric Dzialoshinski-Moriya interaction is of interest in its own right. From spin-orbit coupling theory, it is known to be the cause of "weak" ferromagnetism in certain materials (e.g., hematite,[3] α-Fe_2O_3). Moreover, in a recent Letter, Melcher[4] has shown that the spin-wave dispersion relation includes a linear term, $\omega(q) = aq + bq^2$, where a and b are functions of J, D, and A_3, and $a = 0$ unless $A_3 \neq 0$, leading one to suspect possible effects of nonzero A_3 on thermodynamic properties in general and on *critical* properties in particular.

(3) The interaction $\mathcal{H}_3$ provides an opportunity to test the effect of breaking exchange symmetry on critical properties,[5-6] since the antisymmetric interaction $\vec{A} \cdot \vec{S}_i \times \vec{S}_j$ changes sign upon interchange of $\vec{S}_i$ and $\vec{S}_j$, whereas previously studied models of critical behavior are symmetric under this interchange.

In this work I study the critical behavior of $\mathcal{H}$ using the Wilson renormalization group ap-

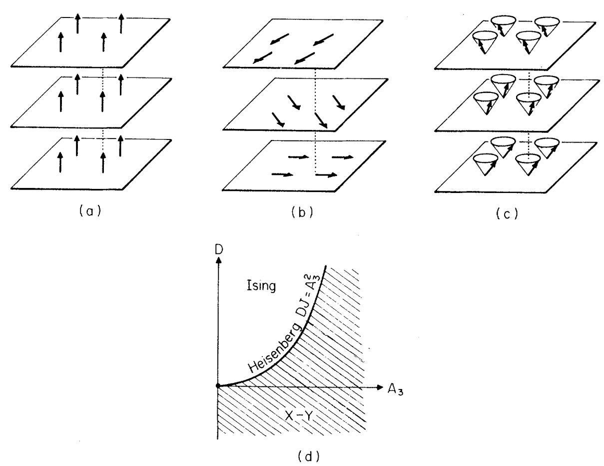

FIG. 1. Pictoral representation of the phase diagram of the Hamiltonian $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3$. (a), (b), (c) The ordered states for the cases (i) $\bar{D} > A_3^2$, (ii) $\bar{D} < A_3^2$, and (iii) $\bar{D} = A_3^2$, respectively. (d) The critical behavior as obtained from the ϵ expansion.

proach.[7-10] In the continuum limit, $\mathcal{H}$ becomes

$$\mathcal{H} = \int d^3r \{\tfrac{1}{2}J(\nabla S_x\cdot\nabla S_x + \nabla S_y\cdot\nabla S_y + \nabla S_z\cdot\nabla S_z) - dJ|\vec{S}|^2 - \tfrac{1}{2}D(S_z)^2 + A_3[S_x(\partial S_y/\partial z) - S_y(\partial S_x/\partial z)]\}, \tag{2}$$

where the $\vec{r}$ dependence of S_x has been suppressed. The reduced Hamiltonian $\mathcal{H}_R$ is obtained by transforming (2) into the momentum representation,

$$\mathcal{H}_R = -\tfrac{1}{4}\textstyle\sum_\alpha\sum_\beta \int d^3q\, u_2(\vec{q},\alpha;\vec{q}',\beta)S^\alpha(\vec{q})S^\beta(\vec{q}') - u_4\int d^3r\,|\vec{S}(\vec{r})|^4, \tag{3}$$

where $\vec{S}(\vec{q}) \equiv V^{-1/2}\int d^3r \exp(i\vec{q}\cdot\vec{r})\vec{S}(\vec{r})$, and α, β run over the components x, y, z of the three-dimensional classical spins. The matrix elements u_2 appearing in (3) are zero when $\vec{q}+\vec{q}'\neq 0$, while if $\vec{q}+\vec{q}'=0$, $u_2(\vec{q},\alpha;\vec{q}',\beta)$ are given by the appropriate element of the following matrix (rows are ordered by $\vec{q},x$; $\vec{q},y$; $\vec{q},z$; $-\vec{q},x$; $-\vec{q},y$; $-\vec{q},z$; and the columns similarly):

$$\begin{bmatrix} 0 & 0 & 0 & q^2+\rho & 2i\bar{A}_3q_z & 0 \\ 0 & 0 & 0 & -2i\bar{A}_3q_z & q^2+\rho & 0 \\ 0 & 0 & 0 & 0 & 0 & q^2-\bar{D}+\rho \\ q^2+\rho & -2i\bar{A}_3q_z & 0 & 0 & 0 & 0 \\ 2i\bar{A}_3q_z & q^2+\rho & 0 & 0 & 0 & 0 \\ 0 & 0 & q^2-\bar{D}+\rho & 0 & 0 & 0 \end{bmatrix}. \tag{4}$$

Here I have introduced the notation $\bar{D}\equiv D/J$, $\bar{A}_3\equiv A_3/J$, and $\rho\equiv BkT/J-2d$, where B is a dimensionless positive number, k is the Boltzmann constant, and T is the temperature.

