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LOCAL STATE REPRESENTATION
IN STATISTICAL MECHANICS
OF CLASSICAL SYSTEMS.
1. DISCRETE SET OF STATES

Local State Representation in Statistical Mechanics of Classical Systems.
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Abstract

We offer a method to study statistical mechanics of classical systems described in terms of local states. The local state is represented by a multicomponent vector in a state space. Equations for the probabilities of the local states are derived in the mean probability approximation. This equations are solved for models with discrete set of states, where new phase transitions occur due to a structure of a state space.

1.Introduction

In the theory of phase transitions the concept of order parameter allows to simplify the description of a system. A coarse graining up to some intermediate scale makes all freedoms except for few ones irrelevant, those few being components of the order parameter field. In the simplest case the order parameter has only one component (a scalar order parameter). Systems with a scalar local order are the most studied. The probability of a configuration of the scalar order parameter field ϕ may be written as

$$w\{\phi\} = \frac{1}{Z}\exp(-\frac{H\{\phi\}}{T}), \quad Z = \int \exp(-\frac{H}{T})D\phi. \tag{1}$$

In (1), T is the temperature, $\int ..D\phi$ denotes the sum over all configurations of $\phi(r)$, r is the point of the real space occupied by the system, and $H(\phi)$ is the effective Hamiltonian of the field ϕ. Near a second order phase transition, only small deviations of the local value $\phi(r)$ near $\phi = 0$ are probable, so for $H(\phi)$ one get the Landau Hamiltonian [1]

$$H = \frac{1}{2}\int \{c(\nabla\phi)^2 + \tau\phi^2 + g\phi^4 - h\phi\}dV. \tag{2}$$

For that scalar system the space of local states is the real axis $\infty > \phi > -\infty$. Examples of those systems are liquid near the critical point, binary solutions, uniaxial ferromagnetics in the vicinity of their second order phase transitions.

For a planar or isotropical ferromagnetics, liquid crystals, crystals at melting point and many other systems the order parameter is a multicomponent

quantity and may be written as a tensor field. An important feature of those systems is the existence of an intermediate scale, on which the order is a physically significant property. The so chosen order parameter describes the local anisotropy of the system. For systems with weak local order, the anisotropy is small and fluctuations of the local form around an isotropical arrangement are important. It results in smallness of order parameter components, so one may still expect to have the effective Hamiltonian in the form of series in order parameter fields. For systems with a hard local order the degree of the local anisotropy is rather a fixed characteristic. The fluctuating quantity is the orientation of local anisotropy considered as a field of orientations. Examples of those systems are classical spin ferromagnetics (vector order parameter), some nematic liquid crystals (order parameter is a tensor rank 2) [2] and crystals and melts near the melting line [3],[4], [5],[6]. For those orientation phase transitions, the simple form of the Hamiltonian is not justified by general physical arguments, but rather it is chosen for the reason of mathematical simplicity. For instance consider a system with an order parameter being a planar vector $M(r)$, as in a classical planar ferromagnetics. The set of local states here is a circle, it may be parameterized with the aid of an angle coordinate $\psi, -\pi < \psi < \pi$. The simple form interaction energy is

$$E_{int} \sim (\nabla \psi)^2. \tag{3}$$

At the phase transition temperature, vortex points for 2D systems and vortex lines for 3D systems are important, where gradients of orientation are large and one have to change the form (3) for a more adequate description of the vortex energy. At the phase transition, the presence and important role of topologically nontrivial configurations is a common property of systems with the orientation local order.

As a result of a strong interaction that fixes the local anisotropy those arguments leading to the universal Landau form of the effective Hamiltonian are no more valid. To understand the phases and phase transitions in this systems one have to consider more general models.

It is worth to mention that a quadratic form of the interaction in the model

$$E_{int}(r, \tilde{r}) \sim S(r)S(\tilde{r}) \tag{4}$$

makes it easy to get a simple mean field approximation (MFA) by replacing the actual Hamiltonian with the MFA one

$$H_{MFA} = hS, \quad h = \nu(S). \tag{5}$$

It would be helpful to have such a simple approximation for more general forms of E_{int}.

The aim of the present paper is to study ordering systems in connection with their local state sets. We offer a method to formulate such a model using a representation of points of the state set as an order parameter. The study of the generating functional for the local state field leads to the mean probability approximation. This approximation is applied to models of

2.Local state representation.

The mathematical construction of a general model considered here is based on the representation in terms of local states. Namely, our system consists of points r, and in each point r of the system some (local) state is realized. Possible local states will be referred as points $\alpha, \beta...$ of the state set. The interaction energy is supposed to be a sum of 2-point, 3-point etc energies

$$E_{2,int}(\alpha; r \mid \tilde{\alpha}; \tilde{r}); \quad E_{3,int}(\alpha; r \mid \tilde{\alpha}; \tilde{r} \mid \tilde{\tilde{\alpha}}; \tilde{\tilde{r}}). \tag{6}$$

In (6), $\alpha, \tilde{\alpha}, \tilde{\tilde{\alpha}}$ are states at points $r, \tilde{r}, \tilde{\tilde{r}}$ correspondingly. We consider only systems with two point interactions $E = E(\alpha, \tilde{\alpha})$. Known examples of systems with continuous state set are planar and 3D classical spin systems (space set is a circle and a sphere respectively), nematics with hard local order (state set is a sphere with points on the same diameter equivalent), the locally crystalline liquids (states is all possible nonequivalent orientations of a lattice), etc. Known models with a discrete state space are the Ising model (two states system), N-states Potts model [7], clock models etc.

