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Pseudospin-electron model in the self-consistent gaussian fluctuation approximation

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Самоузгоджене врахування гаусових флуктуацій в псевдоспін-електронній моделі

І.В.Стасюк, К.В.Табунщик

Анотація. В роботі пропонується аналітична самоузгоджена схема розрахунку термодинамічних і кореляційних функцій в псевдоспін-електронній моделі при відсутності кореляцій. Отримано аналітичні вирази для псевдоспінової кореляційної функції, середнього значення оператора псевдоспіну та термодинамічний потенціал в узагальненому наближенні хаотичних фаз при врахуванні поправок типу середнього поля, що виникають внаслідок ефективної взаємодії псевдоспінів через електрони провідності, а також при врахуванні гаусових флуктуацій середнього поля.

Pseudospin-electron model in the self-consistent gaussian fluctuation approximation

I.V.Stasyuk, K.V.Tabunshchyk

Abstract. An analytical method of the consistent calculation of the thermodynamical and correlation functions of pseudospin-electron model is proposed. Approach is based on the generalized random phase approximation scheme with the self-consistent inclusion of mean field type contributions coming from the effective pseudospin interaction via conducting electrons as well as gaussian fluctuations of the mean field. With the help of the approximation proposed the formulas for the pseudospin correlation function, pseudospin mean value, as well as for the grand canonical potential are obtained.

1. Introduction

Pseudospin-electron model (PEM) was proposed to describe, on the one hand, the strong single–site electron correlation in the spirit of Hubbard model and, on the other hand, the interaction of the conducting electrons with some two level subsystem represented by pseudospins (e.g. anharmonic vibrations of the apex oxygen ions in YBaCuO-type crystals [1], proton-electron interaction in the molecular and crystalline systems with hydrogen bonds [2]). The Hamiltonian of PEM has the following form

$$H = H_0 + \sum_{ij\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma}, \qquad (1)$$

$$H_0 = \sum_i \left\{ U n_{i\uparrow} n_{i\downarrow} - \mu \sum_\sigma n_{i\sigma} + g \sum_\sigma n_{i\sigma} S^z_i - h S^z_i \right\},$$

and includes, besides the terms describing electron transfer ($\sim t_{ij}$), the strong single-site electron correlation U and energy of the subsystem of pseudospins placed in longitudinal field h and interacting with conducting electrons (g-term).

On the basis of PEM a possible connection between the superconductivity and lattice instability of the ferroelectric type in HTSC was discussed [3,4]. The description of the electron spectrum and the electron statistics of the PEM was given in [5] in the framework of the temperature two-time Green's function method in the Hubbard-I approximation. An investigation of dielectric susceptibility of the model was performed in [6,7] within the generalized random phase approximation (GRPA) [14] in the limit $U \to \infty$. The case of absence of the term describing electron transfer ($t_{ij} = 0$) with the inclusion of the direct interaction between pseudospins was considered within the mean field approximation [8,9]. The analysis of ferroelectric type instabilities in the two-sublattice model of the apex oxygen subsystem in high temperature superconducting systems was made [10]. The influence of oxygen nonstoichiometry on localization of apex oxygen in YBaCuO type crystals was studied in the work [11].

From the other point of view, the Hamiltonian of PEM in the $U = 0$ limit (simplified PEM) can be transformed, after some simplification, into the Hamiltonian of the electron subsystem of binary alloy type model as well as the Falicov-Kimball model. The main difference between these models is in the way how an averaging procedure is performed (thermal statistical averaging in the case of PEM and Falicov-Kimball model, configurational averaging for binary alloy) [12,13]. The

Hamiltonian of PEM is, also, invariant with respect to the transformation $\mu \to U - \mu$, $h \to 2g - h$, $n \to 2 - n$, $S^z \to -S^z$. It allows us to use (2) for description of hole-pseudospin system as well.

In the previous papers [15,16] a self-consistent scheme for calculation of mean values of pseudospin and electron number operators, grand canonical potential as well as correlation functions of simplified PEM was proposed. The main idea of the approach was based on the GRPA scheme with the inclusion of the mean field type contributions coming from effective pseudospin interactions via conducting electrons [16]. On the basis of this self-consistent mean field type approximation the energy spectrum, thermodynamics of phase transitions, possibility of phase separations as well as appearance of the chess-board phase were investigated. It was shown that: in the $\mu = \text{const}$ regime (then it is supposed that the electron states of other structure elements, which are not included explicitly into the PEM, play a role of a thermostat, that ensures a constant value of the chemical potential μ) the interaction between the electron and pseudospin subsystems leads to the possibility of either first or second order phase transitions between different uniform phases (bistability) as well as between the uniform and the chess-board ones; in the regime $n = \text{const}$ (this situation is more customary at the consideration of electron systems and it means that the chemical potential is now the function of T, h etc. and depends on the electron concentration) an instability with respect to phase separation in the electron and pseudospin subsystems can take place.

