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LOCAL STATE REPRESENTATION IN STATISTICAL MECHANICS OF CLASSICAL SYSTEMS. 2. PHASE TRANSITIONS IN $O(2)$–SYSTEMS

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НОВОСИБИРСК

Local State Representation in Statistical Mechanics of Classical Systems. 2. Phase Transitions in $O(2)$-Systems

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ABSTRACT

The phase transition in $3D$ systems having $O(2)$ symmetry is studied as a function of the form of interaction. Conditions of a first order phase transitions are found. Probabilities of occupation at a point and their correlations are calculated in a mean-probability approximation.

1 Introduction

The order in systems with a continuous symmetry group has been intensively studied. The simplest case is the $O(2)$ symmetry, realized in superfluid He^4 [1, 2], superconductors [3], magnets with an easy plane and other systems [6]. In all mentioned systems, a coarse graining from the initial atomic scale a to some intermediate scale $R_0 \gg a$ allows to describe the order in the system in terms of a two-component order parameter which can be chosen in the form of a complex scalar field $\psi(r)$. The quantity $\psi(r)$ in a given point r describes the local order in a cluster of the size R_0 with the center in r, the absolute value $\mid \psi \mid$ and the phase (orientation) $\phi(r)$:

$$\psi(r) = \mid \psi \mid \exp(i\phi). \tag{1}$$

At the scale R_0, fluctuations of $\mid \psi \mid$are supposed to be small,

$$\mid \psi \mid = \psi_0 + \delta, \mid \delta \mid \ll \psi_0, \tag{2}$$

hence $\phi(r)$ is a well defined quantity. The orientation order in a cluster of the size R is represented by the orientation order parameter

$$\tilde{\psi}(r) = \exp(i\phi(r)), \tag{3}$$

r is the center of the cluster. The some orientation may be described by the phase $\phi, \phi+2\pi, \phi+4\pi, ...$ In the ordered phase, at temperatures $T < T_c$, $\phi(\mathbf{r})$ fluctuates around some value ϕ_0 ("the phase of the condensate"). In the

disordered phase ($T > T_c$) the long range orientation order is lost. The latter features are the common ones for continious models in $3D$ [4, 5].

The probability distribution of a configuration of orientations $\phi(\mathbf{r})$ may be written as

$$Dw(\mathbf{r}) = exp(-\frac{H\{\phi\}}{T})D\phi(\mathbf{r}), \tag{4}$$

$H\{\phi\}$ is the Hamiltonian of the orientation order, $D\phi$ is an element of the configuration space

$$D\phi(\mathbf{r}) = \prod_{\mathbf{r}_i} d\phi_i, \tag{5}$$

for a lattice system with lattice sites $\mathbf{r}_i$. For configurations having $\mid \nabla\tilde{\psi} \mid \ll 1$ in all space the Hamiltonian has the universal form

$$H = \int \{\frac{c}{2} \mid \nabla\tilde{\psi} \mid^2 - h\cos(\phi - \phi_0)\}dV. \tag{6}$$

h plays the role of the external field conjugated to $\tilde{\psi}$. For larger $\mid \nabla\tilde{\psi} \mid$, the Hamiltonian is not universal. The form (6) appears in Landau theory of second order phase transitions [7, 6].

The concept of the order parameter is more general than in Landau theory, it assumes only the existence of the intermediate scale R_0 mentioned above. The nature of the phase transition depends upon the form of the Hamiltonian at this intermediate scale. For systems considered below some general features are supposed. The general form of the Hamiltonian is

$$H = H_0\{\phi(r)\} - \int h(r,\phi)dV. \tag{7}$$

The $O(2)$ symmetry means that

$$H_0\{\phi + \phi_0\} = H_0\{\phi\} = H_0\{-\phi\}. \tag{8}$$

The exact form of H is expected to make statistically insignificant configurations with the most part of the volume occupied by large values of $\mid \nabla\tilde{\psi} \mid$. Let us consider a configuration with $\mid \nabla\tilde{\psi} \mid \ll 1$ in the most part of the volume. This part of the volume (good material) is supposed to be an infinite multiconnected cluster. The rest of the volume (bad material) occupies a small fraction of the total volume. The absolute minimum of $H\{\phi\}$ is the $T = 0$ configuration (ground state) $\phi(r) = \phi(0)$, the low-energy excitations are those having $\mid \nabla\tilde{\psi} \mid \ll 1$ with probabilities given by (6).