The model we consider is a lattice in (real) space with points (sites) r. Each site may be in one of the states α and the energy of a configuration $\{\alpha(r)\}$ is

$$H\{\alpha\} = -\sum_{r,\tilde{r}} E^{\alpha(r),\beta(r)}(r - \tilde{r}). \tag{7}$$

The summation in (7) goes over all sites $r, \tilde{r}$ of the lattice. Let us now write (7) in an alternative form. For the sake of simplicity we consider a discrete state set with N states. We define an N dimensional euclidean space having an euclidean coordinate frame with unit vectors $e^{(\mu)}$, $\mu = 1, 2, ..., N$. This unit vectors are in one-to-one correspondence with local states: $e^{(\mu)} \Leftrightarrow \mu$. The local state in a site r is represented by a vector σ in this state, namely

$\sigma(r) = e^{(\mu)}$ if the state is μ. For the projections σ^β of σ one has $\sigma^\beta = \delta^{\mu\beta}$. In a case of continuous state space one has a functional space for σ instead of the euclidean one described above and δ-functions instead of Kronecker symbols.

The energy (7) may be now written as

$$H\{\sigma\} = -\frac{1}{2} \sum_{r,\tilde{r}} \sigma^\alpha(r) E^{\alpha\beta}(r - \tilde{r}) \sigma^\beta(\tilde{r}), \qquad (8)$$

where the summation over repeating state set indexes is supposed. The quantity $E^{\alpha\beta}$ is a symmetrical tensor of rank 2 in the state space. We will consider mainly the case

$$E^{\alpha\beta}(r - \tilde{r}) = J(r - \tilde{r}) E^{\alpha\beta} \qquad (9)$$

The form (9) is always valid for models with nearest neighbors interaction.

For the 2-states model (9) coincides with the Ising model, for $E^{\alpha\beta} = \varepsilon\delta^{\alpha\beta}$ and $N > 2$ it is the Potts model. For this model the structure of the state space is irrelevant because of the dependence of the energy only on coincidence or non coincidence of states α and β. In the more general model $E^{\alpha\beta}$ reflects the neighborhood relations in the state space, so topology of this space become important -see below.

Note that the average value of the state vector $<\sigma>$ represent the probability of states at a site: if $w(\alpha; r)$ is the probability to have the state α at a site r then

$$w(\alpha; r) = <\sigma^\alpha(r)>, \qquad \sum_\alpha \sigma^\alpha(r) = 1. \qquad (10)$$

Correlation functions of $\sigma(r)$ are probabilities of simultaneous occupation of states at corresponding points:

$$<\sigma_\alpha(r_1)\sigma_\beta(r_2)...\sigma_\gamma(r_n)> = w\{\alpha; r_1 \mid \beta; r_2 \mid ...\gamma; r_n\} \qquad (11)$$

As in (5), the form of the energy (8) allows to formulate the mean probability approximation (MPA).

3. The Hubbard-Stratanovich transformation. Mean probability approximation.

The generating functional for the state parameter field $\sigma(r)$ for the system with Hamiltonian (8) is

$$Z\{h\} = Tr[\exp(-\frac{H\{\sigma\}}{T} + \sum_r \sigma^\alpha(r)h^\alpha(r))]_\sigma; \qquad w(\alpha; r) = \frac{\delta \ln Z}{\delta h^\alpha(r)}. \qquad (12)$$

$H\{\sigma\}$ is defined by (8), and the trace is taken over all states α in each site r. Let us perform the Hubbard-Stratanovich transformation for Z. We introduce in each site r an N-component vector $\psi(r)$. Formula (12) may be replaced by

$$Z\{h\} = \int \prod_{\alpha;r} D\psi^{\alpha;r} \exp\{-\frac{1}{2T} \sum_{r,\tilde{r}} J^{-1}(r - \tilde{r}) E^{\alpha\gamma} \psi^\alpha(r)\psi^\gamma(\tilde{r})\} \times$$
$$\times \prod_{\alpha;r} Tr \exp[\frac{1}{T}(E^{\alpha\gamma}\psi^\alpha(r)\sigma^\gamma(r)) + h^\alpha(r)\sigma^\alpha(r)]. \qquad (13)$$

In (13), the integration $D\psi$ goes over all components ψ^α of $\psi(r)$ in each site r. The Tr denotes the sum over all local states σ^α in all sites. The actual path of integration in the complex planes of ψ^α is to be chosen as to make the integral convergent. The condition of convergence of (13) is

$$\sum_{r,\tilde{r}} J^{-1}(r - \tilde{r}) E^{\alpha\beta} \psi^\alpha(r)\psi^\beta(\tilde{r}) > 0$$

along the integration in complex ψ planes. To get the eigenvalues of the quadratic form one introduces new variables $\psi_{k,\lambda}$:

$$J(r) = \sum_k J_k \exp(-ikr),$$
$$\psi^\alpha(r) = \sum_{k,\lambda} \psi_{k,\lambda} \exp(-ikr)v^\alpha_\lambda, \qquad E^{\alpha\gamma}v^\gamma_\lambda = \lambda v^\alpha_\lambda. \qquad (14)$$

