

INVESTIGATION OF PHASE DIAGRAM OF HARD-CORE BOSON MODEL WITH NON-ERGODIC CONTRIBUTIONS

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The hard-core boson model which is isomorph to the XXZ anisotropic Heisenberg model is investigated in the self-consistent field approach. The Helmholtz free energy, the set of self-consistency equations and the pseudospin Green's functions are obtained. The approach used corresponds to random phase approximation with the inclusion of non-ergodic contributions. Their influence on the shape of phase diagram and position of the phase transition lines is analysed.

Key words: XXZ anisotropic Heisenberg model, RPA.

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I. INTRODUCTION

The hard-core boson model is of great interest due to its universality in the theory of condensed matter. It is successfully applied to describe different physical phenomena: upper λ point in ^4He [1], supersolid state [2, 3], ionic conductivity [4], bipolaronic superconductivity [5]. The exact mapping of Pauli operators on spin operators makes the model isomorph to the XXZ anisotropic Heisenberg model. The model was intensively studied by Rudoy, Tserkovnikov and Lymar' [6], basing on the original method for the two-time Green's functions (usually named as Zubarev GF) developed by Tserkovnikov [7]. Also the method of equations of motion for the two-time Green's functions was used when considering quantum criticality [8]. Some questions were examined within the random phase approximation (RPA) by different authors [9, 10]. Starting with pioneering works of Landau and Binder [11] Monte Carlo simulations have become a conventional method of the investigation of the XXZ model [12] partially connected with an interesting critical behavior and existence of multicritical points [13], also because of some opened questions concerning thermodynamic stability of supersolid phase [14].

In this work we pay our attention to the so-called "non-ergodic contributions" to the thermodynamics of the model. Isothermal response is expressed in terms of the Matsubara Green's function as

$$\chi_T(\omega_n, \mathbf{q}) = \int_0^\beta \langle T_\tau M(0)M(\tau) \rangle_{\mathbf{q}} \times e^{i\omega_n \tau} d\tau - \beta \langle M \rangle^2 \delta(\omega_n) \quad (1)$$

and isolated response is described by means of the two-time Green's function

$$\chi_I(\omega, \mathbf{q}) \sim \langle\langle M | M \rangle\rangle_{\omega, \mathbf{q}} \quad (2)$$

When $\chi_T(0, \mathbf{q}) \neq \chi_I(0, \mathbf{q})$ it means that the ergodicity does not hold [15, 16]. It has been known for a good while that isothermal and isolated susceptibility for the transverse Ising model does not coincide [16, 17], it has been also shown for the pseudospin-electron model [18].

Here we show that similar differences in responses appear for the XXZ model too. There are some tricks which allow one to take into account static contributions when applying the two-time Green's functions, but then it is not always clear if one keeps to the same precision in different approximations. Common methods of the two-time Green's functions for spin operators suppose the use of kinematical identities and spectral representation for correlation functions. Obviously the paper of Kozitskij and Levitskij [19] has been left unnoticed and a puzzle with discrepancies when using different kinematical identities remains unclear and controversial sometimes [20]. In contrast, our approach is straight and self-consistent as equations for order parameters and susceptibilities are obtained from the Helmholtz free energy determining all thermodynamic properties of system.

According to the sign of interaction constants in the Hamiltonian the phase diagram of the model admits different phases. Owing to the fact that the model is applicable in various fields of the condensed matter theory there is discrepancy in terms. The following groups refer to the same phases: disordered, normal liquid, paramagnetic; superionic, superfluid, canted ferromagnetic, spin-flop; mixed, supersolid, canted antiferromagnetic, biconical; and normal solid, charge ordered, antiferromagnetic. In this paper we stick to the usual magnetic thesaurus — paramagnetic, spin-flop, biconical and antiferromagnetic.

