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Calculation of the Phase Transition Characteristics of a Magnetically Ordered System by the Renormalization Group Method

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Abstract—The phase transition "collapse" of magnetic moments of sublattices in segnetoantiferromagnetics in a strong magnetic field is considered. It is shown that spin fluctuations play an essential role and determine the characteristics of the phase transition. Consecutive accounting for the spin fluctuations by the renormalization group method and ε-expansion results in a phase transition in segnetoantiferromagnetics in a strong magnetic field that occurs at a first-order phase transition, which is close to second order for a nonzero relativistic constant of the magnetoelectric bond and any inductive capacity.

Keywords: phase transition, renormalization group, segnetoantiferromagnetics.

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The study of phase transitions in ordered structures is of significant interest. It is noteworthy that near a phase transition fluctuations of the order parameter are not small; they increase with proximity to the transition point and are necessary for considering it correctly.

We examine the binding magnetic, segnetoelectric, and elastic subsystems and show that during the "disruption" of a phase transition and the transformation of a second-order phase transition into a first-order phase transition that is close to second order, the relativistic magnetoelectric bond energy plays a greater role than the exchange magnetoelastic energy [1, 2].

In order to study the behavior of substances in the field of phase transitions near the critical point, ε-expansion, which has been successfully applied for the description of phase transitions on the basis of the renormalization group method [6–8], has been developed [3–5].

The idea of the renormalization group method and ε-expansion consists in the reduced description of a system, which contains a larger number of degrees of freedom, i.e., the set of initial microscopic degrees of freedom is replaced with a smaller set of effective degrees of freedom. The main assumption of this method consists in the idea that in the phase transition field the behavior of physical magnitudes can only be described by the interaction of long-wave fluctuations and, consequently, the consideration of a system in areas with L that are much smaller than the correlation length r_C gives the correct size of an area in which the properties of a substance correctly transfer to the properties of the entire microscopic sample. The correlation length is defined by the condition of the system $r_C \approx |H - H_C|^{-\nu}$, $\nu > 0$, and if the phase transition is characterized by a critical point, then in the nearby field the correlation length r_C is much more than the internuclear distance and at the point $r_C \longrightarrow \infty$. Therefore, an area of r_C magnitude contains a large number of degrees of freedom and solving the problem directly is not obviously possible.

In [9–11] during the consideration of magnetic structure it was suggested to break the spin system into blocks of several spins. Near the phase transition point, r_C is very large and all spins in the small block should be correlated, i.e., it is possible to pass from the consideration of separate spins to the consideration of spin blocks. The effective correlation length has thus decreased: $r_C = \frac{l_0}{l_1} r_C^{(0)}$, where $r_C^{(0)}$ and l_0 are the correlation length and the distance between spins in the initial microscopic system, respectively, l_0 is the distance between the spin blocks after the first "approximation," and $l_j > l_0$.

The repetitive application of the procedure of grouping neighboring blocks leads to a further decrease of the effective correlation length:

$r_C^{(2)} = \frac{l_1}{l_2} r_C^{(1)} = \frac{l_0}{l_2} r_C^{(0)}$, $l_2 > l_1 > l_0$. Eventually, the task is reduced to effective $r_C \approx 1$, $r_C^{(n)} = \frac{l_0}{l_n} r_C^{(0)}$, $l_n \gg l_0$.

Let us examine the system of free spins. Passing to the Fourier transform, the Hamiltonian of free spins can be written as follows:

$$H^{(0)} = \frac{1}{2}\int \frac{d^{\alpha}\mathbf{q}}{(2\pi)^{\alpha}}(\tau^{(0)} + q^2)\mathbf{S}^{(0)}(\mathbf{q})\mathbf{S}^{(0)}(-\mathbf{q}),$$

where α is the spatial dimension and $\tau^{(0)} = 1 - H_C/H$. Here the integration domain $0 \le |\mathbf{q}| \le q_0$, q_0 is the pulse cutoff $q_0 \approx a^{-1}$. According to the idea of the renormalization group method and ε-expansion the spin blocks depend only on the long-wave spin component $S|q|$ with small q. Let us divide the integration domain into two ranges: $0 \le |\mathbf{q}| \le \lambda q_0$ and $\lambda q_0 \le |\mathbf{q}| \le q_0$, $\lambda < 1$. Then the first range corresponds to a small q of the long-wave components $\mathbf{S}(\mathbf{q})$ and the second range corresponds to a larger q of the short-wave components. It is possible to integrate $\mathbf{q}$ by the second change range. This will be an integration of the quickly fluctuating components of the spin field $\mathbf{S}(\mathbf{x})$. Then:

