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Модель Бозе-Хаббарда в границі жорстких бозонів: вихід за рамки наближення середнього поля

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I.V.Stasyuk, T.S.Mysakovych

HARD-CORE BOSE-HUBBARD MODEL BEYOND MEAN FIELD APPROXIMATION

ЛЬВІВ

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Модель Бозе-Хаббарда в границі жорстких бозонів: вихід за рамки наближення середнього поля

І.В.Стасюк, Т.С.Мисакович

Анотація. У цій роботі розвинуто аналітичний підхід, що дозволяє досліджувати фазові переходи в моделі Бозе-Хаббарда в границі жорстких бозонів виходячи за рамки наближення середнього поля. Виконано розклад по степенях параметра бозонного перескоку та отримано рівняння для бозонної концентрації. Побудовано фазову діаграму та виконано порівняння отриманих результатів із наближенням середнього поля.

Hard-core Bose-Hubbard model beyond mean field approximation

I.V.Stasyuk, T.S.Mysakovych

Abstract. In this work we develop the approach which allows us to investigate the phase transitions in the hard-core Bose-Hubbard model beyond the mean-field approximation. We perform the expansion in powers of the boson hopping parameter and obtain the equation for the boson concentration. We build phase diagram and compare our results with the results of the mean field approximation.

1. Introduction

Both boson atoms and mixtures of boson and fermion atoms (e.g., ^{6}Li-^{7}Li, ^{40}K- ^{87}Rb, ^{6}Li- ^{87}Rb atoms) in optical lattices are intensively investigated in last 10 years. Such systems can be described by the Bose-Hubbard or Bose-Fermi-Hubbard model and different theoretical approaches have been used to study these models [1–11]. The existence of Mott insulator and superfluid phases and transition between them were observed experimentally [12]. The bosonic kinetic energy term is usually considered in the mean-field approximation (MFA). When the kinetic energy dominates the ground state of the system is superfluid (SF). There are also many generalizations of the Bose-Hubbard and Bose-Fermi-Hubbard models, for example, extended models with long-range direct intersite interaction between particles [13], models on superlattices [14–17], two-state Bose-Hubbard models [18], inhomogeneous version of the model [4, 19].

Besides optical lattices the Bose-Hubbard and Bose-Fermi-Hubbard-type models can also be applied for the description of intercalation of ions in crystals (for example, lithium intercalation in TiO_2 crystals). It is known that in such systems Li is almost fully ionized once intercalated and reconstruction of electron spectrum at intercalation takes place [20–22], thus ion-electron interaction can play a significant role.

In our previous work [23] we calculated bosonic Green's function $G_{\boldsymbol{q}}(\omega_n)$ in the random phase approximation (RPA) using the formalism of the Hubbard operators and investigated phase transitions at finite temperature. The divergence of $G_{\boldsymbol{q}=0}(\omega_n = 0)$ was the condition of the transition to the superfluid phase, this condition coincides with the one obtained in the mean field approximation at the calculation of the thermodynamical potential of the system. In this work we want to develope the approximation which allows us to investigate transition to the superfluid phase in the Bose-Hubbard model (we consider a particular case of hard-core bosons) beyond the mean filed approximation.

2. Method and results

The Hamiltonian of the hard-core Bose Hubbard model can be written in the following form

$$\begin{aligned} H &= H_0 + H_{\rm int}, \\ H_{\rm int} &= -\sum_{ij} J_{ij} S_i^+ S_j^-, \quad H_0 = -\sum_i h S_i^z. \end{aligned} \tag{2.1}$$

Here we use the pseudospin formalism and the bosonic occupation number n can be written as $n = S^z + 1/2$; J term in Eq. (2.1) is responsible for nearest neighbour boson hopping. The bosonic chemical potential h is introduced to control the number of bosons. It should be noted that the term $H_{\rm int}$ is often treated in the mean field approximation.

In this paper calculating the bosonic Green's function in the normal, so-called Mott-insulator (MI), phase we want to go beyond the mean field approximation and for this purpose we develope the following approach.

At the calculation of average pseudospin value $\langle S^z\rangle$ we perform an expansion in powers of $H_{\rm int}$:

$$\exp(-\beta H) = \exp(-\beta H_0)\sigma(\beta), \tag{2.2}$$

$$\sigma(\beta) = T_\tau \exp\left(-\int_0^\beta H_{\rm int}(\tau)d\tau\right), \tag{2.3}$$

$$\langle S^z\rangle = \langle S^z\sigma(\beta)\rangle_0^c, \tag{2.4}$$

where T_τ is the imaginary time ordering operator and $\beta = 1/T$ is the inverse temperature. The averaging $\langle ...\rangle_0^c$ is performed over the H_0 Hamiltonian and we take into account connected diagrams.