II. RPA WITH NON-ERGODIC CONTRIBUTIONS

Hamiltonian of hard-core bosons on lattice reads

$$H_{\text{HCB}} = -\mu \sum_i n_i - \frac{1}{2} \sum_{ij} V_{ij} n_i n_j - \frac{1}{2} \sum_{ij} t_{ij} b_i^\dagger b_j$$

where μ is chemical potential, sums over $\{i, j\}$ describe interaction and hopping of particles, respectively, and b_i, b_i^\dagger are Pauli operators of annihilation and creation of

particles. Using pseudospin representation for the occupation number of lattice gas and Pauli operators

$$\begin{cases} S_i^z = n_i - \frac{1}{2} \\ S_i^+ = b_i \\ S_i^- = b_i^+ \end{cases} \quad (3)$$

we can consider an equivalent XXZ anisotropic Heisenberg model

$$H_{\text{XXZ}} = -h \sum_i S_i^z - \frac{1}{2} \sum_{ij} J_{ij} S_i^z S_j^z - \frac{1}{2} \sum_{ij} K_{ij} S_i^+ S_j^-$$

with magnetic the field h and sums over $\{i, j\}$ describing the interaction between spins (we consider nearest neigh-

bors only). Making the following unitary transformation we pass to coordinate system with the only one order parameter $\langle \sigma^z \rangle$ in the mean-field approximation (MFA)

$$\begin{cases} S_i^x = \sigma_i^x \cos \theta_i - \sigma_i^z \sin \theta_i \\ S_i^y = \sigma_i^y \\ S_i^z = \sigma_i^x \sin \theta_i + \sigma_i^z \cos \theta_i \end{cases} \quad (4)$$

So we rewrite the Hamiltonian as

$$H_{\text{XXZ}} = -h \cos \theta \sum_i \sigma_i^z - h \sin \theta \sum_i \sigma_i^x - \frac{1}{2} \sum_{ij} V_{ij}^{\alpha\beta} \sigma_i^\alpha \sigma_j^\beta$$

where

$$\begin{aligned} V^{++} &= \frac{1}{4} (J_{\mathbf{q}} \sin^2 \theta + K_{\mathbf{q}} (\cos^2 \theta - 1)), & V^{++} &= V^{--}, \\ V^{+-} &= \frac{1}{4} (J_{\mathbf{q}} \sin^2 \theta + K_{\mathbf{q}} (\cos^2 \theta + 1)), & V^{+-} &= V^{-+}, \\ V^{+z} &= \frac{1}{2} (J_{\mathbf{q}} - K_{\mathbf{q}}) \cos \theta \sin \theta, & V^{+z} &= V^{-z} = V^{z+} = V^{z-} \\ V^{zz} &= J_{\mathbf{q}} \cos^2 \theta + K_{\mathbf{q}} \sin^2 \theta, \end{aligned} \quad (5)$$

Now $\langle \sigma^x \rangle = 0$ is the condition for the angle θ in the MFA. Thus we have

$$\sin \theta = -\frac{K_0 \xi}{\lambda}, \quad \cos \theta = \frac{h + J_0 \eta}{\lambda} \quad (6)$$

with the introduced notations

$$\begin{aligned} \eta &= \langle S^z \rangle, & \xi &= \langle S^x \rangle, \\ J_0 &= \sum_j J_{ij}, & K_0 &= \sum_j K_{ij}, \\ \lambda &= \sqrt{(h + J_0 \eta)^2 + K_0^2 \xi^2}. \end{aligned} \quad (7)$$

The approach can be presented in a general form also applicable in the antiferromagnetic case when two sublattices are to be introduced, but in the following we restrict our selves to the uniform paramagnetic and spin-flop phases only.

To obtain the first correction to MFA results due to the finite interaction radius we apply a diagrammatic technique based on Wick's theorem for spin operators developed by Vaks *et al.* [21] and slightly modified by Izyumov and Skriabin [22]. After making all possible pairing of σ^+ and σ^- operators, the semi-invariant expansion must be done to calculate the mean values of the remaining products of σ^z operators, i.e.

$$\begin{aligned} \langle T_\tau \sigma_i^z(\tau_i) \sigma_j^z(\tau_j) \rangle_0 &= b^2 + b' \delta_{ij} \\ \langle T_\tau \sigma_i^z(\tau_i) \sigma_j^z(\tau_j) \sigma_k^z(\tau_k) \rangle_0 &= b^3 + bb' (\delta_{ij} + \delta_{ik} + \delta_{jk}) + b'' \delta_{ij} \delta_{jk}, \end{aligned} \quad (8)$$

etc. Here

$$\begin{aligned} b &= b(\beta\lambda) = \frac{1}{2} \tanh \left(\frac{\beta\lambda}{2} \right), \\ b' &= \frac{\partial b}{\partial(\beta\lambda)}, & b^{[n]} &= \frac{\partial^{[n]} b}{\partial(\beta\lambda)^{[n]}}. \end{aligned} \quad (9)$$