We will consider a rather general form of a two point interaction

$$H\{\phi\} = \frac{1}{2}\int E(\mathbf{r} - \tilde{\mathbf{r}}; \cos(\phi(\mathbf{r}) - \phi(\tilde{\mathbf{r}})))dVd\tilde{V} - \int h(\mathbf{r}; \phi(\mathbf{r}))dV. \tag{9}$$

The interaction energy $E(\mathbf{r}; \cos\phi)$ is assumed to have a minimum at $\phi = 0$. At any $\mathbf{r}$ $E(\mathbf{r}; \cos\phi)$ increases with $\mid \cos\phi \mid$ increasing, it depends on r but not on the orientation of $\mathbf{r}$. The $r \to 0$ behavior of $E(\mathbf{r}; \cos\phi)$ determines the probabilities of states with high $\mid \nabla\tilde{\psi} \mid$. To depress probabilities of those configurations, $E(\mathbf{r}; \cos\phi)$ has to increase as $r \to 0$ except for a narrow vicinity of $\phi = 0$:

$$E(\mathbf{r}; \cos\phi) \approx \epsilon(r)\phi^2, \quad \phi \ll 1. \tag{10}$$

The Landau-kind behavior $H \sim V \mid \nabla\tilde{\psi} \mid$ means $\epsilon_k \sim k^2$, or for a $3D$ system

$$\epsilon(r) = \frac{c}{r}. \tag{11}$$

The form of $E(r; \cos\phi)$ may be described with the aid of coefficients ϵ_n:

$$E(\mathbf{r}; \cos\phi) = \sum_{n=0}^{\infty} \epsilon_n(r)\cos n\phi. \tag{12}$$

The case $\epsilon_n = 0, n \neq 1$ is the X-Y model one. The phase transition in X-Y-model is continuous (of second order).

The aim of this paper is to study the phase transition as a function of the form of $E(r; \phi)$. The potential well $E(\mathbf{r}; \phi)$ as a function of ϕ is supposed to have the minimal value at $\phi = 0$ and increase monotonous for $\mid \phi \mid < \pi$. As a function of r, $E(\mathbf{r}; \phi)$ characterized by the interaction radius R_c. Main characteristics of $E(\mathbf{r}; \phi)$ are the depth of the well and the width s. For the X-Y model $s \sim \pi$. In the opposite limit of a very narrow well $E(\mathbf{r}; \phi)$, the attraction of orientations is only for almost parallel orientations $s \ll \pi$. As an example we consider

$$E(\mathbf{r}; \cos\phi) = \epsilon(r)\exp(-\frac{\cos\phi - 1}{s^2})/A, A = \frac{1}{2}\int \exp(-\frac{\cos\phi - 1}{s^2})d\phi. \tag{13}$$

As will be shown, a finite such deformation of the X-Y model results in a change of the order of phase transition.

2 Mean Probability Approach

Let us reformulate the statistical mechanics of the system (10) in terms of local state vector representation as it was described in our paper [8]. We will

treat the continuous cyclic variable $\phi^\alpha = \frac{2\pi n}{N}, n = 0, 1, 2, ...$ We define a N-dimensional Euclidean space spanned on orthonormal vectors $e^{(\alpha)}, e^{(\alpha)}e^{(\beta)} = \delta^{\alpha\beta}$. The state vector $\sigma^\alpha(r)$ is defined to coincide with $e^{(\alpha)}$ if the state in point r is α. The idea is a straightforward generalization of the Ising variable in a two-state system. Quantities $E(\mathbf{r}_i - \mathbf{r}_j; \cos(\phi_i^\alpha - \phi_j^\beta))$ and $h\cos(\phi_i^\alpha)$ are represented by a tensor with components $E_{ij}^{\alpha\beta}$ and a vector with components h_i^α consequently in the N-dimensional state space.