First consider the Gaussian model, for which $u_4=0$. The two off-diagonal submatrices in (4) may be diagonalized in the representation of $S^+(\vec{q})$, $S^-(\vec{q})$, and $S^z(\vec{q})$, where $S^\pm(\vec{q})\equiv 2^{-1/2}[S^x(\vec{q})\pm iS^y(\vec{q})]$, with the result

$$\mathcal{H}_R(u_4=0) = -\tfrac{1}{2}\int d^3q\,\{(q^2+2\bar{A}_3q_z+\rho)S^+(\vec{q})[S^+(\vec{q})]^* + (q^2-2\bar{A}_3q_z+\rho)S^-(\vec{q})[S^-(\vec{q})]^* + (q^2-\bar{D}+\rho)S^z(\vec{q})[S^z(\vec{q})]^*\}. \tag{5}$$

Here the asterisk denotes complex conjugate. The nonvanishing spin-spin correlation functions (i.e., the Gaussian propagators) are, from (5),

$$\Gamma^{++}(\vec{q}) = \langle S^+(\vec{q})[S^+(\vec{q})]^*\rangle = [(\vec{q}+\bar{A}_3\hat{z})^2+\rho-\bar{A}_3^{\,2}]^{-1}, \tag{6a}$$

$$\Gamma^{--}(\vec{q}) = \langle S^-(\vec{q})[S^-(\vec{q})]^*\rangle = [(\vec{q}-\bar{A}_3\hat{z})^2+\rho-\bar{A}_3^{\,2}]^{-1}, \tag{6b}$$

$$\Gamma^{zz}(\vec{q}) = \langle S^z(\vec{q})[S^z(\vec{q})]^*\rangle = (q^2-\bar{D}+\rho)^{-1}. \tag{6c}$$

Note that at high temperature ($\rho\gg 1$), all propagators are finite and the system is disordered. To study the behavior near T_c, we consider three different situations: (i) $\bar{D}>\bar{A}_3^{\,2}$. As T (and hence ρ) decreases, $\Gamma^{zz}(\vec{q}=0)$ is the first propagator of (6) to diverge—it diverges at $\rho=\bar{D}$, while all other propagators are still finite at this temperature. Therefore the order parameter is $S^z(\vec{q}=0)$ and the ordered state is given in Fig. 1(a). (ii) $\bar{D}<\bar{A}_3^{\,2}$. In this case, as we lower the temperature the propagators $\Gamma^{++}(-\bar{A}_3z)$ and $\Gamma^{--}(\bar{A}_3z)$ diverge first, at $\rho=\bar{A}_3^{\,2}$. There are two independent order parameters responsible for the transition, viz., $S^+(-\bar{A}_3\hat{z})$ and $S^-(\bar{A}_3\hat{z})$. Note that although they are indistinguishable statically [Fig. 1(b)], they are independent dynamically (and mathematically). Note also that the conventional $\vec{q}=0$ "susceptibilities," $\Gamma^{xx}(\vec{q}=0)$, do not diverge. However, $\Gamma^{xx}(\vec{q})$ and $\Gamma^{yy}(\vec{q})$ are both diverging at $\vec{q}=\pm\bar{A}_3\hat{z}$. (iii) $\bar{D}=\bar{A}_3^{\,2}$. Here all three propagators diverge simultaneously at $\rho=\bar{D}=\bar{A}_3^{\,2}$, and the order parameter may be either $S^z(\vec{q}=0)$, $S^+(\vec{q}=-\bar{A}_3\hat{z})$, or $S^-(\vec{q}=\bar{A}_3\hat{z})$ [cf. Fig. 1(c)].