If the interaction constants J_{ij} and K_{ij} have an effective range R_0 , their Fourier transforms $J_{\mathbf{q}}$ and $K_{\mathbf{q}}$ are effectively non-zero when $|\mathbf{q}| < R_0^{-1}$. Hence every sum over momentum is proportional to $(a/R_0)^3$, where a is some typical distance, for instance lattice constant. The simplest approximation implies that analytical expressions of the considered quantities do not hold the sum over momentum. It is realized when the diagrams do not contain the closed loops formed by the lines of Green's functions, interactions or blocks, for example Fig. 1.

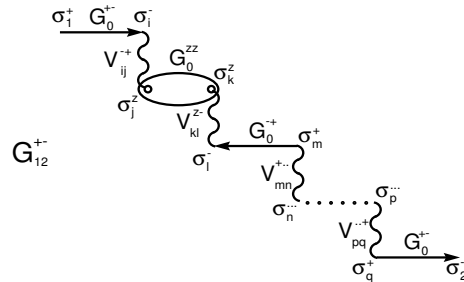


Fig. 1. The diagram corresponding in RPA to G_{ij}^{+-} in coordinate space (an example).

The selection for Green's functions of this class of diagrams only corresponds to the random phase approximation. Diagrammatically, the RPA correction to the Helmholtz free energy calculated in MFA looks like

$$\text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \dots = \frac{1}{2\beta N} \sum_{\mathbf{q}} \sum_{\omega_n} \ln \det \|\hat{1} - \hat{\Sigma} \hat{V}\|$$

The wavy lines refer to interactions $V^{\alpha\beta}$ and filled blocks to $\Sigma^{\alpha\beta}$ – irreducible (according to Larkin) parts. So we write for the Helmholtz free energy

$$F = F_{\text{MFA}} + \Delta F_{\text{RPA}}, \quad \begin{cases} F_{\text{MFA}} = \frac{1}{2} J_0 \eta^2 + \frac{1}{2} K_0 \xi^2 - \frac{1}{\beta} \ln \left(2 \cosh \left(\frac{\beta \lambda}{2} \right) \right) \\ \Delta F_{\text{RPA}} = \frac{1}{2\beta N} \sum_{\mathbf{q}} \sum_{\omega_n} \ln \det \|\hat{1} - \hat{\Sigma} \hat{V}\| \end{cases} \quad (10)$$

Only the next three irreducible parts are nonzero in the lowest approximation

$$\begin{aligned} \Sigma_0^{+-} &= -2bg^0(i\omega_n) = -\frac{2b}{i\omega_n - \lambda} = G_0^{+-} \\ \Sigma_0^{-+} &= -2bg^0(-i\omega_n) = \frac{2b}{i\omega_n + \lambda} = G_0^{-+} \\ \Sigma_0^{zz} &= \beta b' \delta(\omega_n) = G_0^{zz} \end{aligned}$$

After summation over Matsubara's frequencies one gets

$$\begin{aligned} \Delta F_{\text{RPA}} &= \frac{1}{\beta N} \sum_{\mathbf{q}} \left[\ln \left(\sinh \left(\frac{\beta \Lambda_{\mathbf{q}}}{2} \right) \right) - \ln \left(\sinh \left(\frac{\beta \lambda}{2} \right) \right) \right. \\ &\quad \left. + \frac{1}{2} \ln \left(1 - \beta b' \frac{\lambda (\cos^2(\theta) J_{\mathbf{q}} + \sin^2(\theta) K_{\mathbf{q}}) - b J_{\mathbf{q}} K_{\mathbf{q}}}{\lambda - b (\sin^2(\theta) J_{\mathbf{q}} + \cos^2(\theta) K_{\mathbf{q}})} \right) \right] \end{aligned} \quad (11)$$

here

$$\Lambda_{\mathbf{q}} = \sqrt{(\lambda - bK_{\mathbf{q}})(\lambda - bP)}, \quad \begin{aligned} P &= J_{\mathbf{q}} \sin^2 \theta + K_{\mathbf{q}} \cos^2 \theta \\ R &= J_{\mathbf{q}} \cos^2 \theta + K_{\mathbf{q}} \sin^2 \theta \end{aligned} \quad (12)$$

and the last term in the sum corresponds to non-ergodic contributions. The quasiparticle spectrum $\Lambda_{\mathbf{q}}$ coincides with the one obtained in [9].