An approach, that takes into account only mean field type contributions, is reasonable only when deviations from the average self-consistent field are small or in other words – in the area where fluctuation's effects are unimportant. Therefore, the method which was proposed previously [15,16] gives the possibilities to obtained an accurate results outside the vicinity of the critical point.

In the vicinity of the critical points the effects of the mean field fluctuations become significant (i.e. fluctuations of mean field increase infinitely near the second order phase transition point). Hence, for the better description of critical properties of our system we must correct the approach by taking into account the contribution of the fluctuations of the self-consistent field of pseudospins.

For this purpose we build the consistent scheme (using the diagram method), for calculation of pseudospin operator mean value, grand canonical potential as well as pseudospin correlation function of simplified PEM, which allows one to takes into account the gaussian fluctuations of the self-consistent mean field. Root–mean–squares (r.m.s.)

gaussian fluctuations of the field are calculated in a self-consistent way. Within the high density expansion method the r.m.s. of gaussian fluctuations of molecular field were applied previously to spin models [17,18]. In the present paper we generalize this scheme on the case of pseudospin-electron model (when, with respect to spin models with direct interaction, we have an effective many–body one between pseudospins via conducting electrons). Proposed here approach can be used, also, to investigate the above mentioned electron models when it is convenient (or possible) to introduce pseudospin operators (i.e. Falicov-Kimball model).

2. Mean field approximation

We perform the calculations in the strong coupling case ($g \gg t$) using single-site states as the basic ones. We rewrite the initial Hamiltonian of the the simplified PEM in the second quantized form using projecting electron annihilation (creation) operators [15,16] $a_{i\sigma} = c_{i\sigma}P_i^+$, $\tilde{a}_{i\sigma} = c_{i\sigma}P_i^-$ ($P_i^{\pm} = \frac{1}{2} \pm S_i^z$) acting at a site with the certain pseudospin orientation:

$$H_0 = \sum_i \{\varepsilon(n_{i\uparrow}+n_{i\downarrow}) + \tilde{\varepsilon}(\tilde{n}_{i\uparrow}+\tilde{n}_{i\downarrow}) - hS_i^z\}, \qquad (2)$$

$$H_{\rm int} = \sum_{ij\sigma} t_{ij}(a_{i\sigma}^+ a_{j\sigma} + a_{i\sigma}^+ \tilde{a}_{j\sigma} + \tilde{a}_{i\sigma}^+ a_{j\sigma} + \tilde{a}_{i\sigma}^+ \tilde{a}_{j\sigma}).$$

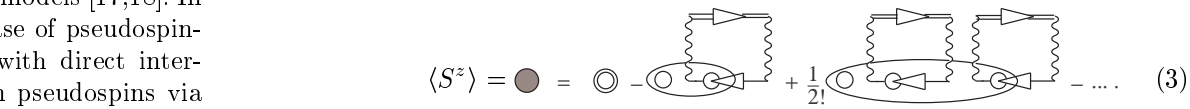
Here $\varepsilon = -\mu + g/2, \quad \tilde{\varepsilon} = -\mu - g/2$ are energies of the single–site states. The introduced operators satisfy the following commutation rules:

$$\{\tilde{a}_{i\sigma}^+, \tilde{a}_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}P_i^-, \quad \{\tilde{a}_{i\sigma}^+, a_{j\sigma'}\} = 0,$$
$$\{a_{i\sigma}^+, a_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}P_i^+, \quad \{a_{i\sigma}^+, \tilde{a}_{j\sigma'}\} = 0.$$

Expansion of the calculated quantities in terms of the electron transfer leads to an infinite series of terms containing the averages of the T-products of the $a_{i\sigma}$, $\tilde{a}_{i\sigma}$ operators. The evaluation of such averages is made using the corresponding Wick's theorem. The results are expressed in terms of the products of the nonperturbed Green's functions and averages of the projection operators $P_i^{\pm}$ which are calculated by means of the semi-invariant expansion [15].

From such an infinite series we are summing up a certain partial sum of diagrams (in the spirit of the traditional mean field approach [15]) characterized by the inclusion of the mean field type contributions (loop fragments) coming from the effective many–body interaction between

pseudospins via conducting electrons in all basic semi-invariants. The corresponding diagram series for pseudospin mean value has the form:

$\langle S^z \rangle =$  $- \ldots .$ (3)

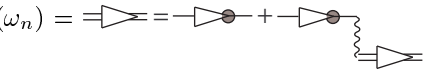
Here we use the following diagram notations: $\bigcirc - S^z$, $\multimap\!\!\circ\!\!\multimap - g_i(\omega_n)$, wavy line is the Fourier transform of hopping $t_{\boldsymbol{k}}$. Basic semi-invariants are represented by ovals and contain the δ-symbols on site indexes:

$$\text{◎} = \langle S^z \rangle_0 = b(h) = \frac{\mathrm{Sp}(S^z \mathrm{e}^{-\beta H_0})}{\mathrm{Sp}(\mathrm{e}^{-\beta H_0})}, \quad \text{⬭} = \langle S^z S^z \rangle_0^c = \frac{\partial b(h)}{\partial \beta h}. \quad (4)$$