Next consider the more general situation with $u_4\neq 0$. The critical behavior of (3) may be obtained by using exact recurrsion relations in $d=4-\epsilon$ dimensions or by using the Feynman diagram expansion.[7-9] We find that with suitable choices of order parameters and diverging quantities (cf. preceding paragraph), the critical behavior may again be categorized as above, with cases (i), (ii), and (iii) corresponding, respectively, to Ising-like, xy-like, and Heisenberg-like critical behavior [cf. the phase diagram of Fig. 1(d)].

This result is rendered plausible by the following analogy between our Hamiltonian $\mathcal{H}=\mathcal{H}_1+\mathcal{H}_2+\mathcal{H}_3$ and the conventional Ising, xy, and Heisenberg systems. For case (i) there is only one order parameter, $S^z(0)$, whose fluctuation diverges at T_c, while the same is true for the Ising model (or the anisotropic Heisenberg model with $J_z>J_x, J_y$). Similarly, for case (ii) there are two independent order parameters $S^+(-\overline{A}_3\hat{z})$ and $S^-(\overline{A}_3\hat{z})$, and the same is true [with different order parameters, $S^x(0)$, $S^y(0)$] for the xy model (or anisotropic Heisenberg model with $J_x=J_y>J_z$). Finally, for case (iii) there are three independent order parameters [$S^z(0)$, $S^+(-\overline{A}_3\hat{z})$, and $S^-(\overline{A}_3\hat{z})$] just as for the isotropic Heisenberg model [$S^x(0)$, $S^y(0)$, and $S^z(0)$]. The exact recursion relation for ρ and u_4 (and hence the critical exponents) for our system in $d=4-\epsilon$ dimensions may be obtained in analogy with conventional systems, namely, by iterations which integrate out half of the variables $\vec{S}(\vec{q})$. However, the integration ranges in $\vec{q}$ space are now different for the three independent variables $S^+(\vec{q})$, $S^-(\vec{q})$, and $S^z(\vec{q})$. For example, the $S^+(\vec{q})$ are now integrated over the range $1\geq|\vec{q}+\overline{A}_3\hat{z}|\geq\frac{1}{2}$, instead of $1\geq|\vec{q}|\geq\frac{1}{2}$. ($\overline{A}_3$ is assumed to be much smaller than the cutoff momentum.)

The phase diagram of $\mathcal{H}$ is given in Fig. 1(d). It is gratifying to note that the condition $\overline{D}\leq\overline{A}_3^2$ (i.e., $DJ\leq A_3^2$) is exactly the condition that determines the instability of the ferromagnetic ground state—cf. Eq. (13) of Ref. 4. The critical behavior for the special case $A_3=0$ [the y axis of Fig. 1(d)] is also consistent with previous work (cf. Ref. 5). Furthermore, for $D=0$ and $A_3\neq0$ [the x axis of Fig. 1(d)], the xy-like behavior is plausible, since the interaction Hamiltonian $\mathcal{H}_1+\mathcal{H}_3$ possess rotational symmetry about the $\hat{z}$ direction of *spin* space (although it is neither symmetric nor antisymmetric under exchange of $\vec{r}_i, \vec{r}_j$ in the *lattice* space). This observation may serve as evidence that exchange symmetry is not one of the "basic symmetries" that affect the nature of critical behavior.

Consider finally the crossover behavior.[11-13] We find two symmetrized anisotropy parameters about the Heisenberg fixed points ($\overline{D}=\overline{A}_3^2$). The first is

$$\mathcal{O}^{(1)}\equiv\sum_{\langle ij\rangle}[S_{iz}S_{jz}-\tfrac{1}{2}(S_{ix}S_{jx}+S_{iy}S_{jy})]+\tfrac{1}{2}\overline{A}_3{\sum_{\langle ij\rangle}}'(S_{ix}S_{jy}-S_{iy}S_{jx})-\frac{\overline{D}}{2}\sum_{i=1}^{N}S_{iz}^2, \tag{7a}$$

with crossover exponent given by the $n=3$ value of

$$\varphi^{(1)}=1+\frac{n}{2(n+8)}\epsilon+\frac{(n^3+24n^2+68n)}{4(n+8)^3}\epsilon^2+O(\epsilon^3). \tag{7b}$$

The second symmetrized operator is

$$\mathcal{O}^{(2)}\equiv{\sum_{\langle ij\rangle}}'(S_{ix}S_{jy}-S_{iy}S_{jx})+\overline{A}_3\sum_{i=1}^{N}[S(S+1)-S_{iz}^2], \tag{8a}$$

with crossover exponent given by the $n=3$ value of

$$\varphi^{(2)}=\frac{3}{2}+\frac{3n+2}{4(n+8)}\epsilon+\frac{3n^3+72n^2+164n+104}{8(n+8)^3}\epsilon^2+O(\epsilon^3). \tag{8b}$$

