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GAUSSIAN AND NONGAUSSIAN BASIC MEASURE DENSITIES IN THE THEORY OF CLUSTER FERROELECTRICS

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The problem of application of Gaussian and non-Gaussian basic measure densities of collective variables for integration a cluster ferroelectric partition function functional is discussed. Starting from the conver- gence of functional integrals in the phase transition point vicinity the first Brillouin zone is divided into layers. Every layer consists of two parts. In the first one the Gaussian measure density is sufficient and in the second one the non-Gaussian measure density must be used. The partition function obtained as a result of layer by layer integration is finite in the temperature region which contains the neighbourhood of phase transition point. The critical behaviour of a thermodynamic functions is studied.

1. Introduction

There are two recently unsolved problems in the description of the phase transition point neighbourhood in cluster ferroelectrics. The first one is the rigorous treatment of dipole-dipole interaction between particles of system and influence of it on the critical behaviour of thermodynamic functions. The second problem is connected with complex intra-and inter clusters short-ranging interactions, including the transverce field influence. The role of dipolar interaction in forming the critical behaviour of isotropic ferromagnets was discussed in [1-6]. The investigations have been performed using both numerical methods and ε-expansion in field renormalization group theory.

Some problems of simultanious coexistence of short range and long range dipolar interactions in ferromagnetic systems was discussed in [7,8].

In the microscopic theory of ferroelectricity there are well known investigations based on taking into account long-range dipolar interactions [9-11]. For calculation Gaussian integrals the procedure of diagram summation in perturbation theory was developed [9,10]. The logarithmic corrections to some thermodynamical functions were obtained. The renormalization group method and it's application to investigation the thermodynamical properties of ferroelectrics near phase transition point were developed in [11]. The role of short-range interactions in the phase transition was not discused. New interesting results of experimental investigation of ferroelectric crystals are presented in [12].

In the present paper the regular method for calculation of different thermodynamic functions of uniaxial cluster ferroelectrics in the phase transition

point vicinity is proposed. The knowledge of characteristic functions like free energy or thermodynamic potential is a basis to obtain all thermodynamic functions [13]. Therefore. considering the phase transition from one thermodynamic state to another one within the frames of equilibrium statistical physics, we shall deal with free energy which is a characteristic function of system under volume and temperature as an independed variables. For this the Yukhnovskii's method of layer by layer integration of partition function functional over collective variables (CV) is used [14]. We propose modificated layer by layer integration method [15], which is based on the taking into account fine peculiarities of CV distributions in cluster ferroelectric system. Short-range intracluster interactions will be considered exactly, but intercluster short-range interactions renormalize spherically-symmetric part of long-range patential.

2. Hamiltonian and initial relations

We shall consider a crystalline system of volume V containing f_0N particles. There are f_0 particles in every of N unit cells of crystal. They form a cluster. So, we have a N-clusters system. For every particle there occurs the possibility to be in one of two quantum states. These states are determined by the S^z Pauli matrix. The transition from one state to another one is discribed by the S^x operator. The probability of such a transition is determined by the extermal tranverse field value, or by so-called tunneling parameter Γ. The pair potential of interparticle interaction consists of two terms: a short-range potential of nearest neighbours $V_{ff'}$ and a long-range potential $J_{ff'}(\mathbf{R}_i - \mathbf{R}_j)$; where f, f' are numbers of particles in cluster, $\mathbf{R}_i$ is a radius-vector of cluster center.

As it was showh in [16] the Hamiltonian of such cluster system may be presented in a Ising-like form using deneralized Hubbard-Stasyuk operators $Y^\lambda(\mathbf{R}_i)$:

$$H = \sum_{\lambda=1}^{2^{2f_0}} \left\{ \sum_{i=1}^{N} \Lambda_\lambda Y^\lambda(\mathbf{R}_i) - \frac{1}{2} \sum_{i,j=1}^{N} \Phi_\lambda(\mathbf{R}_i - \mathbf{R}_j) Y^\lambda(\mathbf{R}_i) Y^\lambda(\mathbf{R}_j) \right\}. \quad (2.1)$$

Here

$$Y^\lambda(\mathbf{R}_i) = \sum_{m=1}^{2^{2f_0}} U_{\lambda m} X^m(\mathbf{R}_i), \qquad \lambda = 1, 2, \ldots 2^{2f_0},$$
$$m = 2^{f_0}(p-1) + q, \qquad p, q = 1, 2, \ldots 2^{f_0}. \quad (2.2)$$

$X^m \equiv X^{pq}$ is a Hubbard-Stasyuk operator, which discribes "transition" of a cluster from q-state into p-state [17,18]. $U_{\lambda m}$ are a matrix elements of U-matrix, which is a eigenmatrix of equation:

$$\sum_{m,m'=1}^{2^{f_0}} \left\{ \sum_{f,f'=1}^{f_0} \left[V_{ff'}\delta(\mathbf{R}_i - \mathbf{R}_j + \mathbf{r}_{ff'} - \right.\right.$$
$$\left.\left. - \frac{1}{2} J_{ff'}(\mathbf{R}_i - \mathbf{R}_j) \right] \alpha_m^{(f)} \alpha_{m'}^{(f')} U_{m\lambda} U_{m'\lambda'} \right\} =$$
$$\Phi_\lambda(\mathbf{R}_i - \mathbf{R}_j)\delta_{\lambda\lambda'}. \quad (2.3)$$

Here $\mathbf{r}_{ff'}$ is a radius-vector of the nearst neighbours f and f', $\alpha_m^{(t)}$ are matrix elements of the transition from two-component individual particle spinor basis to 2^{f_0}-component diagonal onto S^z and S^x spinor basis of cluster. $\Phi_{ff'}(\mathbf{R}_i - \mathbf{R}_j)$ are the eigenvalues of the intercluster interaction matrix, including long-range interactions $J_{ff'}(\mathbf{R}_i - \mathbf{R}_j)$ and short-range interactions of the nearest neighbours $V_{ff'}\delta(\mathbf{R}_i - \mathbf{R}_j + \mathbf{r}_{ff'})$. Λ_λ are energies of isolated cluster. δ is a Kronecher symbol. For more details about representation (2.1)-(2.3) see ref. [15].

Generalized Hubbard-Stasyuk operators satisfy the commutation relation

$$\left[Y^\lambda(\mathbf{R}_i), Y^{\lambda'}(\mathbf{R}_j)\right] = \sum W^\mu_{\lambda\lambda'}, Y^\mu(\mathbf{R}_i)\delta(\mathbf{R}_i - \mathbf{R}_j), \tag{2.4}$$

where

$$W^\mu_{\lambda\lambda'} = \sum_{r,s,t} \left\{U_{rs\lambda}U_{st\lambda'} - U_{st\lambda}U_{rs\lambda'}\right\}U_{rt\mu}, \tag{2.5}$$

r, s, t are ordinary and λ, μ are double indices.