For the quadratic term one gets now

$$\sum_{r,\tilde{r}} J^{-1}(r - \tilde{r}) E^{\alpha\gamma} \psi^\alpha(r)\psi^\beta(\tilde{r}) = \sum_{k,\lambda} \frac{\lambda}{J_k} \psi_{k,\lambda}\psi_{-k,\lambda}, \qquad (15)$$

For $\frac{\lambda}{J_k} > 0$ the convergence condition is $\psi_{k,\lambda} = \psi^*_{-k,\lambda}$ as for real function $\psi(r)$ but for those k, λ with $\frac{\lambda}{J} < 0$ integration path is as for a pure imaginary function: $\psi_{k,\lambda} = -\psi^*_{-k,\lambda}$. In the last case we change the $\psi_{k,\lambda} \Rightarrow i\psi_{k,\lambda}$. The result is that one is able to use function with $\psi_k = \psi^*_{-k}$ when changing the sign of λ if $\frac{\lambda}{J_k}$ is negative. In (13), it is easy to take the Tr, summing up over all local states. The resulting formula is

$$Z\{h\} = \int \prod_{\alpha;r} D\psi^\alpha(r) \exp\{-\frac{F}{T}\},$$
$$F = \frac{1}{2} \sum_{r,\tilde{r}} J^{-1}(r - \tilde{r}) E^{\alpha\gamma} \psi^\alpha(r)\psi^\gamma(\tilde{r}) -$$
$$-T \sum_r \ln[\sum_\alpha \exp\{\frac{1}{T}(E^{\alpha\gamma}\psi^\gamma(r) + h^\alpha(r))\}]. \qquad (16)$$

The essential difference in (13) from (16) is that $\psi^\alpha(r)$ is a continuous variable, so one is able to apply to (16) the well known method of analysis - to find the most probable configuration that minimize the expression in the

exponent, then study fluctuations of $\psi(r)$ by expanding this expression in the vicinity of the minima etc. In this paper we restrict ourselves with the first step, that gives the approximation of mean probabilities. The configuration of $\psi(r)$ that minimizes F in (16) (the most probable configuration) obeys the condition

$$\sum_{\tilde{r}} J^{-1}(r-\tilde{r})\psi^{\alpha}(\tilde{r}) = Z_0^{-1}\exp[\frac{E^{\alpha\gamma}\psi^{\gamma}(r)}{T}+h^{\alpha}],$$

$$Z_0 = \sum_{\alpha}\exp[\frac{E^{\alpha\gamma}\psi^{\gamma}(r)}{T}+h^{\alpha}]. \qquad (17)$$

The substitution of the solution ψ of (17) in F (16) gives the generating functional Z , namely $F(\psi) = -T\ln Z$. The probability $w(\alpha;r) = -\frac{\delta F}{\delta h^{\alpha}(r)}$ coincide with the right side of (17). It gives the expression for $w(\alpha;r)$

$$w(\alpha;r) = <\sigma^{\alpha}(r)> = \sum_{\tilde{r}} J^{-1}(r-\tilde{r}) >< \psi^{\alpha}(\tilde{r})> . \qquad (18)$$

The quantity F of the formula (16) has the properties of the nonequilibrium thermodynamic potential of the Landau theory, and the field $\psi^{\alpha}(r)$ plays the role of an order parameter in the theory. F has its minimal value in equilibrium. Let us define $w(\alpha;r)$ for nonequilibrium values of ψ by formula (18). In terms of this new field one has for $F(w)$

$$F = \frac{1}{2}\sum_{r,\tilde{r}} J(r-\tilde{r})E^{\alpha\gamma}w(\alpha;r)w(\gamma;\tilde{r}) -$$

$$-T\sum_r \ln(\sum_{\alpha}\exp(\frac{E^{\alpha\gamma}\sum_{\tilde{r}}J(r-\tilde{r}w(\gamma;\tilde{r})}{T}+h^{\alpha})). \qquad (19)$$

The equilibrium value of w is at minimum of F

$$\frac{\delta F}{\delta w(\alpha;r)} = 0. \qquad (20)$$

the condition for probability

$$\sum_{\alpha} w(\alpha;r) = 1 \qquad (21)$$

is automatically fulfilled for solutions of (20). In explicit form one obtain ($h(\alpha;r) = h^{\alpha}(r)$)

$$w(\alpha;r) = Z_0^{-1}\exp(\frac{E(\alpha;r)}{T}),$$

$$E(\alpha;r) = \sum_{\tilde{r}} J(r-\tilde{r})E^{\alpha\gamma}w(\gamma;\tilde{r}) + h(\alpha;r). \qquad (22)$$

An interpretation of (22) is that the energy $E(\alpha;r)$ is the energy of a site r when the local state is α, and the surrounding sites $\tilde{r}$ are occupied with the mean probability $w(\gamma;\tilde{r})$. The approximation is an exact solution of the statistical problem in the limit of infinite range of interaction $J(r)$.For the homogeneous field $h(r) = h(0)$ one gets for site independent $E(\alpha), w(\alpha)$:

$$E(\alpha) = J_0\sum_{\alpha} E^{\alpha\gamma}w(\alpha) + h^{\alpha}, \quad J_0 = \sum_r J(r-\tilde{r}). \qquad (23)$$

MPA-Equations may have a set of solutions depending on additional parameters not specified by the equations- this is a rather known property of approximations which are neglecting fluctuations. In the vicinity of a first order phase transition one expect to have at least two solutions corresponding to stable and metastable phases. The stable solution corresponds to the lowest minimum of F as a functional of $w(\alpha;r)$ with an additional condition $\sum_{\alpha} w(\alpha;r) = 1$.