Nonperturbated electron Green's function is equal to

$$\multimap\!\!\circ\!\!\multimap = g(\omega_n) = \langle g_i(\omega_n) \rangle, \quad g_i(\omega_n) = \frac{P_i^+}{\mathrm{i}\omega_n - \varepsilon} + \frac{P_i^-}{\mathrm{i}\omega_n - \tilde{\varepsilon}}. \quad (5)$$

Single-electron Green's function is

$G_{\boldsymbol{k}}(\omega_n) =$  $= \left(g^{-1}(\omega_n) - t_{\boldsymbol{k}}\right)^{-1},$ (6)

and determines the spectrum of single-electron excitations. This spectrum was investigated in details in [15].

$$\varepsilon_{\rm I,II}(t_{\boldsymbol{k}}) = \frac{1}{2}(2E_0 + t_{\boldsymbol{k}}) \pm \frac{1}{2}\sqrt{g^2 + 4t_{\boldsymbol{k}}\langle S^z \rangle g + t_{\boldsymbol{k}}^2}\,. \qquad (7)$$

Expression for the loop fragment of diagram has the following form

 $= \dfrac{2}{N}\displaystyle\sum_{n,\boldsymbol{k}} \frac{t_{\boldsymbol{k}}^2}{g^{-1}(\omega_n) - t_{\boldsymbol{k}}} \left(\frac{P_i^+}{\mathrm{i}\omega_n - \varepsilon} + \frac{P_i^-}{\mathrm{i}\omega_n - \tilde{\varepsilon}}\right) = \beta(\alpha_1 P_i^+ + \alpha_2 P_i^-).$

This quantity creates an internal effective self–consistent field acting on the pseudospin. Now, we can introduce the following mean field Hamiltonian:

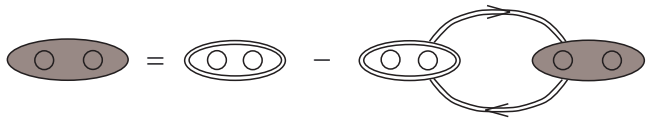
$$H_{\rm MF} = \sum_i \{\varepsilon(n_{i\uparrow}+n_{i\downarrow}) + \tilde{\varepsilon}(\tilde{n}_{i\uparrow}+\tilde{n}_{i\downarrow}) - yS_i^z\}, \qquad (8)$$

where $y = h + \alpha_2 - \alpha_1$ is an effective field.

Summation of the diagram series (3) is equivalent to the averaging with the Hamiltonian (8). The result can be expressed in the form

$$\langle S_l^z \rangle = b(y) = \frac{1}{2} \tanh \left\{ \frac{\beta}{2} y + \ln \frac{1 + \mathrm{e}^{-\beta\varepsilon}}{1 + \mathrm{e}^{-\beta\tilde{\varepsilon}}} \right\}. \tag{9}$$

Diagram equation for the pseudospin correlation functions $\langle S^z S^z \rangle_{\boldsymbol{q}}$ (within the framework of GRPA with the insertion of the mean field type contributions in all zero-order correlators) is following [15]:



(10)

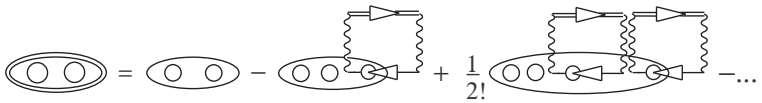
This equation differs from the one for the Ising model in MFA by the replacement of the exchange interaction by the electron loop

which describes an effective many–body interaction between pseudospins via conducting electrons. The corresponding analytical expression is following:

$$\begin{aligned} \boxed{\Pi}_{\boldsymbol{q}} &= \frac{2}{N} \sum_{n,\boldsymbol{k}} t_{\boldsymbol{k}} \left(1 + \frac{t_{\boldsymbol{k}}}{g^{-1}(\omega_n) - t_{\boldsymbol{k}}} \right) \left[\frac{1}{\mathrm{i}\omega_n - \varepsilon} - \frac{1}{\mathrm{i}\omega_n - \tilde{\varepsilon}} \right] \\ &\quad \times t_{\boldsymbol{k}+\boldsymbol{q}} \left(1 + \frac{t_{\boldsymbol{k}+\boldsymbol{q}}}{g^{-1}(\omega_n) - t_{\boldsymbol{k}+\boldsymbol{q}}} \right) \left[\frac{1}{\mathrm{i}\omega_n - \varepsilon} - \frac{1}{\mathrm{i}\omega_n - \tilde{\varepsilon}} \right] \\ &= \frac{2}{N} \sum_{n,\boldsymbol{k}} \Lambda_n^2 \tilde{t}_n(\boldsymbol{k}) \tilde{t}_n(\boldsymbol{k}+\boldsymbol{q}), \end{aligned} \tag{11}$$

$$\text{where} \quad \Lambda_n = \frac{g}{(\mathrm{i}\omega_n + \mu)^2 - g^2/4}, \quad \tilde{t}_n(\boldsymbol{k}) = \frac{t_{\boldsymbol{k}}}{(1 - g_n t_{\boldsymbol{k}})}.$$

