Critical thermodynamics of antiferromagnets with two pairs of magnetic sublattices

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A simple model is used to consider the critical behavior of crystals with two antiferromagnetic subsystems, and an explanation is proposed for the recently observed effect of the "splitting" of the critical exponent β. This splitting is due to specific corrections that must be introduced into the scaling because of the presence of an interaction bilinear in the fluctuations between the antiferromagnetic subsystems.

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It is known that a large number of antiferromagnets (AFM) have in the ordered phase four pairwise collinear (or almost collinear) magnetic sublattices. These include iron orthoborate Fe_3BO_6, in whose structure it is possible to separate below the Néel temperature $T_N = 508$ K two pairs of magnetic sublattices made up of iron ions.[1] The Mössbauer effect was recently used[1] to measure in this crystal the local magnetic fields at the nuclei of the iron ions in the critical temperature region.[2] It turned out that the temperature dependences of the magnetizations of different sublattices, determined in this manner, possess an unexpected singularity: the critical exponents of the magnetization of the sublattices of one pair differ somewhat from the exponents of the magnetization of the sublattices of the other pair, whereas the temperautres at which the AFM order sets in are the same for the two pairs, within the limits of experimental accuracy (for details see[2]). In the present communication we consider, with a simple model of an example, the static critical behavior of AFM of the indicated type and propose, in particular, an explanation of the "splitting" of the critical exponent β, an effect observed in[2].

Let $\phi_i(x)$ be the field of the fluctuations of the AFM-ordering parameter of the ith pair of sublattices, with $i=1$ and 2. We assume the fields ϕ_i to be scalar, i.e., that our AFM is effectively uniaxial with respect to both pairs of sublattices; it appears that this is exactly the situation realized in Fe_3BO_6. The fact that the condensate-formation tempreatures coincide for the fields ϕ_1 and ϕ_2 points to the presence of a coupling between these fields, and furthermore such that the corresponding Hamiltonian of the interaction contains a term bilinear in ϕ_1 and ϕ_2. Thus, the effective Hamiltonian of the critical-fluctuation field takes in this case the form

$$H = \int dx\, [(\nabla\phi_1)^2 + (\nabla\phi_2)^2 + r_1\phi_1^2 + r_2\phi_2^2 + \lambda\phi_1\phi_2 + \sum_{k=0}^{4} \gamma_k \phi_1^k \phi_2^{4-k}]. \tag{1}$$

Here r_1 and r_2 are certain smooth monotonically increasing functions of the temperature and go through zero at the points $T_{N1}^{(0)}$ and $T_{N2}^{(0)}$, respectively, and γ_k are the bare coupling constants. In the Landau theory, $T_{N1}^{(0)}$ and $T_{N2}^{(0)}$ play the role of phase-transition points for each pair of sublattices separately, i.e., in the absence of an interaction of the type $\lambda\phi_1\phi_2$.

To bring to light the manner in which this interaction influences the character of the phase transition, we diagonalize the harmonic part of the Hamiltonian (1). After a suitable orthogonal transformation, the Hamiltonian (1) takes the form

$$H = \int d\mathbf{x}\,[(\nabla\psi)^2 + (\nabla\xi)^2 + r_0\psi^2 + R_0\xi^2 + \sum_{k=0}^{4} \gamma_k \psi^k \xi^{4-k}], \qquad (2)$$

where

$$\psi = a\phi_1 - b\phi_2,\quad \xi = b\phi_1 + a\phi_2,\quad a = \sqrt{1-b^2} = \frac{1}{\sqrt{2}}\sqrt{1 + \frac{r_2 - r_1}{\sqrt{(r_2-r_1)^2+\lambda^2}}}, \qquad (3)$$

$$r_0 = \frac{1}{2}[r_1 + r_2 - \sqrt{(r_2-r_1)^2+\lambda^2}], \qquad R_0 = r_1 + r_2 - r_0 . \qquad (4)$$

The bare "masses" r_0 and R_0, just like r_1 and r_2, increase monotonically with temperature. We denote by $T_N^{(0)}$ and $T_c^{(0)}$ the points at which they vanish. It is easily seen that $T_N^{(0)} > \max(T_{N1}^{(0)}, T_{N2}^{(0)})$ and $T_c^{(0)} < \min(T_{N1}^{(0)}, T_{N2}^{(0)})$. We are interested in the vicinity of the point $T_N^{(0)}$ $[r_0(T_N^{(0)})=0]$ where the field ψ fluctuates strongly and can form a condensate[1)] at a certain temperature $T_N \approx T_N^{(0)}$, while the field ξ is noncritical, with $\langle\xi\rangle=0$. It follows from (3), at $\langle\psi\rangle\neq0$ and $\langle\xi\rangle=0$ both AFM ordering parameters $\langle\phi_1\rangle$ and $\langle\phi_2\rangle$ are simultaneously different from zero. Thus, the two pairs of sublattices do indeed go over into the AFM state at the same temperature T_N.