Representation of the ferroelectric cluster system Hamiltonian in the form (2.1) is convenient for the application of modern functional methods to its investigation. Among different functional methods which are widely used in theory of phase transitions the collective variables method is very powerfull. CV is a collective name of a special class of variables, specific for every physical system. For example, for ferroelectrics CV are modes of a site dipole momentum vibration. The set of CV contains a variable, the mean value of which is connected directly with the order parameter, therefore the phase space of CV is a most natural one for the discription of phase transition. The method provides the possibility to formulate rigorously the phase transition problem without any additional parameters artificially introduced into the partition function [14].

Because the generalized Hubbard-Stasyuk operators are non-commuting we must use an interaction representation and introduce CV in a frequency - momentum representation [15]

$$\rho_\lambda(\mathbf{k}, \nu) = \frac{1}{\sqrt{N}\beta}\int_0^\beta d\beta' e^{-i\beta'\nu}\mathrm{Sp}\left[\sum_{i=1}^N e^{-\beta' H_0}Y^\lambda(\mathbf{R}_i)e^{\beta' H_0} \times \right.$$

$$\left. e^{i\mathbf{k}\mathbf{R}_i}J(\rho_\lambda, Y^\lambda)\right]\left\{\mathrm{Sp}\left[J(\rho_\lambda, Y_\lambda)\right]\right\}^{-1}, \tag{2.6}$$

where $J(\rho_\lambda, Y^\lambda)$ is a transition operator from the set of variables $\mathbf{R}_i$ to CV space, $\nu = \frac{2\pi}{\beta}n (n = 0, \pm1, \pm2, ...)$ are Matsubara's frequencies, $\beta = \frac{1}{kT}$, k is the Bolzman constant,

$$H_0 = \sum_{\lambda=1}^{2^{2f_0}}\sum_{i=1}^N \Lambda_\lambda Y^\lambda(\mathbf{R}_i). \tag{2.7}$$

For partition function functional in CV representation we have an expression

$$Z = Z_0 \int (d\rho_\lambda(\mathbf{k}, \nu)) \prod_{\lambda=1}^{2^{2f_0}} \prod_{k\leq\beta} \prod_\nu J\left(\rho_\lambda(\mathbf{k}, \nu)\right) \times$$

$$\exp\left\{\frac{\beta}{2}\sum_{\lambda=1}^{2^{2f_0}}\sum_{k\leq B_1}\sum_{\nu}\Phi_\lambda(\mathbf{k})\rho_\lambda(\mathbf{k},\nu)\rho_\lambda(-\mathbf{k},-\nu)\right\}. \tag{2.8}$$

Here

$$J\left(\rho_\lambda(\mathbf{k},\nu)\right) = \langle J(\rho_\lambda, Y^\lambda\rangle_{H_0} =$$
$$\int (d\omega_\lambda(\mathbf{k},\nu))\exp\left\{i2\pi\sum_{\lambda=1}^{2^{2f_0}}\sum_{k\leq B_1}\sum_{\nu}\omega_\lambda(\mathbf{k},\nu)\rho_\lambda(\mathbf{k},\nu)\right\}\times$$
$$\exp\left\{\sum_{n=0}^{\infty}\frac{(-i2\pi)^n}{(2n)!}\sum_{\lambda_1,k_1,\nu_1}\cdots\sum_{\lambda_{2n},k_{2n},\nu_{2n}}\mathfrak{M}_{\lambda_1\ldots\lambda_{2n}}(\mathbf{k}_1,\nu_1\ldots\mathbf{k}_{2n},\nu_{2n})\times\right.$$
$$\left.\omega_{\lambda_1}(\mathbf{k}_1,\nu_1)\ldots\omega_{\lambda_{2n}}(\mathbf{k}_{2n},\nu_{2n})\right\} \tag{2.9}$$

is a transition Jacobian, $\mathfrak{M}_{\lambda_1\ldots\lambda_{2n}}(\mathbf{k}_1,\nu_1\ldots\mathbf{k}_{2n},\nu_{2n})$ are cluster cumulants, $\omega_\lambda(\mathbf{k},\nu)$ being variables conjugated to $\rho_\lambda(\mathbf{k},\nu)$

$$Z_0 = \mathrm{Sp}e^{-\beta H_0}, \quad \langle\ldots\rangle_{H_0} = \mathrm{Sp}\left\{\ldots e^{-\beta H_0}\right\}/\mathrm{Sp}\left\{e^{-\beta H_0}\right\}, \tag{2.10}$$

B_1 is a Brillouin zone boundary.

The functionals of the type (2.8),(2.9) related to other problems are usually called Ginzburg-Landau functionals [19]. The coefficients of Ginzburg-Landau functionals are given from phenomenological considerations. We have managed to construct this functional *ab initio*, using only the Hamiltonian of the system.

3. Gaussian and non-Gaussian measure densities for CV

The main problem of integration (2.8),(2.9) consists in the presense of infinite number of $\omega_\lambda(\mathbf{k},\nu)$ in exponential form (2.9). There is no regular recept to calculate such integral exactly. To perform integration of (2.8),(2.9) approximately we may use different measure densities. The simplest nontrivial basic measure density is a Gaussian one (all products of ω up to ω^2 in exponential form (2.9)). The first non-Gaussian measure density is a quartic one (all products of ω up to ω^4 in exponential form (2.9)). Using a perturbation theory based on Gaussian integrals one can obtain results, which a good in wholle temperature interval exepted phase transition point. Non-Gaussian measure density enables us to integrate (2.8) and to obtain results, which are continuous in very transition point. For integrals with quartic measure density we have rather simple formulas [14,20]. So, it is a simplest stright way to obtain an analytic expression for partition function.

It is well known that in cluster systems one may observe different types of arranged structures and corresponding phase transitions [21,22]. Among them the homogeneous arrangement, which is characterized by zero vector, is always present. It is a ferroelectric arrangement of the crystal ($\lambda = 1$). Because only the ferroelectric phase transition is of interest for us we have the possibility to integrate (2.8), (2.9) over $\rho_\lambda(\mathbf{k},\nu)(\lambda \neq 1)$ which are not connected directly with the order parameter of this transition using the Gaussian measure density.

The other difficulty of the integration in (2.8), (2.9) consists in the fact that the CV $\rho(\mathbf{k},\nu)$ are determined in phase space of momenta and frequencies, while for the usual Ising model $\rho(\mathbf{k})$ depends only on momentum. Due to the using the interaction representation, transition from N variables $Y^{\lambda}(\mathbf{R}_i)$ to CV is acompained by appearing of infinite number of variables $\rho(\mathbf{k},\nu)$. But only variables $\rho(\mathbf{k},0)$ are "physical" ones. Passing through the critical temperature, the displacement of the probability distribution maximum takes place only for these variables [14]. They form the order parameter of the system. Variables $\rho(\mathbf{k},\nu\neq 0)$ are "unphysical", the probability of their distribution is indifferent with respect to Tc.