$$H^{(0)} = \frac{1}{2}\int\limits_{0 \le |\mathbf{q}| \le \lambda q_0} \frac{d^{\alpha}\mathbf{q}}{(2\pi)^{\alpha}}(\tau^{(0)} + q^2)\mathbf{S}^{(0)}(\mathbf{q})\mathbf{S}^{(0)}(-\mathbf{q})C. \quad (1)$$

The appearance of the multiplicate constant C, which is independent of spin fields, but is dependent exclusively on the temperature, in (1) during the calculation of the fluctuation free energy can be ignored, since C results in constant free energy. Thus, the effective Hamiltonian is the following:

$$H^{(1)} = \frac{1}{2}\int\limits_{0 \le |\mathbf{q}| \le \lambda q_0} \frac{d^{\alpha}\mathbf{q}}{(2\pi)^{\alpha}}(\tau^{(0)} + q^2)\mathbf{S}^{(0)}(\mathbf{q})\mathbf{S}^{(0)}(-\mathbf{q}). \quad (2)$$

In order that the effective interaction (2) has the same appearance as the initial one, we have to change the scale of pulses. We bring the value $\mathbf{q}' = \lambda^{-1}\mathbf{q}$. Then $\mathbf{q}'$ changes within the limits of $0 \le |\mathbf{q}'| \le \lambda q_0$, i.e., in the same way as in the initial Hamiltonian. We also change the scale of the spin field: $\mathbf{S}^{(0)}(\mathbf{q}) = \mathbf{S}^{(0)}(\lambda\mathbf{q}') = \alpha^{-1}\mathbf{S}^{(1)}(\mathbf{q}')$. Then

$$H'^{(1)} = \frac{1}{2}\alpha^{-2}\lambda^{\alpha+2} \times \int\limits_{0 \le |\mathbf{q}| \le \lambda q_0} \frac{d^{\alpha}\mathbf{q}'}{(2\pi)^{\alpha}}(\tau^{(1)} + q'^2)\mathbf{S}^{(1)}(\mathbf{q}')\mathbf{S}^{(1)}(-\mathbf{q}),$$

where $\tau^{(1)} = \lambda^{-2}\tau^{(0)}$. To obtain a Hamitonian that is conterminous with the initial one, we determine $\alpha = \lambda^{\frac{\alpha+2}{2}}$. We finally receive:

$$H'^{(1)} = \frac{1}{2}\int\limits_{0 \le |\mathbf{q}| \le \lambda q_0} \frac{d^{\alpha}\mathbf{q}'}{(2\pi)^{\alpha}}(\tau^{(1)} + q'^2)\mathbf{S}^{(1)}(\mathbf{q}')\mathbf{S}^{(1)}(-\mathbf{q}').$$

The correlation length r_C that corresponds to $H'^{(1)}$ is determined by the expression:

$$r_C^{(1)} = \frac{1}{\sqrt{\tau^{(1)}}} = \lambda\frac{1}{\sqrt{\tau^{(0)}}} = \lambda r_C^{(0)}.$$

The appearance of a such a connection between $r_C^{(1)}$ and $r_C^{(2)}$ is the consequence of the scale transformation from $\mathbf{q}$ to $\mathbf{q}'$.

The transformation A that translates $H^{(0)}$ into $H^{(1)}$ is the renormalization group transformation. The renormalization group method consists in the iterative transformation of A. $AH^{(0)} = H^{(1)}$, $AH^{(1)} = H^{(2)}$, ... Thus $r_C^{(1)} = \lambda r_C^{(0)}$, $r_C^{(2)} = \lambda^2 r_C^{(0)}$ ... .