The first term in (10) is the second-order semi-invariants renormalized due to the inclusion of 'single-tail' parts, and is thus calculated with the help of H_{MF}:



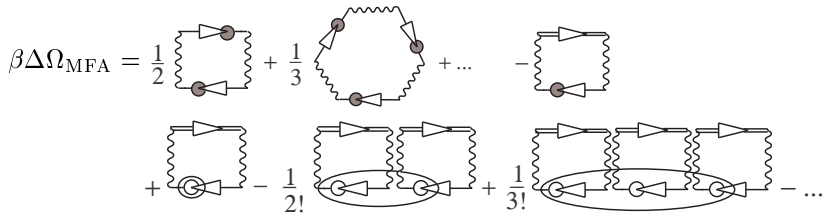
(12)

Finally, the solution of the equation (10) in the analytical form is equal:

$$\langle S^z S^z \rangle_{\boldsymbol{q}} = \frac{1/4 - \langle S^z \rangle^2}{1 + \frac{2}{N} \sum\limits_{n,\boldsymbol{k}} \Lambda_n^2 \tilde{t}_n(\boldsymbol{k}) \tilde{t}_n(\boldsymbol{k}+\boldsymbol{q}) (1/4 - \langle S^z \rangle^2)}, \tag{13}$$

and is different from zero only in a static case ($\omega_n = 0$) (this is due to the fact that pseudospin operator commutes with the Hamiltonian).

In the same approximation the grand canonical potential is [15]:



(14)

The corresponding analytical expression has the following form:

$$\begin{aligned} \Omega_{\mathrm{MFA}} = &- \frac{2}{N\beta} \sum_{n,\boldsymbol{k}} \ln(1 - t_{\boldsymbol{k}} g(\omega_n)) - \frac{2}{N\beta} \sum_{n,\boldsymbol{k}} \frac{g(\omega_n) t_{\boldsymbol{k}}^2}{g^{-1}(\omega_n)) - t_{\boldsymbol{k}}} \\ &- \frac{1}{\beta} \ln \mathrm{Sp}(\mathrm{e}^{-\beta H_{\mathrm{MF}}}). \end{aligned} \tag{15}$$

All quantities can be derived from the grand canonical potential by

$$\frac{\mathrm{d}\Omega_{\mathrm{MFA}}}{\mathrm{d}(-h)} = \langle S^z \rangle, \quad \frac{\mathrm{d}\langle S^z \rangle}{\mathrm{d}(\beta h)} = \langle S^z S^z \rangle_{\boldsymbol{q}=0}, \tag{16}$$

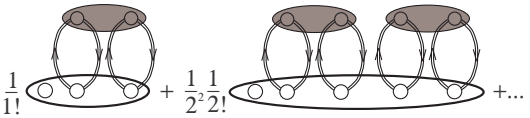
that shows the thermodynamical consistence of the proposed approximations [15].

3. Self–consistent gaussian fluctuation approximation

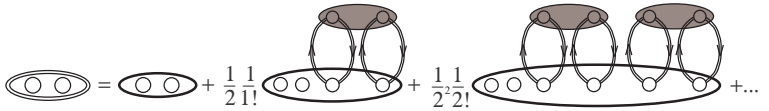
In constructing a higher order approximation, we use MFA as the zero–order one. This means that all 'single-tail' parts of diagrams are already summed over and all semi-invariant is carried out over distribution with the Hamiltonian H_{MF} (8). We represent this graphically by thick ovals:

(17)

As a simplest approximation that goes beyond of the MFA we use the approach that takes into account the so-called 'double-tail' diagrams (which was applied in [18] where the magnetization of the ordinary Ising model was considered). The diagram series for the pseudospin mean value calculated within the approach which include 'double-tail' diagrams is:

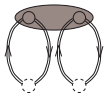
$\langle S^z \rangle =$  $+ \ldots$ (18)

The diagram equation for pseudospin correlator $\langle S^z S^z \rangle_{\boldsymbol{q}}$ within the developed here approximation is given by (10), but now zero-order correlators are renormalized, also, due to the 'double-tail' parts, and thus the corresponding diagram series is:

$\Xi =$  (19)

