Quadrupolar interactions at ferromagnetic critical points

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The critical behavior of d-dimensional ferromagnets with quadrupole-quadrupole short- and long-range interactions is discussed on the basis of renormalization-group calculations to order ϵ^2, with $\epsilon = 4-d$. Such interactions may lead to a first-order transition, to characteristic "cubic" critical behavior, or to the usual isotropic critical behavior.

Pair interactions between magnetic ions which are of fourth order in the spin operators have been known to exist for some time.[1,2] Their origins are rather diverse, and range from multipole expansions of the Coulomb and exchange interactions to effective spin-lattice interactions.[3] Recent work on rare-earth compounds has provided examples where the fourth-order interactions are comparable to the bilinear ones.[4] This work prompted several studies, using mean-field theory and high-temperature-series expansions, for systems which have interactions of fourth order in the spins.[2] These reveal competition between first- and second-order transitions and between quadrupolar and dipolar ordering.

Renormalization-group recursion relations have been applied recently to various bilinear Hamiltonians, leading to a better understanding of the critical behavior.[5,6] This approach has also been used to study the fourth-order terms arising from lattice coupling.[3] In the present note we apply renormalization-group methods to discuss general fourth-order interactions.

We find that if the coefficients of the fourth-order terms are negative, and large enough, the transition is most probably of first order. In addition, we conclude that quadrupole-quadrupole interactions which couple space and spin coordinates will, on cubic lattices, usually introduce cubic symmetric terms, which lead to characteristic cubic critical behavior.[6]

For a rotationally invariant system, the fourth-order terms in the Hamiltonian can generally be written as a sum of two terms,[1,7]

$$\mathcal{H}_1 = -\sum_{i<j} j(R_{ij})(\vec{S}_i \cdot \vec{S}_j)^2 \tag{1}$$

and

$$\mathcal{H}_2 = -\sum_{i<j} k(R_{ij})R_{ij}^{-4}(\vec{S}_i \cdot \vec{R}_{ij})^2(\vec{S}_j \cdot \vec{R}_{ij})^2 \; . \tag{2}$$

For the purely electromagnetic part of the quadrupole-quadrupole interaction, $j(R)$ and $k(R)$ are of order $1/R^{d+2}$ (in d dimensions). However, this long-range interaction is usually negligible compared to the nearest-neighbor contribution to j and to k arising from averaged spin-orbit interactions.[7] We therefore start with the short-range case. If $j(\delta) = yJ$, where $\vec{\delta}$ is a nearest-neighbor vector, and $j(R) = 0$ for all $R > \delta$, with J being the nearest-neighbor exchange, then $\mathcal{H}_1$ may be written as

$$\mathcal{H}_1 = -ycJ\int_{\vec{q}_1}\int_{\vec{q}_2}\int_{\vec{q}_3}[1 + O(q_i^2)](\vec{\sigma}_{\vec{q}_1}\cdot\vec{\sigma}_{\vec{q}_2}) \times(\vec{\sigma}_{\vec{q}_3}\cdot\vec{\sigma}_{-\vec{q}_1-\vec{q}_2-\vec{q}_3}) \; , \tag{3}$$

where c is the coordination number and $\vec{\sigma}_{\vec{q}}$ is the Fourier transform of $\vec{S}_i$. As usual, $\int_{\vec{q}}$ means $(2\pi)^{-d}$ times the integral over the first Brillouin zone. Except for the terms of order q_i^2, this form is exactly similar to the one arising from Wilson's[5] S^4 term in the effective Hamiltonian. As in Ref. 3, we now find that the expansion parameter u_0 (the coefficient of the fourth-order term in Wilson's effective Hamiltonian) is

$$u_0 = (2d)^2 a^{d-4} k_B T (cJ)^{-2} u k_B (T - T_1) \; , \tag{4}$$

where u is the original coefficient of the S^4 term in the weighting factor and

$$k_B T_1 = ycJ/u \simeq 2yk_B T_c / u \; , \tag{5}$$

where we have used $cJ \simeq 2k_B T_c$.[8] Thus u_0 becomes negative if $2y \gtrsim u$. As discussed in Ref. 3, this may lead to a first-order transition if y is sufficiently large. Since u is of order unity at $d = 3$, we find a first order transition for $y \gtrsim \frac{1}{2}$, that is, of the same order of magnitude as found by mean-field theory.[2]