In what follows we apply the mean probability approximation (MPA) to study some models.

4. The Potts model.

The simplest system with a discrete set of local states is the two state system equivalent to an Ising model. In this case the MPA coincide with the mean field approximation. For a N - state model let us correspond local states to points $\alpha, \beta, ...$ of a N- point figure; the energy $E^{\alpha\beta}$ of interaction corresponds to the segment connecting α and β. The resulting graph consists of N vortexes and $\frac{N(N-1)}{2}$ segments. A symmetry of the system courses the symmetry of the graph under permutations of vortexes - the matrix $E^{\alpha\beta}$ is invariant under corresponding permutations of rows and columns of the matrix. It is evident that diagonal elements of the matrix are transformed in diagonal elements.

The most symmetrical model is the Potts model $E^{\alpha\beta} = \varepsilon\delta^{\alpha\beta}$. For Potts model all vortexes are equivalent but disconnected, so the neighborhood relations are not defined for this model. We consider here the case $\varepsilon > 0$ with all points in the same state for $T = 0$: $\alpha = 0$. At high temperatures one expect all states by occupied with equal probability $w = 1/N$. For low temperatures the state 0 has the probability $w(0) > 1/N$. We denote the exceeding probability of the first state as $x = w(0) - 1/N$. All other N-1 states are occupied with equal probabilities $w(1) = w(2) = ... = w(N-1) = \frac{1-w(1)}{N}$. The later assumption reduces the problem to a one parameter one, so MPA coincide with

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a mean field approximation if one uses x as an order parameter-see [7],[3]. Let us use εJ_0 as a unit of energy and temperature. The thermodynamic potential $F(x)$ is now

$$F = \frac{1}{2}((x + \frac{1}{N})^2 + \frac{(1-x-\frac{1}{N})^2}{N-1}) - T \ln Z(x),$$

$$Z(x) = \exp(x + \frac{1}{T}) + (N-1)\exp(\frac{1-x-\frac{1}{N}}{(n-1)T}). \qquad (24)$$

Equation (24) gives for the equilibrium value of x

$$x + \frac{1}{N} = \frac{1}{2}(1 + \tanh(\frac{xN}{2T(N-1)} - \frac{1}{2}\ln(N-1))). \qquad (25)$$

There are three characteristic temperatures for the equation (25). The low temperature solution exists for temperatures $T < T_{ls}$. The high temperature solution $x = 0$ exists for all temperatures but is stable or metastable only for $T > T_{hs}$. The T_{ls} and T_{hs} are the spinodal temperatures of the low and high temperature phases respectively. $F(x)$ has two minima for temperatures $T_{hs} < T < T_{ls}$, and for $T = T_{ls}, T_{hs}$ $\frac{d^2 F}{dx^2} = 0$

$$T_{hs} = \frac{1}{N}; \qquad (26)$$

$$T_{ls} \rightarrow \frac{1}{\ln N}, \quad N \rightarrow \infty. \qquad (27)$$

At the phase transition temperature T_t,

$$F(x_h(T_t), T_t) = F(x_l(T_t), T_t), \qquad (28)$$

where $x_h = 0$, $x_l(T) \neq 0$ are the solutions of (25). One gets

$$T_t = \frac{N-2}{2(N-1)\ln(N-1)}. \qquad (29)$$

Note that the relative difference $\Delta_l \equiv \frac{T_{ls} - T_t}{T_{ls}}$ is a small number of the order 10^2 for $N = 4$ but $\Delta \rightarrow \frac{1}{2}$ for $N \rightarrow \infty$. There is a high asymmetry in the ranges of metastability of two phases.

Let us now consider small deviations from the homogeneous solution w_0. Linearizing (19) near w_0 and treating r as continuous variable one gets for $\varphi = w - w_0$ in the high temperature phase

$$\sum_\gamma (\delta^{\alpha\gamma}T - \frac{J_k}{J_0}(\frac{\delta^{\alpha\gamma}}{N} - \frac{1}{N^2}))\varphi_k^\alpha \equiv M_k^{\alpha\gamma}\varphi_k^\alpha = 0. \qquad (30)$$

J_k is the Fourier transform of $J(r)$,

$$J(r) = \int d^3 k J_k \exp(i\vec{k}\vec{r}), \quad J_k = \frac{J_{k=0}}{1 + (R_0 k)^2}. \qquad (31)$$

R_0 is the radius of interaction. The correlation radius R_c is $R_c = \frac{i}{k_c}$, where

$$Det\{M_{k_c}^{\alpha\gamma}\} = 0, \qquad (32)$$

$$R_c = \frac{R_0}{\sqrt{1 - \frac{2(N-1)\ln(N-1)}{N(N-2)}}}. \qquad (33)$$

For $N > 2$ the phase transition is a jump from a good ordered low temperature phase to the noncorrelated high temperature one.