The fact that the field $\xi(\mathbf{x})$ is not critical near T_N does not make it possible, generally speaking, to neglect immediately the ξ-containing terms in the Hamiltonian (2). The point is that the interaction between the critical and the weakly fluctuating fields may turn out to be substantial in the critical region and lead, for example, to a transformation of the continuous phase transition into a first-order transition.[3] We, however, will assume that the "crossing" coupling constants in (2) are small enough and that there exists a wide range of temperatures where the critical behavior of the system is determined exclusively by the self-action of the field ψ. In this temperature interval, the effective Hamiltonian of the crystal can be taken in the form (2) with $\xi\equiv0$, while the order $\langle\psi\rangle$, the susceptibility χ_ψ, and other quantities as functions of $\tau=|T-T_N|/T_N$ are given by the usual power-law expressions

$$\langle\psi\rangle \sim \tau^\beta, \qquad \chi_\psi \sim \tau^{-\gamma}. \qquad (5)$$

We obtain next the temperature dependences of the magnetizations of the sublattices $\langle\phi_1\rangle$ and $\langle\phi_2\rangle$ of the two AFM subsystems. From (3) under the condition $\langle\xi\rangle=0$ we obtain immediately

$$\langle\phi_1\rangle = a\langle\psi\rangle \sim a\tau^\beta, \qquad \langle\phi_2\rangle = -b\langle\psi\rangle \sim b\tau^\beta. \qquad (6)$$

The coefficients a and b, as seen from (3), vary with temperature, so that $\langle\phi_1\rangle$ and $\langle\phi_2\rangle$ are not strictly power-law functions of τ. Within the limits of the critical region, however, where τ runs through the values from $\tau_1 \ll 1$ and $\tau_2 \ll \tau_1$, the quantities a and b, being smooth functions of the temperature, should vary insignificantly. As a result, the products $a(\tau)\tau^{\beta}$ and $b(\tau)\tau^{\beta}$, will behave over a certain finite (and small) interval of variation of the argument (τ_1,τ_2) like power-law functions of τ, but with exponents slightly different from β:

$$a(\tau)\tau^{\beta} \approx a_0\tau^{\beta'}, \qquad b(\tau)\tau^{\beta} \approx b_0\tau^{\beta''}. \tag{7}$$

Since $a^2+b^2=1$, the signs of the increments a and b are always positive and consequently $\mathrm{sign}(\beta'-\beta)=-\mathrm{sign}(\beta''-\beta)$.

Thus, the critical exponent β splits, as it were, into two effective exponents β' and β'', which characterize the temperature dependence of the magnetization of the sublattices of the two AFM subsystems. Let us estimate numerically the magnitude of this splitting, assuming, as in[1], $\tau_1=0.1$ and $\tau_2=10^{-3}$. Since $(\tau_1-\tau_2)\ll 1$, we can linearize the radical in (3) and represent a and b in the form

$$a \approx \sqrt{\frac{1+A}{2}} + \frac{B\tau}{\sqrt{1+A}} \qquad b \approx \sqrt{\frac{1-A}{2}} - \frac{B\tau}{\sqrt{1-A}}, \tag{8}$$

where the numbers A and B are expressed in elementary fashion in terms of the parameters of the model. At $T_{N1}^{(0)}/T_{N2}^{(0)} \sim \lambda \sim 1$ we have $A \sim B \sim 1$; we assume for the sake of argument $A=B=\frac{1}{2}$. Then, using the relation

$$\beta' - \beta'' \approx \left[\frac{a(\tau_1)\,b(\tau_2)}{b(\tau_1)\,a(\tau_2)} - 1\right] \Big/ \ln\frac{\tau_1}{\tau_2}, \tag{9}$$

we obtain $\beta'-\beta'' \approx 0.05$. In the Fe_3BO_6 crystal we have $\beta'-\beta''=0.045$.[2]

Thus, the considered splitting mechanism of the critical exponents ensures the required order of magnitude of the difference $\beta'-\beta''$.

The described effect is obviously not restricted to AFM with two pairs of magnetic sublattices. Corrections to scaling and "splitting" of critical exponents should be observed also in other substances having several ordered subsystems that are coupled with one another. Calculation of the effective exponent γ_{eff} shows that the splitting may be accompanied also by a shift of the effective value of the exponent relative to the true value, as a result of subsystem interactions that are bilinear in the fluctuations.

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