If $2y \simeq u$, we must allow for a sixth-order spin term in the continuous-spin Hamiltonian. For a particular choice of parameters, near three dimensions, we find the Riedel-Wegner "classical" tricritical point, with $T_t \simeq T_1$ and with logarithmic corrections to the classical tricritical behavior.[3,9]

For long-range interactions one has $j(R) \sim 1/R^{d+2}$, and the Fourier transform behaves as $A + Bq^2 \ln q + Cq^2 + O(q^4 \ln q)$. The $q^2 \ln q$ and the q^2 terms enter into the $O(q_i^2)$ terms in (3), and are irrelevant for determining the critical behavior (at least near $d = 4$). The behavior therefore remains as for the short-range case.

We turn now to the Hamiltonian (2). For nearest-neighbor interactions on cubic lattices $\mathcal{H}_2$ is equivalent to

$$\mathcal{H}_2 = -\sum_{\alpha\beta\gamma\delta} \int_{\vec{q}_1} \int_{\vec{q}_2} \int_{\vec{q}_3} A^{\alpha\beta\gamma\delta}(\vec{q}_1 + \vec{q}_3) \times \sigma^{\alpha}_{\vec{q}_1} \sigma^{\beta}_{\vec{q}_2} \sigma^{\gamma}_{\vec{q}_3} \sigma^{\delta}_{-\vec{q}_1-\vec{q}_2-\vec{q}_3} , \quad (6)$$

where

$$A^{\alpha\beta\gamma\delta}(\vec{q}) = \sum_{\vec{R}=\vec{\delta}} k(\vec{R}) \frac{R^\alpha R^\beta R^\gamma R^\delta}{R^4} e^{-i\vec{q}\cdot\vec{R}} . \quad (7)$$

The coefficients $A^{\alpha\beta\gamma\delta}(\vec{q})$ depend on the lattice structure. For sc lattices one finds

$$A^{\alpha\beta\gamma\delta}(\vec{q}) = 2k\delta_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\alpha\delta} + O(q^2) ,$$

whereas for fcc lattices in three dimensions one has

$$A^{\alpha\beta\gamma\delta}(\vec{q}) = k(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\alpha\delta}) + O(q^2) .$$

In all cases we see that, in addition to the rotationally invariant term, related to $\sum_{\vec{R}} S^4_{\vec{R}}$, there appears a term of only cubic symmetry, having the form of the Fourier transform of $\sum_{\vec{R}}\sum_\alpha (S^\alpha_{\vec{R}})^4$. Such terms were investigated in detail in Ref. 6. For a system with spin having $n = d = 4 - \epsilon$ components [we must take $n = d$, because the product $\vec{S}\cdot\vec{R}$ enters in (2)], the isotropic Heisenberg fixed point was found to be unstable in order ϵ^2. The critical behavior is thus determined by a new "cubic" fixed point, which has slightly different exponents.[6] In addition, negative $|S|^4$ terms may again lead to a first-order transition, just as in the first case discussed above.

For long-range quadrupole-quadrupole interactions, $k(R) \sim 1/R^{d+2}$, and again the deviations of $A^{\alpha\beta\gamma\delta}$ from the momentum-independent terms discussed above are of $O(q_i^2 \ln q_i)$ and thus are irrelevant (at least near $d = 4$).

In general, the quartic terms will appear in addition to the bilinear terms. Thus, as T approaches T_c one must expect a crossover from the usual isotropic critical behavior to the various new types of behavior presented here. As discussed in Ref. 6, the crossover to the "cubic" behavior is expected to be very slow. The crossover from the isotropic behavior to the tricritical behavior is quite complicated, since our discussion is valid near $d = 4$, while the Riedel-Wegner treatment of the tricritical point is valid near $d = 3$.[9] A general treatment of this crossover,[10] as well as a calculation of the crossover function (without which no numerical estimates are possible), is a subject for future investigation. In the meanwhile, experiments and high-temperature series may be very helpful in checking the predicted effects.

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