Using the $\sigma(r)$ field, we may write the Hamiltonian (9) as

$$H = \frac{1}{2}\int \sigma^\alpha(\mathbf{r})E^{\alpha\gamma}(\mathbf{r}-\tilde{\mathbf{r}})\sigma^\gamma(\tilde{\mathbf{r}})dVd\tilde{V} - \int h^\alpha(\mathbf{r})\sigma^\alpha(\mathbf{r})dV. \qquad (14)$$

The sum over all states in the Gibbs ensemble (4) means now the sum over all values of $\sigma(\mathbf{r})$ in all points r of the system. An important feature of the vector σ is that its averages are probabilities. Namely, if $w(\mathbf{r};\alpha)$ is the probability to have a state α at point $\mathbf{r}$, then

$$w(\mathbf{r};\alpha) = < \sigma^\alpha(\mathbf{r}) > . \qquad (15)$$

Correlation functions of σ

$$w(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_n; \alpha_1, \alpha_2, ..., \alpha_n) = < \sigma^\alpha(\mathbf{r}_1)\sigma^\alpha(\mathbf{r}_2)...\sigma^\alpha(\mathbf{r}_n) > . \qquad (16)$$

are probabilities of simultaneous occupation of points $\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_n$ by states $\alpha_1, \alpha_2, ..., \alpha_n$ simultaneously. The bilinear form of the Hamiltonian (14) allows one to formulate a mean field approximation for σ the Mean Probability Approximation (MPA)-see [8]. The approximation is valid if the interaction radius R_{int} is large. The regular way to obtain the MPA- equations is to perform the Hubbard-Stratanovich transformation to the Gibbs ensemble with the energy (14). In MPA, the free energy is given by the formula $F = H - TS$, where H is the energy and S is the combinatorical entropy:

$$H = \int\int\int\int E(\mathbf{r}-\tilde{\mathbf{r}}; cos(\phi-\tilde{\phi}))w(\phi;r)w(\tilde{\phi};\tilde{r})d\phi d\tilde{\phi}dVd\tilde{V} - \int\int h(\phi;r)w(\phi;r)dVd\phi, \qquad (17)$$

$$S = -\int\int w\ln(w)d\phi dV. \qquad (18)$$

The equilibrium $w(\mathbf{r};\phi)$ minimize the thermodynamic potential Φ

$$\Phi = H - TS + \int \nu(\int wd\phi - 1)dV. \qquad (19)$$

ν is the Lagrange multiplier field to fulfill at each point $\mathbf{r}$ the condition

$$\int wd\phi = 1. \qquad (20)$$

In formulas (17,18,19) the limit $N \to \infty$ is performed.The MPA-equations have the form

$$w(\mathbf{r};\phi) = \frac{\exp(-\frac{E(\phi;r)}{T})}{\int \exp(-\frac{E(\phi;r)}{T})d\phi}, \qquad (21)$$

$$E(\phi;\mathbf{r}) = \int\int E(\mathbf{r}-\tilde{\mathbf{r}}; cos(\phi-\tilde{\phi}))w(\tilde{\phi};\tilde{r})d\tilde{\phi}d\tilde{V} - h(\phi;r)w(\phi;r), \qquad (22)$$

An interpretation of (21) is that $E(\mathbf{r};\phi)$ is the energy of a state ϕ in point $\mathbf{r}$ when surrounding points are occupied corresponding probabilities $w(\tilde{\mathbf{r}};\tilde{\phi})$. The generalization of (14-22) for a given group $\mathbf{G}$ instead of $O(2)$ is straightforward. One has to replace $\phi \to \mathbf{g}$, $d\phi \to d\mathbf{g}$, $\mathbf{g}$ being a point on the group manifold, and $d\mathbf{g}$ is an invariant volume element on the group $\mathbf{G}$ manifold.