The problem has special interest if the transformation A exists at one or several motionless points. In other words, if the sequence $H^{(n)}$ converges to the some $H^{(*)}$ there is a motionless point of transformation A that satisfies the condition $AH^{(*)} = H^{(*)}$. This equation is used to obtain all motionless points. It practically does not depend on the choice of the initial Hamiltonian.

It is possible to show that if the spatial dimension $d > 4$, $d = 4 - \varepsilon$, then $\tau^* \approx 4/9\varepsilon\ln\lambda$, and for small ε the value τ^* is also insignificant.

For a segnetoantiferromagnetic with the Hamiltonian:

$$H = H_M + H_F + H_U + H_{MF} + H_{MU},$$

$$H_M = \int d\mathbf{x}\Bigg\{\delta(\mathbf{M}^1\mathbf{M}^2) + \alpha\frac{\partial\mathbf{M}^1}{\partial x_i}\frac{\partial\mathbf{M}^2}{\partial x_i} + \frac{\alpha'}{2}\left[\left(\frac{\partial\mathbf{M}^1}{\partial x_i}\right)^2 + \left(\frac{\partial\mathbf{M}^2}{\partial x_i}\right)^2\right] + \beta M_z^1 M_z^2 + \frac{\beta'}{2}(M_z^{12} + M_z^{22}) - (\mathbf{H}_0, \mathbf{M}^1 + \mathbf{M}^2)\Bigg\},$$

$$H_F = \int d\mathbf{x}\left[-\frac{1}{2}xP^2 + \frac{1}{4}xP^4 + \frac{1}{2}s\left(\frac{\partial\mathbf{P}}{\partial x_i}\right)^2\right],$$

$$H_U = \frac{1}{2}\int d\mathbf{x}c_{ii}u_{ii}^2,$$

$$H_{MF} = \int d\mathbf{x}\gamma_1 P^2(\mathbf{M}^1, \mathbf{M}^2),$$

$$H_{MU} = \int d\mathbf{x}\gamma_{zii}u_{ii}(\mathbf{M}^1, \mathbf{M}^2),$$

where $\mathbf{P} = \mathbf{n}P_0(1 + p)$ is the spontaneous polarization, p is the deviation of the polarization from the spontaneous value caused by the presence of fluctuation, similarly $u_{ii} = u_{ii}^0 + \tilde{u}_{ii}$, u_{ii}^0 is the spontaneous deformation, $\tilde{u}_{ii}$ is the deviation of the deformation from a spontaneous deformation, and the equations of the renorm group are as follow:

$$\frac{\partial\tau}{\partial x} = \left[2-\left(\frac{n+2}{n+8}\right)k_n\Gamma_1\right]\tau,$$

$$\frac{\partial\omega}{\partial x} = -\frac{1}{2}\frac{n}{n+8}k_n\Gamma_2^2,$$

$$\frac{\partial c}{\partial x} = -\frac{3}{2}\frac{n}{n+8}k_n\Gamma_3^2, \qquad (3)$$

$$\frac{\partial\Gamma_1}{\partial x} = \varepsilon\Gamma_1 - k_n\Gamma_1^2,$$

$$\frac{\partial\Gamma_2}{\partial x} = \left[\frac{\varepsilon}{2}-\left(\frac{n+2}{n+8}\right)k_n\Gamma_1\right]\Gamma_2,$$

$$\frac{\partial\Gamma_3}{\partial x} = \left[\frac{\varepsilon}{2}-\left(\frac{n+2}{n+8}\right)k_n\Gamma_1\right]\Gamma_3.$$

With initial conditions: $\tau(0)=\tau_0$, $\omega(0)=\omega_0$, $c(0)=c_0$, $\Gamma_1(0)=\Gamma_{10}-\frac{\Gamma_{20}^2}{\omega_0}-\frac{3\Gamma_{30}^2}{c_0}\equiv\tilde{\Gamma}_{10}$, $\Gamma_2(0)=\Gamma_{20}$, $\Gamma_3(0)=\Gamma_{30}$, where

$$\tau_0 = 1-\frac{H_C}{H_0}, \quad s_0 = \frac{(\alpha'-\alpha)M_0}{H_0}, \quad \omega_0 = \frac{2\chi P_0^4}{H_0M_0},$$