There are two ways to obtain an equation for the order parameter: a) by direct construction using diagrams of certain class; or b) from the extremum condition of the Helmholtz free energy. Either one can be used to verify the results obtained with the other. The state of thermodynamic equilibrium corresponds to the minimum of the Helmholtz free energy, as a function of η and ξ with fixed β and h . Thus

$$\left(\frac{\partial F}{\partial \eta} \right)_{\beta, h} = 0, \quad \left(\frac{\partial F}{\partial \xi} \right)_{\beta, h} = 0 \quad (13)$$

give us

$$\begin{cases} \eta = \frac{\cos \theta}{2} \tanh \left(\frac{\beta \lambda}{2} \right) + \frac{\cos \theta}{2} \frac{1}{N} \sum_{\mathbf{q}} \left(\Lambda_{\mathbf{q}}^h \coth \left(\frac{\beta \Lambda_{\mathbf{q}}}{2} \right) - \coth \left(\frac{\beta \lambda}{2} \right) + C^h \right) \\ \xi = \frac{\sin \theta}{2} \tanh \left(\frac{\beta \lambda}{2} \right) + \frac{\sin \theta}{2} \frac{1}{N} \sum_{\mathbf{q}} \left(\Lambda_{\mathbf{q}}^h \coth \left(\frac{\beta \Lambda_{\mathbf{q}}}{2} \right) - \coth \left(\frac{\beta \lambda}{2} \right) + C_g \right) \end{cases} \quad (14)$$

where

$$\begin{aligned} \Lambda_g^h &= \frac{1}{2\Lambda_{\mathbf{q}}} \left((1 - \beta b' K_{\mathbf{q}})(\lambda - bP) + (\lambda - bK_{\mathbf{q}}) \left(1 - \beta b' P \pm \frac{\sin^2 \theta}{\cos^2 \theta} \frac{2b}{\lambda} (J_{\mathbf{q}} - K_{\mathbf{q}}) \right) \right), \\ C_g^h &= \frac{1}{\lambda - bP + \beta b' (bJ_{\mathbf{q}}K_{\mathbf{q}} - \lambda R)} \left[\beta b'' (bJ_{\mathbf{q}}K_{\mathbf{q}} - \lambda R) + (\beta b' J_{\mathbf{q}}K_{\mathbf{q}} b' - R \right. \\ &\quad \left. \mp \frac{\sin^2 \theta}{\cos^2 \theta} 2(J_{\mathbf{q}} - K_{\mathbf{q}}) - \frac{bJ_{\mathbf{q}}K_{\mathbf{q}} - \lambda R}{\lambda - bP} \left(1 - \beta b' P \pm \frac{\sin^2 \theta}{\cos^2 \theta} 2 \frac{b}{\lambda} (J_{\mathbf{q}} - K_{\mathbf{q}}) \right) \right] \end{aligned} \quad (15)$$

One should take the upper or lower sign and the corresponding factor when the first or second equation is considered. The terms C_g^h are non-ergodic contributions.

Let us consider the first equation only. If we neglect the last term in the sum and formally put $\eta = b \cos \theta$, we come to the equation for order parameter obtained by Alexandov *et al.* [9] within the decoupling approach for the two-time Green's functions. Also it is interesting to consider the self-consistency equation in the limit case $K \rightarrow 0$, when the first two terms of the sum cancel each other, and we have

$$\eta = \frac{1}{2} \tanh\left(\frac{\beta\lambda}{2}\right) - \frac{1}{2N} \sum_{\mathbf{q}} \frac{\beta J_{\mathbf{q}} b''}{1 - \beta J_{\mathbf{q}} b'} \quad (16)$$

that is a well known equation for order parameter of the Ising model with $O(1/z)$ corrections [23].