3 MPA- equations

Let us transform equations (22) to a more suitable form. We will consider the homogeneous case $h = 0, w(r;\phi) = w(\phi)$. By introducing

$$y = Zw - 1, \quad t = ZT, \quad E(\phi) = \int E(\mathbf{r}; cos(\phi))dV \qquad (23)$$

one gets from (22)

$$-tln(1+y) = \int_{-\pi}^{\pi} E(\phi-\tilde{\phi})y(\tilde{\phi})d\tilde{\phi}, \qquad (24)$$

$$Z = 2\pi + \int_{-\pi}^{\pi} y(\phi)d\phi \qquad (25)$$

Here, we fixed the zero level of energy by setting

$$\int_{-\pi}^{\pi} E(\phi)d\phi = 0. \qquad (26)$$

For the homogeneous case, MPA Eqs. (22) have a trivial solution for all t

$$y = 0, \quad w_h = \frac{1}{2\pi}, \quad Z = 2\pi, \quad t = 2\pi T. \qquad (27)$$

This solution describes the symmetric high-temperature phase, it is stable (corresponds to the absolute minimum of the free energy) for $T > T_c$.

The low temperature phase is easy to study for $T \ll T_c$. For that temperatures, the solution $w(\phi)$ is localized near $\phi = \phi_0$, choose $\phi_0 = 0$. The $T = 0$ solution is $w = \delta(\phi)$. The width of the $w(\phi)$ is smaller than those of $E(\phi)$, so we write

$$E(\phi) = E(0) + \frac{\phi^2}{2s^2}, \quad s^{-2} = \frac{d^2E}{d\phi^2}(0). \tag{28}$$

For $w_L(\phi)$ one obtains at $T \ll T_c$

$$w_L = \frac{\exp(-\frac{\phi^2}{2s^2T})}{s\sqrt{2\pi T}}. \tag{29}$$

The approximation (27) is valid if

$$T \ll E(0). \tag{30}$$

For a narrow potential well $E(\phi)$ the solution (27) is valid up to the phase transition temperature T_c. The equilibrium phase transition temperature T_c is determined by the condition of equal values of thermodynamic potentials

$$F_L(w) = F_h(w). \tag{31}$$

In the limit of small s one obtains

$$T_c \approx \frac{E(0)}{2\ln(1/s)}. \tag{32}$$

For the X-Y model $s \sim \pi$, and approximation (28,30) is not applicable at temperatures $T \sim T_c$. To study the order of the phase transition, let us examine the spinodal line of the high-temperature phase, where w_H becomes unstable.

4 The spinodal of the symmetric phase

The trivial solution $w = \frac{1}{2\pi}$ becomes unstable at $T_{hs} = T_c$ for a second order phase transition but $T_{hs} < T_c$ if the phase transition is of the first order. In a mean-field type of an approximation, one expect that the spinodal temperature is the branching point where w_L branches from w_h. The solution

w_L has the maximum at $\phi = \phi_0 = 0$ as expected to be a periodic symmetric function: $w(\phi) = w(-\phi) = w(\phi \pm 2\pi)$. The branch w_L between T_{hs} and low-temperature spinodal T_{lt} does not correspond to any relatively stable spatially homogeneous state. We will study this unstable solution for $\mid w_L - w_h \mid \ll 1$.

The symmetry allows one to write all related function of the angle in Furie-series in the unit circle:

$$E(\phi) = 2\sum_{n=1}^{\infty} \epsilon_n cos(n\phi), \tag{33}$$

$$y(\phi) = y_0 + 2\sum_{n=1}^{\infty} y_n cos(n\phi). \tag{34}$$

The equations (24) in Fourier-representation have the form

$$2\pi\epsilon_n y_n = -t(y - \frac{y^2}{2} + \frac{y^3}{3} - ...)_n, \tag{35}$$

$(B)_n$ stands for corresponding Furie-amplitude

$$B(\phi) = \sum_n B_n \cos(n\phi). \tag{36}$$

At branching, all y_n go to 0. In linear approximation Eq.(35) gives

$$y_n(2\pi\epsilon_n + t) = 0. \tag{37}$$

Solutions of Eq.(37) are

$$t = -2\pi\epsilon_n. \tag{38}$$

For the interaction $E(\phi)$ considered here, $-2\pi\epsilon_1$ gives the highest $T_{hs} \equiv t_{hs}/2\pi$, other solutions are unphysical. Close to $t = -2\pi\epsilon_1 > 0$, in the second order in y_1 one obtains

$$y = 0, t < t_1 \equiv -2\pi\epsilon_1 \tag{39}$$

$$y_0 = \frac{2(2\pi\epsilon_1 + t)(2\pi\epsilon_2 + t)}{t} \approx 2\frac{(\epsilon_1 - \epsilon_2)(t - t_1)}{\epsilon_1}, \quad t > t_1 = -2\pi\epsilon_1. \tag{40}$$