5. Beyond Potts symmetry.

Let us consider a general model (8,9) with all vertexes equivalent. This means by definition that the graph is invariant under special permutations of vertexes exchanging any two vertexes of the graph. In other words it means that all rows of E_{ab} are permutations of one row (the some for columns). A graph with such a symmetry realizes the idea of Platon's figure. One gets those models in the theory of melting as an orientation phase transition by substituting the rotation group with its discrete subgroups, the later one being symmetry groups of regular polyhedrons in 3D case or regular polygons (Z -clock model) in 2D systems.So, the matrix for the N=4 clock model (the symmetry of a square) is

$$E_{(4)}^{\alpha\gamma} = \begin{pmatrix} a & b & b & c \\ b & a & b & c \\ c & b & a & b \\ b & c & b & a \end{pmatrix}, \qquad (34)$$

where b, c energies correspond to the sides and the diagonals of the square. For a model with the symmetry of a cub ($N = 8$) the matrix $E^{\alpha\beta}$ has the form

$$E_{cub}^{\alpha\gamma} = \begin{pmatrix} a & b & b & b & c & c & c & d \\ b & a & c & c & d & b & b & c \\ b & c & a & c & b & b & d & c \\ b & c & c & a & b & d & b & c \\ c & d & b & b & a & c & c & b \\ c & b & b & d & c & a & c & b \\ c & b & d & b & c & c & a & b \\ d & c & c & c & b & b & b & a \end{pmatrix}, \tag{35}$$

where b and c, d energies correspond to the edges of the cub and to the two types of the cub's diagonals.

Let us mention some general properties of discrete models.

1. The largest energy $\Delta = J_0\lambda$, λ being the maximum eigenvalue of $E^{\alpha\beta}$, determines the temperature T_H of the high- temperature phase spinodal. In high temperature phase all local states have equal probabilities $w(\alpha) = \frac{1}{N}$. The solution $w(\alpha) = 1/N$ of MPA - equations exists for all temperatures, but for $T < T_H$ it is unstable.

2. The group G of permutation symmetry of the set of states caused by the symmetry of the graph $E^{\alpha\beta}$ has some important subgroups. Namely, $E^{\alpha\beta}$ is symmetrical under all permutations of G which lives a given state γ unchanged (rotations $O_L(\gamma)$ around γ, L is the number of non coinciding configurations one gets for a graph with marked points). Another set of sub symmetries $Z_2(\alpha\beta)$ consists of pairs of permutations interchanging two given states $\alpha\beta$. The external field h can break some of this symmetries. For $h = 0$ the probability distribution $w(\alpha)$ and other statistical- characteristics may have some of this symmetries. Namely, the high temperature solution $w = \frac{1}{N}$ exhibits all of $O(\alpha)$ and Z_2 symmetries. The low temperature phase has the symmetry O_L of rotation around the state $\alpha = 0$. With the temperature increased the system undergoes a cascade of phase transitions to phase shaving new symmetries or no symmetries until the most symmetric high temperature phase is reached at $T = T_H$. For $T > T_H$, the minimal value of the energy $F(w)$ defined by formula (20) corresponds to $w = w_0 = \frac{1}{N}$. In MPA the expression for F as a function of a small deviation $\varphi = \delta w = w(\alpha) - w_0$ may be written as a power series in φ. Note that the same change of all energy makes no changes in probabilities due to the condition $\sum_\alpha w(\alpha) = 1$. Let us chose the zero level of energy to get the sum of all elements in a row of the interaction matrix $\sum_\alpha E^{\alpha\beta} = 0$. Under this condition

$$F(\varphi) = F(0) + \frac{J_0}{2N} E^{\alpha\gamma}(-\frac{J_0}{T}E^{\gamma\nu} + N\delta^{\gamma\nu})\varphi^\alpha\varphi^\nu + ... \tag{36}$$

The terms replaced by ... are the cubic, quadratic etc. The written quadratic term determines a necessity conditions for the stability of a phase. The matrix $E^{\alpha\beta}$ has a set of eigenvectors $v^{(n)}$ with corresponding eigenvalues λ_n. Due to chosen condition for $E^{\alpha\beta}$ the value of quadratic form in (36) is invariant under a shift of all $\varphi^\alpha \to \varphi^\alpha + c$, and at least one λ is zero corresponding eigenvector is v_0 with all component equal. The physical probability normalization leads to $\sum_\alpha \varphi^\alpha = 0$, hence the projection of φ on v_0 is zero. The eigenvalues μ_n of the matrix of quadratic form in (36) are

$$\frac{2NT}{J_0^2}\mu_n = \frac{\lambda_n}{J_0}(-J_0\lambda_n + NT). \tag{37}$$

As discussed in part 3 (see (15)), the stability condition is $\mu_n > 0$ for $\frac{\lambda_n}{J_0} > 0$ but $\mu_n < 0$ for $\frac{\lambda_n}{J_0} < 0$. In our case $J_0 > 0$ means that all negative λ and positive $\lambda < \frac{NT}{J_0}$ correspond to stable modes but modes ψ_λ with $\lambda > \frac{NT}{J_0}$ are unstable. The largest positive eigenvalue λ_{max} of the matrix $E_{\alpha\beta}$ defines the lower boundary

$$T_H = \frac{\lambda_{max}J_0}{N} \tag{38}$$

of stability or metastability of the high-temperature symmetric phase.