The contribution, which correspond to the 'double-tail' fragment of diagram, can be written in the following analytical form (using the introduced notation (11)):

$$X = \quad (20)$$



$$= \frac{2^2}{N^3} \sum_{n,n'} \sum_{\boldsymbol{k},\boldsymbol{k}'} \sum_{\boldsymbol{q}} \Lambda_n^2 \tilde{t}_n(\boldsymbol{k}) \tilde{t}_n(\boldsymbol{k}-\boldsymbol{q}) \langle S^z S^z \rangle_{\boldsymbol{q}} \Lambda_{n'}^2 \tilde{t}_{n'}(\boldsymbol{k}') \tilde{t}_{n'}(\boldsymbol{k}'+\boldsymbol{q}),$$

here $$\langle S^z S^z \rangle_{\boldsymbol{q}} = \frac{\Xi}{1 + \frac{2}{N} \sum\limits_{n,\boldsymbol{k}} \Lambda_n^2 \tilde{t}_n(\boldsymbol{k}) \tilde{t}_n(\boldsymbol{k}+\boldsymbol{q}) \Xi}, \quad (21)$$

Since the pseudospin correlator (21) is the frequency independent, in the expression (20) we have two independent sums over internal Matsubara frequencies that allows one (using decomposition into simple fractions) to sum over all internal frequencies:

$$\frac{2}{N} \sum_{n,\boldsymbol{k},\boldsymbol{k}'} \Lambda_n^2 \tilde{t}_n(\boldsymbol{k}) \tilde{t}_n(\boldsymbol{k}') = \frac{2\beta}{N} \sum_{\boldsymbol{k},\boldsymbol{k}'} \frac{t_{\boldsymbol{k}} t_{\boldsymbol{k}'} (\varepsilon - \tilde{\varepsilon})^2}{[\varepsilon_{\rm I}(t_{\boldsymbol{k}}) - \varepsilon_{\rm II}(t_{\boldsymbol{k}})][\varepsilon_{\rm I}(t_{\boldsymbol{k}'}) - \varepsilon_{\rm II}(t_{\boldsymbol{k}'})]} \quad (22)$$

$$\times \left\{ \frac{n[\varepsilon_{\rm I}(t_{\boldsymbol{k}})] - n[\varepsilon_{\rm I}(t_{\boldsymbol{k}'})]}{\varepsilon_{\rm I}(t_{\boldsymbol{k}}) - \varepsilon_{\rm I}(t_{\boldsymbol{k}'})} + \frac{n[\varepsilon_{\rm II}(t_{\boldsymbol{k}})] - n[\varepsilon_{\rm II}(t_{\boldsymbol{k}'})]}{\varepsilon_{\rm II}(t_{\boldsymbol{k}}) - \varepsilon_{\rm II}(t_{\boldsymbol{k}'})} \right.$$

$$\left. - \frac{n[\varepsilon_{\rm I}(t_{\boldsymbol{k}})] - n[\varepsilon_{\rm II}(t_{\boldsymbol{k}'})]}{\varepsilon_{\rm I}(t_{\boldsymbol{k}}) - \varepsilon_{\rm II}(t_{\boldsymbol{k}'})} - \frac{n[\varepsilon_{\rm II}(t_{\boldsymbol{k}})] - n[\varepsilon_{\rm I}(t_{\boldsymbol{k}'})]}{\varepsilon_{\rm II}(t_{\boldsymbol{k}}) - \varepsilon_{\rm I}(t_{\boldsymbol{k}'})} \right\}.$$

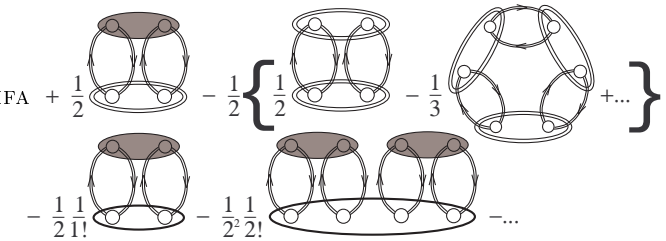
Here $n(\varepsilon) = \dfrac{1}{1 + \mathrm{e}^{\beta\varepsilon}}$ is a Fermi distribution.

Let us now return to the problem of summation of the diagram series (18) and (19). By means of procedure described in [18], and using the introduced here notations (9), (20) we can write:

$$\begin{aligned} \langle S^z \rangle &= b(y) + \frac{1}{1!} b(y)^{[2]} \frac{X}{2} + \frac{1}{2!} b(y)^{[4]} \left(\frac{X}{2}\right)^2 + \frac{1}{3!} b(y)^{[6]} \left(\frac{X}{2}\right)^3 + \cdots \\ &= \frac{1}{\sqrt{2\pi X}} \int\limits_{-\infty}^{+\infty} \exp\left(-\frac{\xi^2}{2X}\right) b(y+\xi) \mathrm{d}\xi, \quad (23) \\ \Xi &= b(y)^{[1]} + \frac{1}{1!} b(y)^{[3]} \frac{X}{2} + \frac{1}{2!} b(y)^{[5]} \left(\frac{X}{2}\right)^2 + \frac{1}{3!} b(y)^{[7]} \left(\frac{X}{2}\right)^3 + \cdots \\ &= \frac{1}{X\sqrt{2\pi X}} \int\limits_{-\infty}^{+\infty} \exp\left(-\frac{\xi^2}{2X}\right) \xi b(y+\xi) \mathrm{d}\xi. \quad (24) \end{aligned}$$

Therefore, the contribution of diagram series with 'double-tail' parts corresponds to the average with the Gaussian distribution where X can be interpreted as the root–mean–squares (r.m.s.) fluctuation of the mean field around the mean value of y. And, thus we obtain a self-consistent set of equations (23), (20) for pseudospin mean value and r.m.s. of gaussian fluctuations of the mean field.