The low-temperature phase corresponds to $t > t_c$. The slope $\frac{dT}{dt}$ at $T = T_{hs} = -\epsilon_1$ is

$$\frac{dT}{dt} = \frac{1}{2\pi}(2\frac{\epsilon_2}{\epsilon_1} - 1). \tag{41}$$

The phase transition is continuous if $\frac{dT}{dt} < 0$. In this case $T_{hs} = T_c$. The phase transition becomes discontinues at $\epsilon_2 = \frac{1}{2}\epsilon_1$. This value corresponds to a finite deformation of the X-Y model. If ϵ_2 is treated as a thermodynamic parameter, the point $\epsilon_2 = \frac{1}{2}\epsilon_1$ is an end point of the line of second order phase transitions. For a narrow function $E(\phi)$, the difference $\epsilon_1 - \epsilon_2$ is small $\mid \epsilon_1 - \epsilon_2 \mid \ll \mid \epsilon_1 \mid$. At the spinodal temperature of low-temperature phase, the width of the function $E(\phi)$ and the width of $w_L(\phi)$ are of the same order.

5 Inhomogeneous Orientation Order

Inhomogeneity in orientation order may be caused by boundaries and by an inhomogeneous external field. Let us consider an external field $h(\mathbf{r};\phi)$. The part of the energy describing the interaction with field h is

$$\delta H = -\int h(\mathbf{r};\phi) w(\mathbf{r};\phi) dV d\phi. \tag{42}$$

The form (42) has the advantage that it allows to obtain the many point probability distributions. The pair connected correlation function
$G(\mid \mathbf{r} - \tilde{\mathbf{r}} \mid; \phi, \tilde{\phi})$

$$G(\mid \mathbf{r} - \tilde{\mathbf{r}} \mid; \phi, \tilde{\phi}) = < \sigma_\phi(r)\sigma_{\tilde{\phi}}(\tilde{\mathbf{r}}) > - < \sigma_\phi(r) >< \sigma_{\tilde{\phi}}(\tilde{\mathbf{r}}) > \tag{43}$$

gives the probability distribution of pairs of values $\phi, \tilde{\phi}$ at the distance r (see formula (16)). From the definition (14) one has

$$G(\mid \mathbf{r} - \tilde{\mathbf{r}} \mid; \phi, \tilde{\phi}) = \frac{1}{T}\frac{\delta w(\mathbf{r};\phi)}{\delta h(\tilde{\mathbf{r}};\tilde{\phi})}. \tag{44}$$

We will study here correlations in the high-temperature phase $T > T_c, w_h = \frac{1}{2\pi}$. Due to the symmetry of high-temperature phase, $G(r;\phi,\tilde{\phi})$ depends only on the difference $\phi - \tilde{\phi}$, $G(r;\phi-\tilde{\phi}) = u(r;\phi-\tilde{\phi})$. Besides, at $r \to \infty$ $G(r;\phi)$ goes to 0. Linearized MPA equations for $u(r;\phi-\tilde{\phi})$ are

$$Tu(\mathbf{r};\phi) = -\int d\tilde{V} \int d\tilde{\phi} E(\mathbf{r} - \tilde{\mathbf{r}}; cos(\phi - \tilde{\phi}))u(\tilde{\mathbf{r}}) + h(\mathbf{r};\phi) - \tilde{E}, \tag{45}$$

$$\tilde{E} = \int\int E(\mathbf{r} - \tilde{\mathbf{r}}; cos(\phi - \tilde{\phi}))u(\tilde{\phi};\tilde{r}) d\tilde{\phi} d\tilde{V}, \tag{46}$$

$$h(\mathbf{r};\phi) = \delta(\mathbf{r} - \tilde{\mathbf{r}})\delta(\phi - \tilde{\phi}) \tag{47}$$