Because the phase transition in a physical system is possible in the thermodynamic limit ($N,V\to\infty$, $\frac{N}{V}=const$)only, the spectrum of wave vectors $\mathbf{k}$ ($k_\alpha=\frac{2\pi n}{N_\alpha c}$, c is a lattice constant, N_α is a number of atoms of the first Brillouin zone in α direction, $n=0,\pm1,\pm2,...$) becomes quasicontinuous, variables $\rho_\lambda(\mathbf{k},\nu)$ do not separate with respect to the $\mathbf{k}$ index, and the problem of integration of (2.8), (2.9) remains similar to that in the Ising model [14].

Another situation takes place for the frequency dependence. The spectrum of values $\nu(\nu=\frac{2\pi n}{\beta},\quad n=0,\pm1,\pm2,...)$ for real ferroelectric phase transition temperatures is discrete, as well as the spectrum of values $\mathfrak{M}_{11}(\mathbf{k},\nu)$ as a function of ν . The maximum of $\mathfrak{M}_{\lambda\lambda}(\mathbf{k},\nu)$ occurs at $\nu=0$ [16]: $\max\{\mathfrak{M}_{\lambda\lambda}(\mathbf{k},\nu)\}=\mathfrak{M}_{11}(\mathbf{k},0)$. Therefore, in the Gaussian approximation for critical temperature we have an estimation

$$T_c\approx\Phi_1(0)\mathfrak{M}_{11}(0,0). \tag{3.1}$$

The integrand of such Gaussian momentum contains a factor like $(æ^2+\nu^2+k^2)^{-1}$, were according to [14] $æ\sim\tau$ $(\tau=\frac{T-Tc}{Tc})$. Because of the discreteness of ν even when æ equals zero the Gausiian momentum is convergent at $\nu\neq 0$. So, when the critical phenomena are investigated in the temperature interval

$$\Delta T\leq\Phi(0)\left[\mathfrak{M}_{11}(0,0)-\mathfrak{M}_{11}(0,\frac{2\pi}{\beta})\right] \tag{3.2}$$

all Gaussian momenta obtained as a result of integration over variables $\rho_1(\mathbf{k},\nu)$ with $\nu\neq 0$ are convergent.

Descreteness of $\rho_1(\mathbf{k},\nu)$ with respect to ν and the fact that in phase transition the leading role is played by CV with zero frequency, allow us to apply the following order of integration of (2.8), (2.9), using different basic measure densities. At the first stage we integrate over variables $\rho_\lambda(\mathbf{k},\nu)$ $(\lambda\neq 1)$ and $\rho_1(\mathbf{k},\nu)$ $(\nu\neq 0)$ using the Gaussian measure density. As it was shown above all obtained integrals will remain convergent at $T=Tc$. At the second stage we integrate over variables $\rho_1(\mathbf{k},\nu)$ (with $\nu=0$), but using non-Gaussian measure density. Such measure density satisfies an essential requirement: all obtained integrals are convergent at $T=Tc$.

Some aspects of using Gaussian and non-Gaussian measure densities connected with the peculiarity of dipole-dipole intercluster interaction will be discussed below.

After performing integration over CV $\rho_\lambda(\mathbf{k},\nu)$ $\lambda\neq 1$ and $\rho_1(\mathbf{k},\nu)$ $\nu\neq 0$ using Gaussian measure density we obtain the following expression for partition function (2.8)

$$Z=Z_0\prod_{\lambda\neq 1}Z_\lambda^G Z_1^G Z_1. \tag{3.3}$$

Here

$$Z_\lambda^G = C_\lambda \prod_{\substack{\mathbf{k}\geq 0\\ \nu\geq 0}} \left[1-\beta\Phi_\lambda(0)\mathfrak{M}_{\lambda\lambda}(0,\nu)\right]^{-\frac{1}{2}} \left[1-\beta\Phi_\lambda(\mathbf{k})\mathfrak{M}_{\lambda\lambda}(\mathbf{k},\nu)\right]^{-1},$$
$$Z_1^G = C_1 \prod_{\substack{\mathbf{k}\geq 0\\ \nu>0}} \left[1-\beta\Phi_1(0)\mathfrak{M}_{11}(0,\nu)\right]^{-\frac{1}{2}} \left[1-\beta\Phi_1(\mathbf{k})\mathfrak{M}_{11}(\mathbf{k},\nu)\right]^{-1}, \tag{3.4}$$

$$C_\lambda = \exp\left\{-\frac{1}{8}\sum_{\substack{\mathbf{k}',\nu'\\ \mathbf{k}'',\nu''}} \mathfrak{M}_{\lambda\lambda\lambda\lambda}(\mathbf{k}',\nu',-\mathbf{k}'-\nu',\mathbf{k}'',\nu'',-\mathbf{k}'',-\nu'')\times\right.$$
$$\left. g_\lambda(\mathbf{k}',\nu')g_\lambda\mathbf{k}'',\nu'')\right\}, \tag{3.5}$$
$$g_\lambda(\mathbf{k},\nu) = \beta\Phi_\lambda(\mathbf{k})\left[1-\beta\Phi_\lambda(\mathbf{k})\mathfrak{M}_{\lambda\lambda}(\mathbf{k},\nu)\right]^{-1}.$$

With accuracy up to quartic basic measure density

$$Z_1 = \sqrt{2}^{N_1-1} Q^{N_1} \int (d\rho_k)^{N_1} \exp\left\{-\frac{1}{2}\sum_{\mathbf{k}\leq B} d_2^{(1)}(\mathbf{k})\rho_{\mathbf{k}}\rho_{-\mathbf{k}} -\right.$$
$$\left. -\frac{1}{4!N}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4\leq B_1} a_4^{(1)}\rho_{\mathbf{k}_1}\rho_{\mathbf{k}_2}\rho_{\mathbf{k}_3}\rho_{\mathbf{k}_4}\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4)\right\}; \tag{3.6}$$

$$d_2^{(1)}(\mathbf{k}) = a_2^{(1)} - \beta\Phi_1(\mathbf{k}), \qquad Q = \int_{-\infty}^{\infty} f(\omega)d\omega,$$
$$a_2^{(1)} = (2\pi)^2 Q^{-1}\int_{-\infty}^{\infty}\omega^2 f(\omega)d\omega,$$
$$a_4^{(1)} = -(2\pi)^4 Q^{-1}\int_{-\infty}^{\infty}\omega^4 f(\omega)d\omega + 3a_2^{(1)},$$
$$f(\omega) = \exp\left\{-\frac{(2\pi)^2}{2}b_2\omega^2 - \frac{(2\pi)^4}{4!}b_4\omega^4\right\},$$
$$\rho_k \equiv \rho_1(\mathbf{k},0). \tag{3.7}$$

b_2, b_4 are renormalized after integration over CV with Gaussian measure density cumulants $\mathfrak{M}_{11}$ and $\mathfrak{M}_{1111}$.