Transverse and longitudinal Green's functions

$$G^{+-}(i\omega_n, \mathbf{q}) = \langle T_{\tau} \sigma^+(\tau) \sigma^-(0) \rangle_{\mathbf{q}, i\omega_n} \quad (17)$$

$$G^{zz}(i\omega_n, \mathbf{q}) = \langle T_{\tau} \sigma^z(\tau) \sigma^z(0) \rangle_{\mathbf{q}, i\omega_n} \quad (18)$$

are obtained from the set of equations which is similar to the Larkin equation written in the matrix form (the corresponding sets for $\{G^{++}, G^{-+}, G^{z+}\}$ and $\{G^{+z}, G^{-z}, G^{zz}\}$ are written by analogy)

$$\begin{pmatrix} 1 - \Sigma_0^{+-} V^{-+}, & -\Sigma_0^{+-} V^{--}, & -\Sigma_0^{+-} V^{-z} \\ -\Sigma_0^{+-} V^{++}, & 1 - \Sigma_0^{+-} V^{+-}, & -\Sigma_0^{+-} V^{+z} \\ -\Sigma_0^{zz} V^{z+}, & -\Sigma_0^{zz} V^{z-}, & 1 - \Sigma_0^{zz} V^{zz} \end{pmatrix} \begin{pmatrix} G^{+-} \\ G^{--} \\ G^{z-} \end{pmatrix} = \begin{pmatrix} \Sigma_0^{+-} \\ 0 \\ 0 \end{pmatrix}. \quad (19)$$

In the paramagnetic phase Green's functions are

$$G^{+-}(i\omega_n, \mathbf{q}) = \frac{\Sigma_0^{+-}}{1 - \Sigma_0^{+-} \frac{K_{\mathbf{q}}}{2}} \quad (20)$$

$$G^{zz}(i\omega_n, \mathbf{q}) = \frac{\Sigma_0^{+-} \Sigma_0^{-+} \Sigma_0^{zz} \frac{K_{\mathbf{q}}^2}{4}}{\left(1 - \Sigma_0^{+-} \frac{K_{\mathbf{q}}}{2}\right) \left(1 - \Sigma_0^{-+} \frac{K_{\mathbf{q}}}{2}\right) (1 - \Sigma_0^{zz} J_{\mathbf{q}})}. \quad (21)$$

We obtain the equations for lines of phase transitions from the instability conditions for susceptibilities and respectively for Green's functions. Namely, from the divergence of $G^{+-}(i\omega_n = 0, \mathbf{q} = 0)$ we get the equation for paramagnetic-spin-flop transition

$$\lambda - K_0 b = 0 \quad (22)$$

and the divergence of $G^{zz}(i\omega_n = 0, \mathbf{q} = \frac{\pi}{a})$ should we take into account that $J_{\mathbf{q}=\frac{\pi}{a}} = -J_0$ gives the equation for paramagnetic-antiferromagnetic transition

$$1 + \beta J_0 b' = 0. \quad (23)$$

They are identical to the equations obtained in the MFA and should be considered together with the set of self-consistency equations (14).

III. DISCUSSION

Below we illustrate some differences in numerical results for the paramagnetic-antiferromagnetic phase transition line irrespective of whether non-ergodic contributions in the set of self-consistency equations (14) are taken into account or not. Here we employ semielliptic density of states for $I_{\mathbf{q}}(K_{\mathbf{q}})$ taken in the model form

$$\frac{1}{N} \sum_{\mathbf{q}} f(I_{\mathbf{q}}) = \int_{-I_0}^{I_0} d\omega \rho(\omega) f(\omega),$$

$$\rho(\omega) = \frac{2}{\pi I_0^2} \sqrt{I_0^2 - \omega^2}. \quad (24)$$

Using equation (23) we can formally express η as a function of h and T

$$\eta = f(h, T). \quad (25)$$

In the paramagnetic phase $\xi = 0$, so we can treat the first equation from the set of self consistency equations (14) as a condition of equality to zero of the function

$$\begin{aligned} \Phi(h, T, \eta) = & \eta - \frac{1}{2} \left(\tanh\left(\frac{\beta\lambda}{2}\right) - \coth\left(\frac{\beta\lambda}{2}\right) \right) \\ & - \frac{1}{N} \sum_{\mathbf{q}} \left(\Lambda^h \coth\left(\frac{\beta\Lambda_{\mathbf{q}}}{2}\right) + C^h \right). \end{aligned} \quad (26)$$

For fixed h , change of sign of $\Phi(h, T, \eta)$ when tabulating over T , corresponds to the temperature of phase transition T^* .