In the Fourier- representation

$$E(\mathbf{r};\cos\phi) = \sum_n \epsilon_n(\mathbf{r})\exp(in\phi), \quad \epsilon_n(\mathbf{r}) = \sum_{\mathbf{k}} \epsilon_{n;\mathbf{k}} \exp(-i\mathbf{kr}), \tag{48}$$

$$u(\mathbf{r};\phi) = \sum_n u_n(\mathbf{r})\exp(in\phi), \quad u_n(\mathbf{r}) = \sum_{\mathbf{k}} u_{n;\mathbf{k}} \exp(-i\mathbf{kr}), \tag{49}$$

here sums over n include all $n = 0, \pm 1, \pm 2, \ldots$. In this representation, the solution of (45) has the form

$$(T + \epsilon_{n;\mathbf{k}})u_{n;\mathbf{k}} = \frac{1}{2\pi}. \tag{50}$$

For $u_n(\mathbf{r})$, we obtain

$$u_n(\mathbf{r}) = \frac{1}{2\pi}\sum_{\mathbf{k}} \frac{\exp(-i\mathbf{kr})}{T + \epsilon_{n;\mathbf{k}}} = c_n \frac{\exp(-k_n r)}{r}, \tag{51}$$

$k = ik_n$ is the solutions of the equation

$$T + \epsilon_{n;\mathbf{k}} = 0; \tag{52}$$

for c_n one gets:

$$c_n = \frac{1}{(2\pi)^4} Re\{k / \frac{d\epsilon_{n;\mathbf{k}}}{dk} \mid_{k=ik_n}\}, \tag{53}$$

where the unit volume of the lattice is supposed to be equal 1. As we see, every partial harmonic u_n has its correlation radius $r_c(n)$:

$$r_c(n) = k_n^{-1}. \tag{54}$$

At the spinodal line Eq. (37) gives $k_1 = 0$, the correlation radius $r_1$is infinite. For functions $E(\mathbf{r};\cos\phi)$ having features described above, the dipole harmonic $n = 1$ has the largest correlation radius, $r_c(n)$ decreases with n increasing as slowly as s is small. At the largest distances

$$r \gg \frac{r_c^2(2)}{r_c(1) - r_c(2)}, \tag{55}$$

taking into account only the first term of the Furie series (49) one obtains

$$u(\mathbf{r};\phi) \approx 2u_1(r)\cos(\phi). \tag{56}$$

At smaller r, the width of $u(\mathbf{r};\phi)$ as a function of ϕ decreases due to other harmonics u_n. At the inverse to (55) limit case, the form of $u(\mathbf{r};\phi)$ is

$$u(\mathbf{r};\phi) = \frac{1}{r} f(\phi), \tag{57}$$

the width of $f(\phi)$ is of the same order as the width of $E(\mathbf{r};\cos\phi)$. The linear approximation is valid if $u \ll 1$, or $r \gg f(0)$.

6 Conclusions

In this and previous [8] papers we have presented the formalism of local state representation intended for models of orientation order. MPA was defined to describe statistical properties of the simplest discrete [8] and continuous models. The most straightforward possibility to investigate $3D$ models is to consider homogeneous MPA. Different phases appear via violation of the interaction symmetry. Both orders of phase transitions are available. So, studies of the narrow width $O(2)$ model show that there is the strong first order phase transition neither in the X-Y model case.

Let us review briefly some of the topics related to the orientation order models that can be studied via the formalism of local state representation but are been out of the scope of this papers. 1.Investigation of other models of orientation order as $SO(3)$ model having much to do with $3D$ melting [9, 10, 11] or S^2 model of nonhaisenberg magnetics [12, 13]. 2.Study of effects of vortexes in abelian and nonabelian continuous models. 3.Investigation of an arbitrary $O(2)$ model in $2D$. Some of these problems are at progress now.

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