$$b_2(\mathbf{k}_1,\mathbf{k}_2) = \mathfrak{M}_{11}(\mathbf{k}_1,0\mathbf{k}_2,0) - \frac{1}{2}\sum_{\mathbf{k}',\nu'}\mathfrak{M}_{1111}(\mathbf{k}',\nu',-\mathbf{k}',-\nu',\mathbf{k}_1,0,\mathbf{k}_2,0)\times$$
$$g_1(\mathbf{k}',\nu')\delta(\mathbf{k}_1+\mathbf{k}_2),$$

$$b_4(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4,) = \mathfrak{M}_{1111}(\mathbf{k}_1,0,\mathbf{k}_2,0,\mathbf{k}_3,0,\mathbf{k}_4,0,) -$$

$$-\frac{3}{2}\sum_{\substack{\mathbf{k}',\nu'\\ \mathbf{k}'',\nu''}} \mathfrak{M}_{1111}(\mathbf{k}',\nu',\mathbf{k}'',\nu'',\mathbf{k}_1,0,\mathbf{k}_2,0)\times$$
$$\mathfrak{M}_{1111}(-\mathbf{k}',-\nu',-\mathbf{k}'',-\nu'',\mathbf{k}_3,0,\mathbf{k}_4,0)\times$$
$$g_1(\mathbf{k}',\nu')g_1(\mathbf{k}'',\nu'')\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4). \tag{3.8}$$

The critical behaviour of ferroelectric cluster system is described by functional (3.6). (3.6) is completely similar to three-dimentional Ising model partition function functional in form [14]. The specific features of investigated system contains in values $d_2^{(1)}(\mathbf{k})$, $a_4^{(1)}$, Q (3.7).

4. Recursion relations. Fixed point

The only condition imposed by the CV method is the existence of the Fourier transform of interparticle potential [23]. The complete intercluster potential of cluster ferroelectrics, as it was mentional in chapter 2, consists of short-range spherically symmetric potential and long-range dipole-dipole part. The Fourier transform of such potential was obtained in [15]. To integrate (3.6) in the neighbourhood of a ferroelectric phase transition point information about the behaviour of the intercluster potential inside the Brillouin zone, that is at $\mathbf{k}\to 0$, is necessary. In the rotational ellipsoid coordinate system:

$$k_x=\frac{|\mathbf{k}|\cos\phi}{\sqrt{\alpha^2+\cot^2\vartheta}},\ k_y=\frac{|\mathbf{k}|\sin\phi}{\sqrt{\alpha^2+\cot^2\vartheta}},\ k_z=\frac{|\mathbf{k}|}{\sqrt{1+\alpha^2\tan^2\vartheta}},\ \alpha^2=\frac{a}{c}. \tag{4.1}$$

We have at small $\mathbf{k}$

$$\Phi_1(\mathbf{k})=\phi_0-\lambda x^2+AK^2. \tag{4.2}$$

Here $x=\cos\vartheta$, ϕ and ϑ are azimuth and polar angles, respectively, ϕ_0, λ, A are constants, a, c, are lattice parameters.

The main idea of integration of (3.6) is based on the fact that there exist a certain region in the Brillouin zone B_1 where $d_2^{(1)}(\mathbf{k})\geq 0$, therefore, in this region (B_1^G) one is able to use the Gaussian measure density for CV. All obtained expressions remain finite under this integration in whole temperature region, including Tc. In other part of the Brillouin zone B_1^q we shall use non-Gaussian quartic measure density and perform integration only in thin layer of CV-replacing $d_2^{(1)}(\mathbf{k})$ by it's mean velue $\langle d_2^{(1)}(\mathbf{k})\rangle_{B_1^q}$. After such two-stage procedure of integration we obtain an expression for Z_1 which is similar to (3.6), but defined in the already reduced Brillouine zone B_2. Than we can find new region of zone B_2, where $d_2^{(2)}(\mathbf{k})\geq 0$, and repeat the same procedure of two-stage integration.

The sequence of subzones B_n, B_n^G, B_n^q (see Fig. 1) is defined by formulae

$$B_n:\left[0<|\mathbf{k}\leq\frac{B_1}{S^{n-1}},\quad \vartheta_n<\vartheta\leq\pi-\vartheta_n,\quad 0<\phi\leq 2\pi\right];$$
$$B_n^G:\left[0<|\mathbf{k}\leq\frac{B_1}{S^{n-1}},\quad \vartheta_{n-1}<\vartheta\leq\vartheta_n,\quad \begin{matrix}\pi-\vartheta_n<\vartheta\leq\pi-\vartheta_{n-1},\\ 0<\phi\leq 2\pi\end{matrix}\right];$$
$$B_n^q:\left[0<|\mathbf{k}\leq\frac{B_1}{S^{n-1}},\quad \vartheta_n<\vartheta\leq\pi-\vartheta_n;\quad 0<\phi\leq 2\pi\right],$$

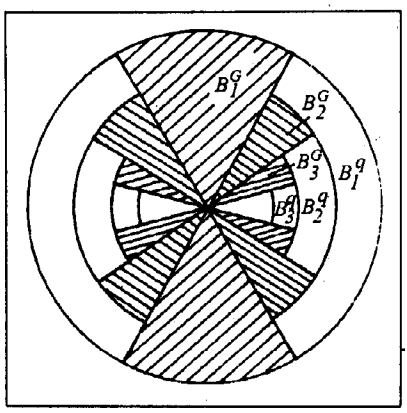


Figure 1. The sequence of subzones B_n, B_n^G, B_n^q.

$$B_n = B_n^G + B_n^q. \tag{4.3}$$

$$\vartheta_n = \arctan\left\{\frac{1}{\alpha}\sqrt{\beta\lambda(\beta\phi_0 - a_2^{(n)})^{-1} - 1}\right\}. \tag{4.4}$$

S is a division parameter of subzones B_n into layers. Corresponding number of sites in these subzones is:

$$N_n = \frac{N_1}{S^{3(n-1)}}\sqrt{\frac{1}{\beta\lambda}\left(\beta\phi_0 - a_2^{(n-1)}\right)},$$

$$N_n^q = \frac{N_1(1-S^{-3})}{S^{3(n-1)}}\sqrt{\frac{1}{\beta\lambda}\left(\beta\phi_0 - a_2^{(n)}\right)},$$

$$N_n^G = \frac{N_1}{S^{3(n-1)}}\left\{\sqrt{\frac{1}{\beta\lambda}\left(\beta\phi_0 - a_2^{(n-1)}\right)} - \sqrt{\frac{1}{\beta\lambda}\left(\beta\phi_0 - a_2^{(n)}\right)}\right\}. \tag{4.5}$$