Note that the operators $\mathcal{O}^{(1)}$ and $\mathcal{O}^{(2)}$ are functions of $\overline{D}=\overline{A}_3^2$, which is the position of the critical line about which the operators are perturbing. On the other hand, the crossover exponents are independent of $\overline{D}$. At $\overline{D}=\overline{A}_3=0$, the operator $\mathcal{O}^{(1)}$ reduces to one of the operators previously considered for this case[12] (and the crossover exponent is the same), while the second operator, $\mathcal{O}^{(2)}$, is just the pure Dzialoshinski-Moriya term.

In summary, then, we have studied a model Hamiltonian which readily yielded the helical ordered state. The order parameters of the phase transition and phase diagram were found. Our results reduce to previous results[4] in special cases. The antisymmetric term $\vec{A}\cdot\vec{S}_i\times\vec{S}_j$ is shown to enchance the fluctuation of the spin components in the plane perpendicular to $\vec{A}$. However, the breaking of exchange symmetry does not change the nature of the phase transition. Finally, the crossover behavior was also studied.

I conclude with the following remarks: (1) The critical behavior of helically ordered materials has yet to be studied experimentally. Guided by our results, one may make some calculated conjectures about the critical behavior of these materials, even though the helically ordered state may not result from the Dzialoshinski-Moriya interaction. For example, the ordered state of $MnAu_2$ is known[14] to be the same as in Fig. 1(b), with a turn angle corresponding to $\vec{q}_0 \cong (0.1\ \text{Å}^{-1})\hat{z}$. I suspect that in the critical region, $\Gamma^{xx}(\vec{q}_0, T) \sim (T-T_c)^{-\gamma}$ and $C_H \sim (T-T_c)^{-\alpha}$ with γ and α given by the $d=3$ value of the xy model. These speculations may be tested experimentally. (2) Unless $\overline{A}_3$ could be adjusted experimentally, I am unable to make any quantitative prediction about the crossover behavior of materials which possess Dzialoshinski-Moriya interaction. The crossover exponents, in particular $\varphi^{(2)}$, may, however, be tested numerically.

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Fluctuation Effects at a Peierls Transition

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The effects of fluctuations on the Peierls transition in one dimension are calculated by taking a functional average over variations in the order parameter. It is found that the transition is suppressed to a temperature of approximately one quarter of the mean-field transition but remains fairly sharp. The coherence length and density of states are calculated as a function of temperature, and brief comparison is made to experimental systems.

It has long been known that a one-dimensional metal is inherently unstable with respect to charge or spin-density waves.[1-3] In recent years a wide range of both inorganic and organic compounds which have characteristic one-dimensional metallic behavior have been discovered and extensively studied.[4-6] Theoretical calculations to date have been carried out only within a mean-field–theory description, although it is well known that fluctuation effects are very important in one-dimensional systems. In this Letter we report theoretical calculations incorporating fluctuation effects on the Peierls transition in a one-dimensional metal.

We consider a model with noninteracting electrons in a linear chain coupled to phonons:

$$H=\sum_{p\sigma}\epsilon_p c_{p\sigma}^\dagger c_{p\sigma}+\sum_q \omega_q b_q^\dagger b_q + (\sqrt{L})^{-1}\sum_{p,\sigma}\sum_q g(q) c_{p+q\sigma}^\dagger c_{p\sigma}(b_q+b_{-q}^\dagger), \quad (1)$$

where $c_{p\sigma}^\dagger$ and $b_q^\dagger$ are creation operators for a Bloch state and longitudinal phonon, respectively, with energies ϵ_p and ω_p, respectively. Because a Fermi surface in one dimension is a point, it is, of necessity, a perfect nesting Fermi surface causing an instability in the lattice with wave vector $2k_F$, where k_F $(=\pi N/2L)$ is the Fermi wave vector. A description of this instability within mean-field theory for the case where k_F is incommensurate with the underlying lattice periodicity (π/a) has been given by Fröhich,[2] Kuper,[7] and Rice and Strassler.[8] The mathematical structure of the theory closely parallels that of the BCS theory of superconductivity. The effects of fluctuations on phase transitions in one dimension have been studied by many authors. It is possible to treat the problem accurately by performing a functional integral over all possible fluctuations described by a Landau expansion of the free energy. Recently Scalapino, Sears, and