3. The highest possible symmetry of the high temperature phase is spontaneously broken in the lower- temperature phase. The phase transition is a second order one in MPA if and only if the φ^3 term in (36) vanishes for $T_H = \frac{\lambda J_0}{N}$ and the φ^4 term is nonnegative. Consider the eigenvector v corresponding to the maximal eigenvalue λ. The phase transition is in MPA a second order phase transition if

$$\sum_\alpha (v^\alpha)^3 = 0, \quad \frac{3}{N}(\sum_\alpha (v^\alpha)^2)^2 - \sum_\alpha (v^\alpha)^4 > 0. \tag{39}$$

For all other cases the phase transition is a first order one in MPA.

4. Let us investigate fluctuations about high-temperature trivial phase for 3D models. One expand the action (16) in a series in fluctuating fields $\varphi^\alpha(r) = \psi^\alpha(r) - \frac{J_0}{N}$ neglecting terms above the second order. The gauss approximation for connected correlation function of probabilities gives $(\sum_\alpha E^{\alpha\beta} = 0)$

$$K^{\alpha\gamma}(r_i - r_j) = \langle\langle \sigma_i^\alpha \sigma_j^\gamma \rangle\rangle \equiv \frac{d^2 \ln(Z)}{d^2 h_i^\alpha h_j^\gamma}\Big|_{h\to 0} = $$
$$= \sum_\nu (\frac{\delta_{ik}\delta^{\alpha\nu}}{N} - \frac{\delta_{ik}}{N^2})L_{kj}^{\nu\gamma}, \tag{40}$$

where

$$(L^{-1})_{ij}^{\alpha\nu} = \delta_{ij}\delta^{\alpha\nu} - \frac{J_{ij}E^{\alpha\gamma}}{NT}, \tag{41}$$

$$(L^{-1})_{ij}^{\alpha\nu} L_{jk}^{\nu\gamma} = \delta_{ik}\delta^{\alpha\gamma}. \tag{42}$$

Poles of fourier transformed correlation function $K^{\alpha\gamma}(\vec{q})$ defining a scale of fluctuations we obtain from equation

$$Det[\delta^{\alpha\gamma} - \frac{J_{k_c}}{NT}E^{\gamma\nu}] = 0, \tag{43}$$

with J_k from (31). The solution of the (42) equation with the smallest $|k_c| = \frac{1}{R_c}$ defining a behaviour of the correlation function on large distances connects with the maximal eigenvalue of matrix E (see also reasonings from the 2 part of this section)

$$J_{k_c} = \frac{NT}{\lambda_{max}}. \tag{44}$$

From (31),(38) and (44) the correlation radius at $T > T_{hs}$ is

$$R_c = \frac{R_0}{\sqrt{1 - \frac{T_{hs}}{T}}}. \tag{45}$$

5. The ground state of the system is determined by the location of largest matrix elements. We study here only systems having all sites in the some local state at zero temperature: it is the case if $J(r) > 0$ and $a > 0, a > b, c, \dots$ -see formula (9). This state is chosen by an infinitely small external field $h \to 0$. We will mark the preferred state as $\alpha = 0$. The lowest energy- excitations are then sites occupied by local states β corresponding to lowest values Δ_0 of excitation energy $\Delta(\beta)$

$$\Delta(\beta) = J_0(E^{0\beta} - E^{00}), \beta \neq 0; J_0 = \sum_r J(r). \tag{46}$$

We will refer those states β as next neighbor states to the state $\alpha = 0$. For every state α there are next neighboring states β with minimal values of $E^{\alpha\beta}$, we will denote those states as $\beta = nn(\alpha)$. At low temperatures $T \ll \Delta_0$ the system has almost all sites in $\alpha = 0$ as a background for a low density gas excitations - sites in states $\gamma \neq 0$, with concentrations $c(\gamma)$,

$$c(\gamma) = \exp(-\frac{\Delta(\gamma)}{T}). \tag{47}$$

All states symmetric under permutations not changing the state 0 have equal densities (probabilities) at $T \ll \Delta_0$, particularly the $nn(0)$ states have the highest but small equal densities $c = \exp(-\frac{\Delta_0}{T})$. It is important to stretch that the symmetry of $c(\gamma)$ is unbroken at low temperatures $T < T_L$. The MPA is not valid for this temperature range because the number of excitations inside the interaction volume is a small number proportional to the density c. One can check the statement by applying to the expression (12) for Z a low density approximation using the $c(\gamma)$ as a small parameter.

6. In the intermediate temperature interval $T_H > T > \Delta_0$ the symmetry of phases depends on details of interaction , e.g on $J(r)$ and $E^{\alpha\beta}$.