The diagram series for the grand canonical potential within the approximation accepted here is:

$\beta\Delta\Omega = \beta\Delta\Omega_{\rm MFA}$  (25)

The grand canonical potential written in this form satisfies the stationary conditions:

$$\frac{\mathrm{d}\Omega}{\mathrm{d}\langle S^z \rangle} = 0, \quad \frac{\mathrm{d}\Omega}{\mathrm{d}X} = 0, \quad (26)$$

which are equivalent to the equations (23), (20) (see the Appendix). The consistency of the approximation made for the pseudospin mean value, pseudospin correlation function and grand canonical potential can be checked explicitly using the relations:

$$\frac{\mathrm{d}\Omega}{\mathrm{d}(-h)} = \langle S^z \rangle, \quad \frac{\mathrm{d}\langle S^z \rangle}{\mathrm{d}(-h\beta)}\Big|_{X=\mathrm{const}} = \langle S^z S^z \rangle_{\boldsymbol{q}=0}. \tag{27}$$

In the limit of vanishing fluctuations our results go over into the ones obtained within the mean field approximation.

In the analytical form the first term in the diagram series for the grand canonical potential (25) is equal to

$$\frac{1}{2}\Xi X = \frac{1}{2}\frac{1}{\sqrt{2\pi X}} \int\limits_{-\infty}^{+\infty} \exp\left(-\frac{\xi^2}{2X}\right) \xi b(y+\xi)\mathrm{d}\xi. \tag{28}$$

The bracketed diagram series can be presented as following:

$$-\frac{1}{2}\left\{\frac{1}{2}\Xi^2\left(\frac{2}{N}\sum_{n,\boldsymbol{k}}\Lambda_n^2\tilde{t}_n(\boldsymbol{k})^2\right)^2 - \frac{1}{3}\Xi^3\left(\frac{2}{N}\sum_{n,\boldsymbol{k}}\Lambda_n^2\tilde{t}_n(\boldsymbol{k})^2\right)^3 + \cdots\right\}$$
$$= -\frac{1}{2}\left\{\Xi\frac{2}{N}\sum_{n,\boldsymbol{k}}\Lambda_n^2\tilde{t}_n(\boldsymbol{k})^2 - \ln\left(1+\Xi\frac{2}{N}\sum_{n,\boldsymbol{k}}\Lambda_n^2\tilde{t}_n(\boldsymbol{k})^2\right)\right\}. \tag{29}$$

The remainder of the diagram in the series (25) can be written as

$$-\left\{b(y)^{[1]}X + \frac{1}{2!}b(y)^{[3]}\left(\frac{X}{2}\right)^2 + \frac{1}{3!}b(y)^{[5]}\left(\frac{X}{2}\right)^3 + \cdots\right\}$$
$$= -\int\limits_0^X \mathrm{d}t\frac{1}{2}\left\{b(y)^{[1]} + \frac{1}{1!}b(y)^{[3]}\frac{t}{2} + \frac{1}{2!}b(y)^{[5]}\left(\frac{t}{2}\right)^2 + \cdots\right\}$$
$$= -\int\limits_0^X \mathrm{d}t\frac{1}{2t\sqrt{2\pi t}} \int\limits_{-\infty}^{+\infty} \exp\left(-\frac{\xi^2}{2t}\right)\xi b(y+\xi)\mathrm{d}\xi$$
$$= -\frac{1}{2}\int\limits_{-\infty}^{+\infty}\left\{1-\mathrm{erf}\left(\frac{|\xi|}{\sqrt{2X}}\right)\right\}\mathrm{sign}(\xi)b(y+\xi)\mathrm{d}\xi, \tag{30}$$

where we use the relation (24) and definition of the erf function. Finally the diagram series for grand canonical potential Ω can be written in the following analytical form:

$$\Omega = \Omega_{MFA} + \frac{1}{2}\frac{1}{\sqrt{2\pi X}} \int\limits_{-\infty}^{+\infty} \exp\left(-\frac{\xi^2}{2X}\right)\xi b(y+\xi)\mathrm{d}\xi$$
$$-\frac{1}{2}\Xi\frac{2}{N}\sum_{n,\boldsymbol{k}}\Lambda_n^2\tilde{t}_n(\boldsymbol{k})^2 + \frac{1}{2}\ln\left(1+\Xi\frac{2}{N}\sum_{n,\boldsymbol{k}}\Lambda_n^2\tilde{t}_n(\boldsymbol{k})^2\right)$$
$$-\frac{1}{2}\int\limits_{-\infty}^{+\infty}\left\{1-\mathrm{erf}\left(\frac{|\xi|}{\sqrt{2X}}\right)\right\}\mathrm{sign}(\xi)b(y+\xi)\mathrm{d}\xi. \tag{31}$$