Performing completely two-stage integration over CV in (3.6) we obtain the final expression for Z_1 in the form of a product of partial partition functions referring to separate layers,

$$Z_1 = \sqrt{2}^{N_1-1} Q^{N_1} Q_1 Q_2 ... Q_n ..., \tag{4.6}$$

where

$$Q_n = \sqrt{2}^{N_n^q} D_n \left[\sqrt[4]{\frac{12Z_n}{a_4^{(n)}}} e^{Z_n} K_{1/4}(Z_n)\right]^{N_n - N_n^G} \times$$

$$\left[\frac{1}{\pi}\sqrt[4]{\frac{Q_4^{(n)}\zeta_n^2}{12K^2(Z_n)}}\sqrt{\zeta_n} e^{\zeta_n} K_{1/4}(\zeta_n)\right]^{N_{n+1}} \tag{4.7}$$

is the partial partition function of n-th layer,

$$D_n = \prod_{\mathbf{k}\in B_n^G} \left\{ \frac{\pi}{d_2^{(n)}(\mathbf{k})} \right\},$$

$$K(Z_n) = \sqrt{Z_n} \left(\frac{K_{3/4}(Z_n)}{K_{1/4}(Z_n)} - 1 \right),$$

$$L(Z_n) = 6K^2(Z_n) + 4\sqrt{Z_n}K(Z_n) - 1,$$

$$Z_n = \frac{3\left(d_2^{(n)}(\frac{B_n}{S}, B_n)\right)^2}{4a_4^{(n)}}, \quad \zeta_n = \frac{3}{2}S^3 \frac{K^2(Z_n)}{L(Z_n)},$$

$$d_2^{(n)}\left(\frac{B_n}{S}, B_n\right) \equiv \langle d_2^{(n)}(\mathbf{k})\rangle_{\frac{B_n}{S}, B_n} = \frac{2}{3}\left(a_2^{(n)} - \beta\phi_0\right) + \frac{q}{S^{2(n-1)}},$$

$$q = \frac{3}{5}\frac{1 - S^{-5}}{1 - S^3}\beta A B_1^2. \tag{4.8}$$

K_ν are modified Bessel functions [15,20].

The coefficients $d_2^{(n)}(\frac{B_n}{S}, B_n)$,$a_4^{(n)}$ corresponding to n-th layer of integration satisfy certain recursion relations, which characterize the behaviour of an investigated system in a critical point.

Using a standard substitution for the terms $d_2^{(n)}(\frac{B_n}{S}, B_n)$ and $a_4^{(n)}$ at $T = T_c$

$$d_2^{(n)}\left(\frac{B_n}{S}, B_n\right) = \frac{r_n + q}{S^{2n}}, \quad a_4^{(n)} = \frac{U_n}{S^{4n}}, \tag{4.9}$$

we have

$$r_{n+1} = S^2(r_n + q)\left\{ \bar{N}^{(n)} + \frac{3}{4Z_n}\left(\bar{N}^{(n)} - \frac{1}{3}\right)\left(1 - S^{-n}\sqrt{\frac{3}{2\beta\lambda}(-r_n)}\right)\right\} -$$

$$-S^2 q, \qquad U_{n+1} = \sqrt{\frac{r_n}{r_{n-1}}}\mathcal{E}^{(n)}U_n. \tag{4.10}$$

Here

$$\bar{N}^{(n)} = \frac{2\sqrt{\zeta_n}K(\zeta_n)}{3\sqrt{Z_n}K(Z_n)} + \frac{1}{3}, \quad \mathcal{E}^{(n)} = S^6\frac{L(\zeta_n}{L(Z_n)}. \tag{4.11}$$

The particular solution of (4.10) is

$$z^{(n)} = z^* = \infty, \quad r_n = r^* = 0, \quad U_n = U^* = 0, \tag{4.12}$$

hence, the cluster ferroelectric system is of Gaussian type.

In order to obtain a general solution of (4.10) we use the fixed point method [14, 15, 24]. Linearizing (4.10) in the neighbourhood of the fixed point (4.12), we obtain

$$r_{n+1} - r^* = R_{11}(r_n - r^*) + R_{12}(U_n - U^*),$$
$$U_{n+1} - U^* = R_{21}(r_n - r^*) + R_{22}(U_n - U^*). \tag{4.13}$$

Here

$$R_{11} = \left(\frac{\partial r_{n+1}}{\partial r_n}\right)^* = S^2\left[\bar{N}(z^*) + \sqrt{z^*}\frac{\partial \bar{N}(z^*)}{\partial\sqrt{z^*}}\right], \tag{4.14}$$

$$R_{12} = \left(\frac{\partial r_{n+1}}{\partial U_n}\right)^* = \mp S^2\frac{z^*}{\sqrt{3U^*}}\frac{\partial \bar{N}(z^*)}{\partial\sqrt{z^*}},$$

$$R_{21} = \left(\frac{\partial U_{n+1}}{\partial r_n}\right)^* = \pm\frac{\sqrt{3U^*}}{2}\frac{\partial \mathcal{E}(z^*)}{\partial\sqrt{z^*}} + \frac{U^*\mathcal{E}(r^*)}{2r^*}\left[1 - \left(\frac{\partial r_{n-1}}{\partial r_n}\right)^*\right],$$

$$R_{22} = \left(\frac{\partial U_{n+1}}{\partial U_n}\right)^* = \mathcal{E}(z^*) - \frac{\sqrt{z^*}}{2}\frac{\partial \mathcal{E}(z^*)}{\partial\sqrt{z^*}} - \frac{U^*\mathcal{E}(r^*)}{2r^*}\left(\frac{\partial r_{n-1}}{\partial U_n}\right)^*.$$

General solution of (4.13),(4.14) was obtained in [25]. They reads

$$d_2^{(n)}\left(\frac{B_n}{S}, B_n\right) = \frac{c_1E_1^{n-1} - c_2RE_2^{n-1} + q}{S^{2(n-1)}},$$

$$a_4^{(n)} = \frac{c_1R^1E_1^{n-1} + c_2RE_2^{n-1}}{S^{4(n-1)}}, \tag{4.15}$$

where

$$c_1 = \left[\frac{2}{3}(a_2^{(1)} - \beta\phi_0) + a_4^{(1)}R\right]w^{-1},$$

$$c_2 = \left[-\frac{2}{3}(a_2^{(1)} - \beta\phi_0)R^1 + a_4^{(1)}\right]w^{-1};$$

$$R = \frac{R_{12}}{R_{11} - E_2}, \quad R^1 = \frac{E_1 - R_{11}}{R_{12}}, \quad w = \frac{E_1 - E_2}{R_{11} - E_2};$$

$$E_1 = \frac{1}{2}\left[S^2 + \sqrt{\frac{3S^4 - 2S^2 - S + 2 + 2S^{-1} - 2S^{-3}}{3 - S^{-3}}}\right],$$

$$E_2 = 1. \tag{4.16}$$

The expressions (4.15), (4.16) will be used for direct calculation of the cluster ferroelectrics free energy.