Some general approach may be applied to the low temperature investigation of a model with an arbitrary discrete space set interaction. For low temperatures only the ground state and the any states nearest by energies to one are significant. The all other states are negligible. This idea allows to simplify an arbitrary discrete model to

6. Model with nearest state interaction.

Consider a system in which the interaction between next neighboring states is added to the Potts interaction energy:

$$E^{\tilde{\alpha}\beta} = \varepsilon\delta^{\alpha\beta} + \varepsilon(1 - \nu)\delta^{\alpha, nn(\alpha)} \tag{48}$$

$\varepsilon > 0, \nu > 0, \nu \ll 1, T \ll \varepsilon$. Let us chose the energy scale by setting $\varepsilon J_0 = 1$. For very low temperatures $T \ll \nu$ almost all sites are occupied by the same state witch we will denote as $\alpha = 0 : 1 - w(0) \ll 1$. Probability (concentration) of all other states is low. For $\beta = nn(0)$ it is $w(\beta) = \exp(-\frac{\nu}{T})$ while for $\gamma \neq nn(0)$ it is $w(\gamma) = \exp(-\frac{1}{T})$ and we can neglect this probability for $T \ll 1$ and reduce the set of local states to those of ground state 0 and L states $nn(0)$. For the reduced system, the initial symmetry of $E^{\alpha\gamma}$ is broken - the state $\alpha = 0$ plays the role of a vacuum for the system.

1. At the lowest temperatures $T \ll \nu$ the system has a O_L symmetry under(discrete) rotations around the $\alpha = 0$ state, the concentration of states $\beta = nn(0)$ is the same

$$w(\beta) = w = exp(-\frac{\nu}{T}). \tag{49}$$

On increasing temperature, O_L symmetry of equilibrium configuration is broken via a phase transition. It is possible to consider this one for two limit

cases: a) radius of interaction is finite, the product of J_0 and ε -the diagonal element of the matrix E is infinite; b) radius of interaction is infinite, the product of J_0 and ε is finite.

1a. At lowest temperatures a probability p for two nn(0) states which are not nn between each other to be at distance of the interaction radius R_0 is

$$p(T) \sim (\frac{R_0}{r})^3 w^2 \ll 1, \qquad (50)$$

where r is the elementary lattice site, $d = 2$ or $d = 3$ is the number of dimensions of the system. At higher temperatures the repulse of excitations with different β is essential - every nn exclude all others nn from the volume R_0^d. For all nn having the some density it results in a lost of the entropy and hence to increase of the free energy. A phase with a symmetry of rotation-surround $\alpha = 0$ broken has a lower value of the free energy. In the new phase the smaller set of states all being nn of each other is preferred. The system undergoes a phase transition to this phase at the temperature of the order $\tilde{T}$

$$\tilde{T} \sim \frac{\nu}{\ln(R_0)}. \qquad (51)$$

We got the latter formula from the crude estimation $p(\tilde{T}) \sim 1$.

1b. In this limit case homogeneous MPA equations (22) with E from (48) are exact. We are going to look for a solution of this equations for probabilities $w(\alpha), \alpha = 0, 1...L$ depending on two variables only

$$w(0) = 1 - (L-1)\pi - w, \quad w(1) = w, \quad w(2) = ... = w(L) = \pi. \qquad (52)$$

This kind of solution of equations (22) realizes an idea of a separation of one of nn(0) states (1 state for example). From (22) and (52) we obtain the equations for equilibrium values of π and w

$$\pi = \frac{1}{1+(L-1)\exp(\frac{J_0(\pi-w)}{T})+\exp(\frac{J_0}{T}(\nu+(L-1)(1-2\nu)\pi+(1-2\nu)w))},$$
$$w = \frac{1}{1+(L-1)\exp(\frac{J_0(\pi-w)}{T})+\exp(\frac{J_0}{T}(\nu-(L-1)(1-2\nu)\pi-2\nu w))}. \qquad (53)$$

There exist some temperature $\tilde{T}$

$$\tilde{T} \sim \frac{J_0\nu}{\ln(\frac{1}{\nu})}, \qquad (54)$$

and the trivial solution of the equations (53) at this temperature

$$\tilde{w} = \tilde{\pi} \sim \frac{\tilde{T}}{J_0}, \qquad (55)$$

such that at $T = \tilde{T} + \Delta, \Delta \ll \nu$ some nontrivial solution (NS) going to trivial $\tilde{w}$ at $\Delta \to 0$ exists. The expressions (54,55) are obtained in the leading order in $\nu \ll 1$. The value $\chi = \frac{\pi-w}{2}$ plays the role of order parameter, which non equal to 0 for NS only. There is the great difference between circle-like $L = 2$ and other $L > 2$ cases.

In the circle-like case the phase transition of O_2 symmetry breach via the separation of 1 state is the second order one. The dependence χ on T for NS near $\tilde{T}$- the temperature of phase transition- points to the strong dumping of the 2 state at temperatures above $\tilde{T}$:

$$\frac{d^2T}{d\chi^2}\big|_{\chi\to0} = \frac{2J_0}{\nu} \to \infty \quad for \quad \nu \to 0. \qquad (56)$$

The same phase transition becomes the first order one for the $L > 2$ case. It is possible to define three characteristic temperatures in this case: the first one $\tilde{T}$ from (54) is the temperature of low-temperature phase spinodal; the second one $\tilde{T} - \delta\tilde{T}$, where

$$\delta\tilde{T} \sim \frac{\tilde{T}^2}{J_0}\frac{(L-2)(L^2+2L-6)}{2L-1}, \qquad (57)$$

is the temperature of high-temperature phase spinodal; the third one is the temperature of the equilibrium phase transition been in between the first and second one. As for $L = 2$ case the strong dumping of the all nn(0) states besides the 1 one for temperatures above the temperature of phase transition takes place too.