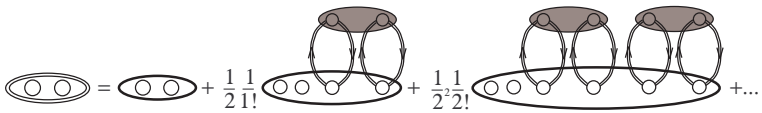
To sum over the Matsubara frequency, the relation (22) must be used in the limit of $\boldsymbol{k}' \to \boldsymbol{k}$.

4. Conclusion

The consistent method, which takes into account the corrections due to the gaussian fluctuation of self–consistent field, for calculation of thermodynamic and correlation functions is presented. The diagram series and corresponding formulas for the pseudospin mean value $\langle S^z \rangle$, pseudospin correlation function $\langle S^z S^z \rangle_{\boldsymbol{q}}$ as well as for the grand canonical potential Ω are obtained. The possibility exists to investigate their behaviour under changes of thermodynamical and model parameters. The parameter X (20) (r.m.s. fluctuation of the mean field) is calculated by means of the self–consistent renormalization of the correlation function (10), (19). From the expression for the grand canonical potential, calculated within the presented here scheme, the equations for $\langle S^z \rangle$ and X parameters satisfying the stationary conditions (26) are obtained.

This approach can be applied for the investigation of phase separation phenomena as well as the transition into a modulated phase in PEM. This question will be the subject of our following work.

It should be noted that the analytical scheme presented in our paper can be easily reduced to the other similar approach (which was successfully used in the case of spin models [19,20]) where the renormalization (18) is performed with the use of the simplest possible pseudospin correlation function which involves gaussian fluctuations of the mean field:



(32)

Within the framework of this approximation grand canonical potential satisfies the stationary conditions (26) and can be written as:

$$\Omega = \Omega_{MFA} + \frac{1}{4}\Xi X - \frac{1}{2}\int\limits_{-\infty}^{+\infty}\left\{1 - \mathrm{erf}\left(\frac{|\xi|}{\sqrt{2X}}\right)\right\}\mathrm{sign}(\xi)b(y+\xi)\mathrm{d}\xi, \quad (33)$$

$$\text{where} \quad X = \Xi\left(\frac{2}{N}\sum_{\boldsymbol{q},n}\Lambda_n^2\tilde{t}_n^2(\boldsymbol{k})\right)^2. \quad (34)$$

This method is more suitable for the numerical calculation then one presented above, but takes into account the narrow class of diagrams.

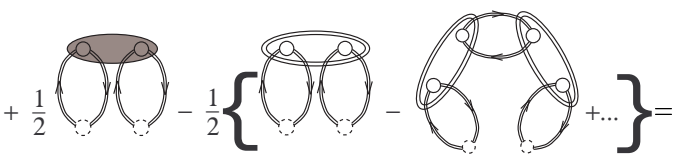
Appendix

Here we would like to prove that the grand canonical potential satisfies the stationary conditions (26) as well as consistency conditions (27).

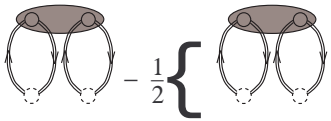
Let us consider the derivative of the grand canonical potential with respect to the pseudospin mean value (18):

$$\frac{\mathrm{d}\Delta\Omega}{\mathrm{d}\langle S^z\rangle} = \frac{\partial\Delta\Omega}{\partial\langle S^z\rangle} + \frac{\partial\Delta\Omega}{\partial\Xi}\frac{\mathrm{d}\Xi}{\mathrm{d}\langle S^z\rangle} + \frac{\partial\Delta\Omega}{\partial X}\frac{\mathrm{d}X}{\mathrm{d}\langle S^z\rangle}, \quad (35)$$

$\beta\dfrac{\partial\Delta\Omega}{\partial\Xi}$ =

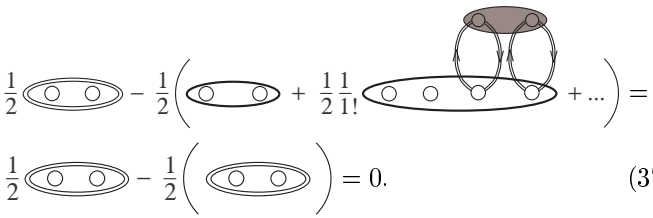


$$= + \frac{1}{2}$$



$$= 0, \quad (36)$$

$\beta\dfrac{\partial\Delta\Omega}{\partial X}$ =

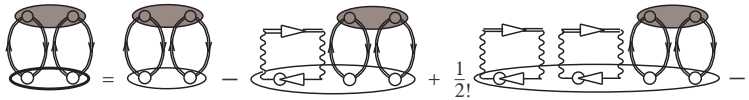


$$= + \frac{1}{2}$$

$$= 0. \quad (37)$$

Here we use the definition (10), (19) respectively.