5. Free enegry. Heat capacity

One of the most important advantagies of the CV method in comparison with the other functional methods, is the possibility to use it for direct calculation of free energy of the investigeted system [14, 23]. According to general rules of statistical physics [13] from (2.3) we obtain a complete value for cluster ferroelectrics free energy as a sum of several terms:

$$-\beta F = \ln z_0 + \sum_{\lambda\neq 1}\ln z_1^G + \ln z_1^G + \ln z_1. \tag{5.1}$$

First three terms in (5.1) describe a regular part of total free energy due to analytic behaviour of (2.10) and (3.4) in the vicinity of a phase transition point. Now we pay attention to calculation the last term in (5.1)

$$F_1 = -\beta^{-1}\ln z_1. \tag{5.2}$$

Substituting (4.6), (4.7) into (5.2) we obtain the expression for free energy in the form of a sum of partial free energies referring to particular layers.

$$F = F^{(1)} + \sum_{n=1}^{m_\tau+1} F_n^G + \sum_{n=1}^{m_\tau} F_n^q. \tag{5.3}$$

Here $F^{(1)} = -\beta^{-1} \ln \frac{(\sqrt{2}Q)^{N_1}}{\sqrt{2}}$ being constant, F_n^G and F_n^q are partial free energies connected with Gaussian and non-Gaussian fluctuations of CV near phase transition point, respectively; m_τ is a number, which fixes the end of coexistence of Gaussian B_n^G and non-Gaussian B_n^q regions in the Brillouin zone.

$$m_\tau = 1 - \frac{\ln c_1 - \ln(c_2 R)}{2 \ln S}. \tag{5.4}$$

$$F_n^G = -\beta^{-1} \ln \left(\sqrt{2}^{N_n^q} D_n \right), \tag{5.5}$$

$$F_n^q = -\beta^{-1} \left\{ (N_n - N_n^G) \ln \left[\sqrt[4]{\frac{12 z_n}{a_4^{(n)}}} e^{z_n} K_{1/4}(z_n) \right] + \right.$$

$$\left. N_{n+1} \ln \left[\frac{1}{\pi} \sqrt[4]{\frac{a_4^{(n)} \zeta_n^2}{12 K^2(z_n)}} \sqrt{\zeta_n} e^{\zeta_n} K_{1/4}(\zeta_n) \right] \right\}. \tag{5.6}$$

Substituting (4.15) into (5.5), (5.6) and performing summation over n accordingly to (5.3), we obtain complete expression for the critical part of free energy

$$F - F^{(1)} = -\beta^{-1} N_1 \{ -A + B \ln \tau \}. \tag{5.7}$$

Coefficients A and B (in the case $S \to 1$) are the following

$$A = \frac{c_1^2}{2\sqrt{\beta\lambda(c_2 R)^3}} \left\{ \left[1 + \frac{3}{4} \frac{c_2 R}{q - c_2 R} - \frac{3}{4} \left(\frac{c_2 R}{q - c_2 R} \right)^2 + \right. \right.$$

$$\left. \left. + \frac{1}{32} \ln \frac{(\beta A)^{18} (q - c_2 R)^{30}}{2^{15} \pi^6} \right] \ln \frac{c_2 R \tau}{c_1} - \frac{11}{8} \ln \beta A \pi + \frac{11}{12} \right\}, \tag{5.8}$$

$$B = \frac{c_1^2}{2\sqrt{\beta\lambda(c_2 R)^3}} \left\{ 1 + \frac{3}{4} \frac{c_2 R}{q - c_2 R} - \frac{3}{4} \left(\frac{c_2 R}{q - c_2 R} \right)^2 + \right.$$

$$\left. + \frac{1}{32} \ln \frac{(\beta A)^{18} (q - c_2 R)^{30}}{2^{15} \pi^6} \right\}.$$

Therefore, we are able to calculate other thermodynamic functions as the derivatives of free energy (5.7). They depend on $\tau = \frac{T - T_c}{T_c}$ through the terms $\ln \tau$ and c_1.

In order to calculate the coefficient c_1 we must obtain a renormalized value of $d_2^{(n)}(k)$ after integration of partition function functional in subzone B_n^G.

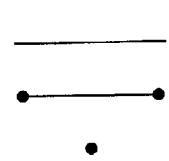
Let us introduce notation: $\mu_n = \frac{1}{\beta}\left(a_2^{(n)} - \beta\varphi_0\right)$, m_n is a complete renormalized value of μ_n ($m_n = 0$ at $T = T_c$). From the Word identity [10]

$$\frac{\partial G_n^{-1}(0)}{\partial m_n} = \mathcal{T}_n(0,0,0), \tag{5.9}$$

where $G_n(k) = \frac{1}{d_2^{(n)}(k)}$ is a Green function and $\mathcal{T}(k_1,k_2,k_3)$ is a vertex part, m_n is easily obtained.

The vertex part $\mathcal{T}(k_1,k_2,k_3)$ is determined by the "scattering amplitude" $\Gamma(k_1,k_2,k_3,k_4) = \langle \rho_{k_1}\rho_{k_2}\rho_{k_3}\rho_{k_4}\rangle$.

Let us introduce the notation



ρ_k is an "external line",

$\rho_k\rho_{-k}$ is a pair correlation function,

$\sum_{k_1,k_2,k_3,k_4}\delta(k_1+k_2+k_3+k_4)$.

With the accuracy up to fourth order in a_4 we have the following diagrams (see Fig.2). Taking into account only diagrams of b, c and d types, for the case when all moments are of the same order in k we obtain a following equation for $\Gamma_n(k)$

$$\Gamma_n(k) = \gamma_n - 3R \int\limits_{\sqrt{\frac{Ak^2+m_n}{A}}}^{\frac{\pi}{S^{n-1}}} p^2dp \int\limits_{\cos\vartheta_n}^{\cos\vartheta_{n-1}} dx \int\limits_0^{2\pi} d\varphi \frac{\Gamma_n^2(p)}{(\beta\lambda x^2 + \beta A p^2)^2}, \tag{5.10}$$

Here

$$\gamma_n = \frac{a_4^{(n)}(1-s^{-1})}{32\pi^2\beta^2\sqrt{\lambda A^3}}\left\{\arctan\frac{\pi(s-1)\sqrt{\frac{3c_2RA}{2\beta}}}{\frac{3c_2Rs}{2\beta} + A\pi^2} - \pi\sqrt{\frac{2\beta A\left(1-s^{-1}\right)^2}{3c_2R}}\right\} \tag{5.11}$$

is so called the constant of anharmonicity.