We plot the results on Fig. 2 with solid (2) and dashed-dot (3) curves for cases without and with non-ergodic contribution in the self-consistency equation, respectively. Curve (1) corresponds to the MFA result, when no RPA corrections in the set of self-consistency equations are taken into consideration. Dashed lines, obtained in MFA, separate different phases: paramagnetic (P), antiferromagnetic (A) and spin-flop (S) ones.

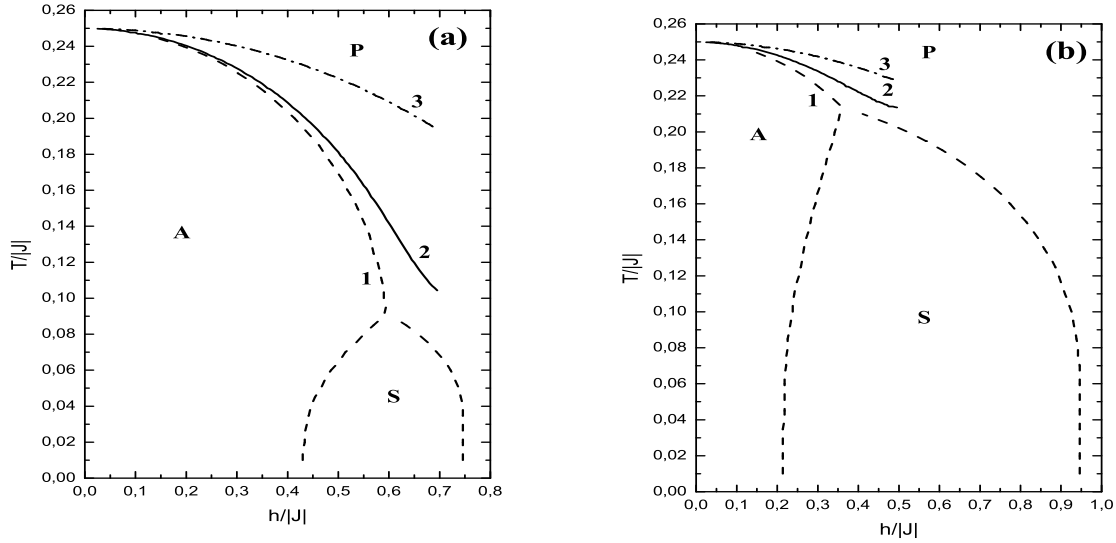


Fig. 2. The (h, T) phase diagram $J < 0$: (a) $\frac{K}{|J|} = 0.5$; (b) $\frac{K}{|J|} = 0.9$.

It is seen that the temperature of A \rightarrow P phase transition is higher due to the non-ergodic contribution. Its influence is stronger in the Ising limit, when K is small, and, vice versa, it weakly affects the phase diagram when approaching the isotropic Heisenberg limit, $K \rightarrow 1$.

CONCLUSIONS

In this paper we propose the self-consistent approach for the description of thermodynamics of the XXZ anisotropic Heisenberg model which allows to take in-

to account the non-ergodic contributions. The approach corresponds to the random phase approximation. In the limit of low temperature it resembles the results of the spin-wave approximation and non-ergodic terms contribute negligibly. One should pay attention to the region of finite temperatures when the phase diagram can be significantly affected. Certainly the method is unsatisfactory in the critical temperature region when the approach of the renorm group to be employed.

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ДОСЛІДЖЕННЯ ФАЗОВОЇ ДІАГРАМИ МОДЕЛІ ЖОРСТКИХ БОЗОНІВ З УРАХУВАННЯМ НЕЕРГОДИЧНИХ ВНЕСКІВ

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Досліджено модель жорстких бозонів, яка є ізоморфною до XXZ анізотропної моделі Гайзенберга, у підході самоузгодженого поля. Отримано вирази для вільної енергії, побудовано системи рівнянь самоузгодження та розраховано псевдоспінові функції Гріна. Використаний метод відповідає наближенню хаотичних фаз з урахуванням неергодичних внесків. Проілюстровано їх вплив на форму фазової діаграми й розташування ліній фазових переходів.