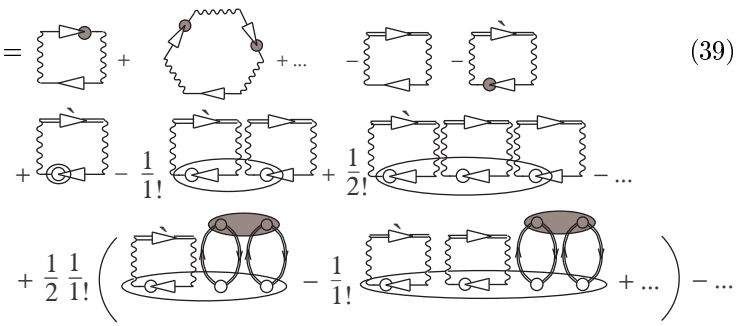
Thick ovals (17) take into account all 'single-tail' parts of diagrams:



(38)

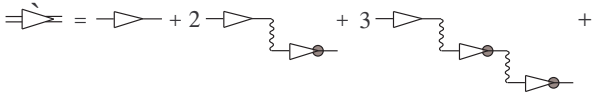
Thus, from the diagram series on grand canonical potential we have:

$\beta\dfrac{\partial\Delta\Omega}{\partial\langle S^z\rangle}$ =



(39)

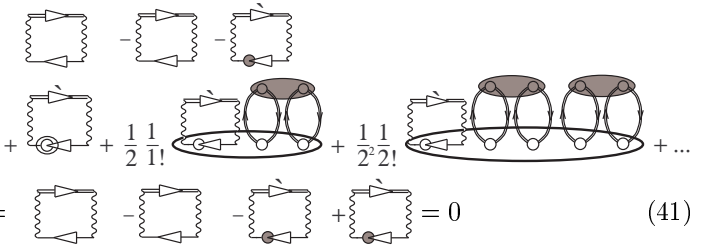
where the following shortened notation are introduced:



(40)

Using the diagram expression for the Green's function and expression for the mean value of pseudospin (18) we can write:

$\beta\dfrac{\partial\Delta\Omega}{\partial\langle S^z\rangle}$ =



(41)

In the same way we can prove that $\mathrm{d}\Delta\Omega/\mathrm{d}X = 0$

Therefore, we have the following conditions:

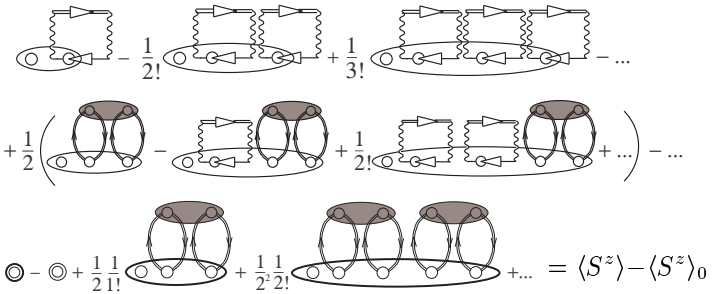
$$\frac{\mathrm{d}\Delta\Omega}{\mathrm{d}X} = \frac{\partial\Delta\Omega}{\partial X} = 0, \quad \frac{\mathrm{d}\Delta\Omega}{\mathrm{d}\langle S^z\rangle} = \frac{\partial\Delta\Omega}{\partial\langle S^z\rangle} = 0. \quad (42)$$

Using them we can check the consistency of the approximation used in the calculation of the pseudospin mean value (18) and grand canonical

potential:

$$\frac{\mathrm{d}\Delta\Omega}{\mathrm{d}(-h)} = \frac{\partial\Delta\Omega}{\partial(-h)} + \frac{\partial\Delta\Omega}{\partial\langle S^z\rangle}\frac{\mathrm{d}\langle S^z\rangle}{\mathrm{d}(-h)} + \frac{\partial\Delta\Omega}{\partial X}\frac{\mathrm{d}X}{\mathrm{d}(-h)} = \frac{\partial\Delta\Omega}{\partial(-h)} \qquad (43)$$

$$\frac{\partial\Delta\Omega}{\partial(-h)} =$$



$$= \langle S^z\rangle - \langle S^z\rangle_0$$

Here we use the definition of semi-invariants (4).

In the same way we can prove that $\left.\frac{\mathrm{d}\langle S^z\rangle}{\mathrm{d}(-h\beta)}\right|_{X=\mathrm{const}} = \langle S^z S^z\rangle_{\boldsymbol{q}=0}$.

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