2. A strong interaction of nn states for temperatures above $\tilde{T}$ leads to the separation one of nn states (1 state) and the strong dumping of other states. So, except some small vicinity of $\tilde{T}$, an influence of 2,..., L states on the Ising-like 0-1 states picture is weak. To clarify this issue it is convenient to study the generating functional (16) with the state matrix $\tilde{E}$ (48) and without lose of generality for $L = 2$. It is our waiting to obtain

$$<\sigma^2> \ll <\sigma^0>, <\sigma^1> \qquad (58)$$

or in accordance with (18) $<\psi^2> \ll <\psi^0>, <\psi^1>$. Again, we work in such temperature region $\tilde{T} < T \sim \frac{\nu J_0}{2}$ where an additional small parameter $\exp(-\frac{<\psi^1>}{T})$ exists. So, let us expand the action in a power series in ψ^2 and $\exp(-\frac{\psi^1}{T})$ neglecting terms above the first and the second order over ψ^2 and $\exp(-\frac{\psi^1}{T})$ accordingly

$$Z\{h\} = \int \prod_{r_i} D\psi^0(r_i)D\psi^1(r_i)D\psi^2(r_i)\exp\{-\tilde{F}\}, \qquad (59)$$

$$\tilde{F} = \tilde{F}_I + \tilde{F}_2 + \tilde{F}_{ext}, \tag{60}$$

$$\tilde{F}_I = \frac{1}{2T} J^{-1}(r_i - r_j) \begin{pmatrix} \psi^0(r_i) & \psi^1(r_i) \end{pmatrix} \begin{pmatrix} \nu & 0 \\ 0 & \nu \end{pmatrix} \begin{pmatrix} \psi^0(r_j) \\ \psi^1(r_j) \end{pmatrix} -$$

$$- \sum_{r_i} \ln[\exp(\tfrac{\psi^0(r_i)\nu}{T}) + \exp(\tfrac{\psi^1(r_i)\nu}{T})], \tag{61}$$

$$\tilde{F}_2 = \frac{1}{2T} J^{-1}(r_i - r_j)\psi^2(r_i)\psi^2(r_j)\nu + \frac{\nu-1}{T}\psi^2(r_i)(J^{-1}(r_i - r_j)\psi^1(r_j) -$$

$$- \frac{\exp(\frac{\nu}{T}\psi^1(r_i))}{\exp(\frac{\psi^0(r_i)\nu}{T}) + \exp(\frac{\psi^1(r_i)\nu}{T})}) - \frac{\nu}{T} \sum_i \psi^2(r_i) \frac{\exp(-\frac{\psi^1(r_i)(1-\nu)}{T})}{\exp(\frac{\psi^0(r_i)\nu}{T}) + \exp(\frac{\psi^1(r_i)\nu}{T})}, \tag{62}$$

$$\tilde{F}_{ext} = - \sum_{r_i} \frac{\exp(-\frac{\psi^1(r_i)(1-\nu)}{T})}{\exp(\frac{\psi^0(r_i)\nu}{T}) + \exp(\frac{\psi^1(r_i)\nu}{T})}. \tag{63}$$

$\tilde{F}_I$ is the action of the Ising model for which a mean-field investigation gives a correct description of a second order phase transition at the temperature $\tilde{T} = \frac{\nu J_0}{2}$. About the phase transition, contribution in the action from $\tilde{F}_{ext}$ is exponentially small $\sim \exp(-\frac{1}{\nu})$. One is equivalent to an action on the Ising system of an unsymmetrical under a permutation of the 0 and 1 states external field. Yet, about the Ising phase transition $< \sigma^0 > \sim < \sigma^1 >$ and we must take into account an influence of states nearest neighbor as to 0 state as to 1 state. This makes an external field at the phase transition point symmetrical under permutation of 0- and 1-state and doesn't change the order of phase transition. The expression for σ^2

$$< \sigma^2 > = \frac{\exp(-\frac{\sigma^1 J_0(1-\nu)}{T})}{\exp(\frac{\sigma^0 J_0\nu}{T}) + \exp(\frac{\sigma^1 J_0\nu}{T})}. \tag{64}$$

obtained after the gauss integration in (59) over ψ^2 fields with a substitution in (62) most probable Ising-like mean-field configurations of ψ^0, ψ^1 fields confirms near the phase transition, where $< \sigma^0 > \sim < \sigma^1 > \sim \frac{1}{2}$, the start approach (58). So, the nearest state interaction model (48) at an increasing temperature above $\tilde{T}$ turns out to be invariant under $Z_2(0,1)$ subgroup of group G of permutation symmetry of the set of states.

Acknowledgments

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Представление локальных состояний
в статистической механике
классических систем.
1. Дискретный набор состояний

A.Z. Patashinski and M.V. Chertkov

Local State Representation
in Statistical Mechanics
of Classical Systems.
1. Discreate Set of States

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