$$c_{ii}^0 = \frac{c_{ii}}{H_0M_0}, \quad \Gamma_{10} = \frac{1}{16}, \quad \Gamma_{20} = -\frac{2\gamma_1P_0^2M_0}{H_0},$$

$$\Gamma_{30} = -\frac{\gamma_{2ii}M_0}{H_0}.$$

Solutions (3) are as follow:

$$\tau(x) = \tau_0 e^{\left(2-\frac{4-n}{n+8}\varepsilon\right)x}\left[\frac{\varepsilon}{\varepsilon e^{-\varepsilon x}+k_n\Gamma_{10}(1-e^{-\varepsilon x})}\right]^{\frac{n+2}{n+8}},$$

$$\omega(x) = \omega_0 - \frac{n\Gamma_{20}^2}{2(4-n)\tilde{\Gamma}_{10}\varepsilon^{\frac{4-n}{n+8}}} \times\left\{\left[\varepsilon-k_n\tilde{\Gamma}_{10}(1-e^{\varepsilon x})\right]^{\frac{4-n}{n+8}}-\varepsilon^{\frac{4-n}{n+8}}\right\},$$

$$c(x) = c_0 = \frac{3n\Gamma_{30}^2}{2(4-n)\tilde{\Gamma}_{10}\varepsilon^{\frac{4-n}{n+8}}} \times\left\{\left[\varepsilon-k_n\tilde{\Gamma}_{10}(1-e^{\varepsilon x})\right]^{\frac{4-n}{n+8}}-\varepsilon^{\frac{4-n}{n+8}}\right\},$$

$$\Gamma_1(x) = \frac{\varepsilon\tilde{\Gamma}_{10}}{\varepsilon e^{-\varepsilon x}+k_n\Gamma_{10}(1-e^{-\varepsilon x})},$$

$$\Gamma_2(x) = \Gamma_{20}e^{\frac{4-n}{2(n+8)}\varepsilon x}\left[\frac{\varepsilon}{\varepsilon e^{-\varepsilon x}+k_n\tilde{\Gamma}_{10}(1-e^{-\varepsilon x})}\right]^{\frac{n+2}{n+8}},$$

$$\Gamma_3(x) = \Gamma_{30}e^{\frac{4-n}{2(n+8)}\varepsilon x}\left[\frac{\varepsilon}{\varepsilon e^{-\varepsilon x}+k_n\tilde{\Gamma}_{10}(1-e^{-\varepsilon x})}\right]^{\frac{n+2}{n+8}},$$

$$x = \frac{2}{\varepsilon q_0^{\varepsilon}}\left\{\left(\frac{q_0}{\max[\lambda(\tau), l_0]}\right)^{\varepsilon}-1\right\}.$$

Phase transition in a system will occur if Γ is zero and the system becomes thermodynamically unstable. This happens at

$$x^* = \frac{1}{\varepsilon}\ln\left\{1+\frac{\varepsilon}{k_n\tilde{\Gamma}_{10}}\left\{\left\{\frac{(4-n)}{2}+\Gamma_{10}\left[\frac{\Gamma_{20}^2}{\omega_0+\frac{n\Gamma_{20}^2}{2(4-n)}}+\frac{3\Gamma_{30}^2}{c_0+\frac{3n\Gamma_{30}^2}{2(4-n)\tilde{\Gamma}_{10}}}\right]^{-1}\right\}-1\right\}^{\frac{n+8}{4-n}}\right\}.$$

In the phase transition point the parameter of the order jumps at

$$H > H_C^*, \quad l_0 = 0,$$

$$\text{at } H < H_C^*, \quad l_0^2 = \left(\frac{2-\varepsilon}{2+\varepsilon x^*}\right)^{\frac{2}{\varepsilon}}.$$

This means that at $\varepsilon \longrightarrow 0$ the value of the jump parameter order is exponentially small, i.e., phase transition occurs in the scaling range. Increasing ε leads to an increase in the values of the jump in the magnitude of the antiferromagnetism vector, as well as the magnitudes of the elasticity and frequency of the soft ferroelectric mode. This testifies to the strengthening of the influence of fluctuation on the phase transition with decreasing spatial dimension. The character of the phase transition remains constant and the phase transition is a first-order phase transition that is close to a second-order one.

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