$$R = \left\{\frac{\pi}{2\beta^2\sqrt{\lambda A^3}}\arctan\frac{\pi(s-1)\sqrt{\frac{3c_2RA}{2\beta}}}{\frac{3c_2Rs}{2\beta} + A\pi^2} + \right.$$

$$\left. + \frac{(S-1)\pi^4}{2\beta^2}\frac{\sqrt{\frac{3c_2R}{2\beta\lambda}}}{\left(\frac{3c_2R}{2\beta} + A\pi^2\right)\left(\frac{3c_2Rs}{2\beta} + A\pi^2\right)}\right\}. \tag{5.12}$$

Introducing logarithmic variables

$$y = \ln\frac{Ak^2 + m_n}{m_n}, \quad L_n = \ln\frac{A\pi^2}{m_n s^{2(n-1)}}$$

and differentiating (5.10) with respect to y we obtain

$$\frac{\partial\Gamma_n(y)}{\partial y} = 3\Gamma_n^2(y). \tag{5.13}$$

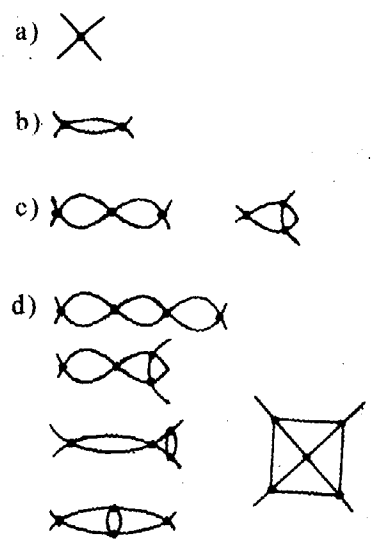


Figure 2. The Gaussian diagrams for "scattering amplitude" $\Gamma(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4,)$.

Performing the integration (5.13) with boundary condition $\Gamma_n(L_n) = \gamma_n$, we obtain

$$\Gamma_n(k) = \frac{\gamma_n}{1 + 3\gamma_n(L_n - y)} = \frac{\gamma_n}{1 + 3\gamma_n \ln \frac{A\pi^2}{(Ak^2+m_n)S^{2(n-1)}}}. \tag{5.14}$$

For the vertex part $\mathcal{T}_n(k)$ the equation similar to (5.14) may be obtained

$$\mathcal{T}_n(k) = 1 - R \int\limits_{\sqrt{\frac{Ak^2+m_n}{A}}}^{\frac{\pi}{S^{n-1}}} p^2 dp \int\limits_{\cos\vartheta_n}^{\cos\vartheta_{n-1}} dx \int\limits_0^{2\pi} d\varphi \frac{\mathcal{T}_n(\rho)\Gamma_n(\rho)}{(\beta\lambda x^2 + \beta A k^2)^2}. \tag{5.15}$$

In a logarithmic variables y and L_n, after differentiation with respect to y we have

$$\frac{\partial \mathcal{T}_n(y)}{\partial y} = \mathcal{T}_n(y)\Gamma_n(y). \tag{5.16}$$

Subsituting (5.14) into (5.16) and integrating (5.16) with boundary condition $\mathcal{T}_n(L_n) = 1$, we obtain

$$\mathcal{T}_n(y) = [1 + 3\gamma_n(L_n - y)]^{-1/3}. \tag{5.17}$$

Therefore, taking into account the identity (5.9) expressions $d_2^{(n)} = m_n + \beta\lambda x^2 + \beta A k^2$ and (5.17), we obtain the equation for m_n

$$\frac{\partial m_n}{\partial \mu_n} = \left[1 + 3\gamma_n \ln \frac{A\pi^2}{m_n s^{2(n-1)}}\right]^{-1/3}. \tag{5.18}$$

We shall obtain the solution of (5.18) correct to the logarithmic divergency, substituting $m_n = \mu_n - \mu_n^c = \frac{3}{2}\frac{c_1 E_1^{n-1} - c_2 R E_2^{n-1}}{s^{2(n-1)}} + \frac{3}{2}\frac{c_2 R E_2^{n-1}}{s^{2(n-1)}}$ accordinly to (4.15). So, at small τ

$$3\gamma_n \ln \frac{A\pi^2}{m_n s^{2(n-1)}} \approx -3\gamma_n \ln \tau. \tag{5.19}$$

Integrating (5.18), (5.19) with boundary condition $m_n = 0$ at $\mu_n = \mu_n^c$, we obtain

$$m_n = [1 - 3\gamma_n \ln \tau]^{-1/3} (\mu_n - \mu_n^c). \tag{5.20}$$

For $d_2^{(n)}(k)$ we have now an expression

$$d_2^{(n)}(k) = \beta\varphi_0 [1 - 3\gamma_n \ln \tau]^{-1/3} \tau + \beta\lambda x^2 + \beta A k^2. \tag{5.21}$$

Substituting (5.21) into (4.16) we have

$$c_1^{(n)} = \frac{2}{3}\beta\varphi_0 [1 - 3\gamma_n \ln \tau]^{-1/3} \tau. \tag{5.22}$$

Hence, $c_1^{(n)}$ at small τ is proportional to $\tau \ln^{-1/3} \tau$. This peculiarity, as compared with behaviour of similar coefficient for isotropic Ising model ($c_1 \sim \tau$) [14], leads to the different character of behaviour of thermodynamic functions near phase transition point.

The critical part of free energy (5.7) together with (5.8) and (5.22), has the following final form

$$F - F^{(1)} = -\beta^{-1} N_1 f_1 \tau^2 (\ln \tau)^{1/3}, \tag{5.23}$$

Here

$$f_1 = \frac{2\left(3^{-4/3}\beta\phi_0\gamma_1^{-1/3}\right)^2}{(\beta\lambda(c_2R)^3)^{1/2}} \left[1 + \frac{3}{4}\frac{c_2R}{q - c_2R} - \frac{3}{4}\left(\frac{c_2R}{q - c_2R}\right)^2 + \frac{1}{32}\ln\frac{(BA)^{18}(q - c_2R)^{30}}{2^{15}\pi^6}\right]. \tag{5.24}$$

It must be noted that free energy (5.23) is obtained in such a way that two everylayer's terms F_n^G and F_n^q are calculated in the same approximation. For calculation F_n^G we had summize (equations (5.10), (5.15)) in infinite series of Gaussian diagrams which arrised from the perturbation theory with respect to $a_4^{(n)}$. This is equivalent to using non-Gaussian measure density for calculation F_n^q.

Using (5.4) it may be shown (see [15]) that for correlation length critical exponent one has

$$\nu = \frac{4}{3}\frac{\ln(SE_2)^{-\frac{1}{8}}}{\ln E - \ln E_2}. \tag{5.25}$$

Substituting here (4.16) we obtain $\nu = \frac{2}{3}$. Accordinghly to a well- known relation [24]

$$\alpha = 2 - d\nu \to 2 - 2. \tag{5.26}$$

so, there are no exponential divergency of heat capacity at $T = Tc$.
For obtaining Cv in explicit form we use an expression

$$Cv = \frac{1}{T}\frac{\partial U}{\partial \tau}, \tag{5.27}$$

where an internal energy U may be obtained from Gibbs-Helmholtz equation

$$U = F - T\frac{\partial F}{\partial T}. \tag{5.28}$$

Using (5.23), (5.24) and (5.27), (5.28) we obtain

$$Cv = -kN_1 f_1 \left\{ 2\left(\tau\frac{T}{Tc} + \frac{T^2}{Tc}\right)\ln^{1/3}\tau + \right.$$
$$\left. \frac{1}{3}\left(\tau\frac{T}{Tc} + 3\frac{T^2}{T_c^2}\right)\ln^{-2/3}\tau + \frac{2}{9}\frac{T^2}{T_c^2}\ln^{-5/3}\tau \right\}. \tag{5.29}$$

At $T - T_c(\tau \to 0)$ the asymptotic behaviour of Cv is determined by the term

$$Cv = -2kN_1 f_1 \frac{T^2}{T^2 c}\ln^{1/3}\tau, \tag{5.30}$$

which posesses a weaker temperature dependence at $\tau \to 0$ as compared with $\ln\tau$ (simpe Gaussian result).

References

[1] Domb C., D. L. Hunter D. L. On the critical behaviour of ferromagnets. // Progr. Phys. Soc., 1965, vol. 86, p. 1147-1151.

[2] Wegner F. Spin-ordering in a planar classical Heisenberg model. // Phys., 1968, vol. 216, p. 433.

[3] Dohm V. Dynamical spin-spin correlation function of an isotropic ferromagnet at T_c in 6-ε dimensions. // Solid. State. Comm., 1976, vol 20, p. 657-660.

[4] Bhattacharjee J.K., Ferrell R. A. Dynamic scaling for the isotropic ferromagnet: ε-expansion to two-loop order. // Phys. Rev. B., 1981, vol. 24, p. 6480-6485.

[5] Folk R., Iro H. Paramagnetic neutron scattering and renormalization-group theory for isotropic ferromagnets at T_c. // Phys. Rev. B., 1985, vol. 32, p. 1880-1882.

[6] Folk R., Iro H. Temperature dependence of paramagnetic neutron scattering from Heisenberg ferromagnets above T_c. // Phys. Rev. B., 1986, vol. 34, p. 6571-6574.

[7] Frey E., Schwabl F., Thoma S. Shape functions of dipolar ferromagnets of the Curie point. // Phys. Lett. A., 1988, vol. 129, p. 343-349.

[8] Schwabl F. Critical dynamics of dipolar ferromagnets (invited). // J. Appl. Phys., 1988, vol. 64 , No 10, p. 5867-5872.

[9] Vaks V. G., Larkin A. I. On the second order phase transitions. // JETP, 1965, vol. 49, p. 975-989 (in Russian).

[10] Larkin A. I., Khmelnitsky D.,E. The phase transition in uniaxial ferroelectrics. // JETP, 1969, vol 56, p. 2087-2098 (in Russian).

[11] Sokolov A. I. Renormalization group equations and thermodynamical peculiarities near three-critical point. // JETP, 1979, vol. 77, p. 1598-1614 (in Russian).

[12] Vysochansky Yu. M., Slivka B. Yu. Lifshits point on the state diagrams of ferroelectrics. // Usp. phys. nauk, 1992, vol. 162, p. 163-184 (in Russian).

[13] Leontovich M. A. Introduction into thermodynamics. Statistical physics. Moskva, Nauka, 1983, p. 416 (in Russian).

[14] Yukhnovskii I. R. Phase transition of the second order. The collective variables method. Singapore, World Scientific, 1987, p. 400.

[15] Yukhnovskii I. R., Korynevskii N. A. The investigation of the ferroelectric phase transition in cluster systems of order-disorder. I. Partition function functional. // Phys. Stat. Sol. B., 1989, vol. 153, p. 583-593;
II. Two particle cluster system. // Phys. Stat. Sol., 1989, vol. 154, p. 519-534;
III Free energy. // Phys. Stat. Sol., B., 1991, vol. 163, p. 355-367.

[16] Korynevskii N. A. On calculation of free energy of two-particle cluster system. // TMP, 1983, vol. 55, p. 291-304 (in Russian).

[17] Stasyuk I. V., Glauberman A. E. Method of Knot elementary exitation in the semiconductors theory. // Ukr. Phys. J., 1964, vol. 9, p. 3-13 (in Ukrainian).

[18] Hubbard J. Electron correlations in narrow energy bands. IV. The atomic representation. // Proc. Roy. Soc., 1965, vol. A. 285, p. 542-560.

[19] Stanley E. Phase transitions and critical phenomena. Moskva, Mir, 1968, p. 420, (in Russian).

[20] Gradshtein I. S., Ryzhyk, Tables of integrals, sum, series and products. Moskva, Nauka, 1971, 1108 p. (in Russian).

[21] Vaks V. G. Introduction to microscopic theory of ferroelectrics. Moskva, Nauka, 1973, 327 p. (in Russian).

[22] Levitskii R. R., Korynevskii N. A., Stasjuk I. V. Distribution functions and thermodynamical properties of KH_2PO_4 and $ND_4D_2PO_4$ type crystals. // Phys. Stat. Sol. B., 1978, vol. 88, p. 51-63.

[23] Yukhnovskii I. R., Holovko M. P. Statistical theory of classic equilibrium systems., Kiev, Naukova dumka, 1980, 372 p. (in Russian).

[24] Wilson K., Kogut J. Renormalization Group and ε-expantion. 1975, 256 p. (in Russian).

[25] Korynevskii N. A. Solution of linearized recursion equations for uniaxial cluster ferroelectrics., Lviv, 1993, 13 p. (Preprint/ Nat. Acad. Scien. Ukr., ICMP; ICMP-93-13U) (in Ukrainian).

ГАУСОВІ ТА НЕГАУСОВІ ГУСТИНИ МІРИ В ТЕОРІЇ КЛАСТЕРНИХ СЕГНЕТОЕЛЕКТРИКІВ

М.А. Кориневський

Досліджено проблему застосування гаусових і негаусових густин мір колективних змінних за інтегруванням функціонала статистичної суми кластерного сегнетоелектрика. Виходячи з умови збіжності функціональних інтегралів в околі точки фазового перетворення запропоновано спосіб поділу першої зони Брілюена на шари. Кожен шар складається з двох частин. В першій частині достатньою є гаусова густина міри, в той час як в другій необхідно застосовувати негаусову. Отримана як результат пошарового інтегрування статистична сума є скінченною в температурному інтервалі, що включає окіл точки фазового перетворення. Вивчена критична поведінка термодинамічних функцій.