We take into account diagrams shown in Fig. 1; taking as skeleton the diagrams which formally correspond to the first order of our expansion in powers of $H_{\rm int}$. It should be noted that such expansion also can be obtained when we calculate the thermodynamical potential of the system in the random phase approximation and the derivative of this potential over the chemical potential h gives us the value of $(-\langle S^z\rangle)$. We use the diagrammatic technique based on Wick's theorem for the spin operators [24]. To calculate the remaining product of the diagonal S^z operators we perform the semi-invariant expansion. Here we have introduced the unperturbed bosonic Green's function (thin solid line with arrow in diagram shown in Fig. 1) $\langle T_\tau S_i^+(\tau)S_j^-\rangle_0 = -2\langle S^z\rangle K_0(\tau)_{ij}$,

$$K(\boldsymbol{q},\omega_n) = \frac{1}{N}\sum_{ij} e^{i\boldsymbol{q}\boldsymbol{R}_{ij}}\int_0^\beta d\tau e^{i\omega_n\tau}K_{ij}(\tau),$$

$$K_0(\boldsymbol{q},\omega_n) = \frac{1}{i\omega_n - h}, \tag{2.5}$$

with imaginary discrete Matsubara frequency $i\omega_n = i2n\pi T$ ($n = 0, \pm 1, ...$). The bosonic Green's function in random phase approximation (thick solid line with arrow in diagram shown in Fig. 1) is equal

$$K_{\rm RPA}(\boldsymbol{q},\omega_n) = \frac{1}{i\omega_n - h + \langle S^z\rangle J_{\boldsymbol{q}}}. \tag{2.6}$$

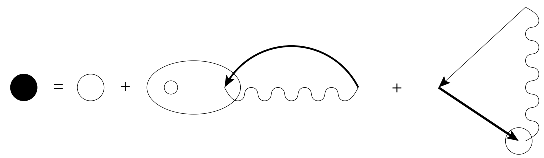

Figure 1. Diagrams for average value of the pseudospin $\langle S^z\rangle$ (it is presented by the dark filled circle). Thick solid line with arrow denotes Green's function in random phase approximation, thin solid line with arrow denotes unperturbed Green's function. Wavy lines indicate the Fourier transform of the boson hopping parameter, unfilled circles and ovals denote the average value of $\langle S^z\rangle_0$ and semi-invariants, respectively.

In this approximation we take into account chain-like diagrams at the calculation of the correlator

$$\langle T_\tau S_m^+(\tau)S_n^-\rangle = \langle T_\tau S_m^+(\tau)S_n^-\sigma(\beta)\rangle_0^c = -2\langle S^z\rangle K_{\rm RPA}(\tau)_{mn}$$
$$= \langle T_\tau S_m^+(\tau)S_n^-\rangle_0$$
$$+\frac{1}{2}\sum_{ij} J_{ij}\int_0^\beta d\tau_1\langle T_\tau S_m^+(\tau)S_n^- S_i^+(\tau_1)S_j^-(\tau_1)\rangle_0^c + \ldots, \tag{2.7}$$

such as the diagram (5) in Figure 2. It should be noted that diagrammatic technique allows us to take into account non ergodic terms which are missed if one uses equation of motion method, see [11], [25]. Semi-invariant in the zero approximation is written as $\langle T_\tau S^z(\tau)S^z\rangle_0 = \langle S^z\rangle_0^2 + M(\tau)$, $M(\omega_n) = \beta\delta_{\omega_n,0}(\frac{1}{4} - \langle S^z\rangle_0^2)$, and $\langle S^z\rangle_0 = \frac{1}{2}\tanh(\frac{\beta h}{2})$. In Figure 2 we show the skeleton diagrams which originate from the first order of the mentioned above expansion at the calculation of the correlator $\langle T_\tau S^+(\tau)S^-\rangle$. The diagram (5) in this figure corresponds to the random phase approximation.

The diagrams (1) and (2) in Figure 2 correspond to the renormalization of the pseudospin mean value (see Fig. 1). In this work we do not take into account the diagrams of (3) and (4) types in Figure 2.

In analytical form we have the following expression for the average value of $\langle S^z\rangle$:

$$\langle S^z\rangle = \frac{1}{2}\tanh\left(\frac{\beta h}{2}\right) - \Phi\beta\left(\frac{1}{4} - \langle S^z\rangle_0^2\right)$$
$$-\frac{1}{2}\sum_{\boldsymbol{q}}\left[\coth\left(\beta\frac{E_{\boldsymbol{q}}}{2}\right) - \coth\left(\beta\frac{h}{2}\right)\right], \tag{2.8}$$

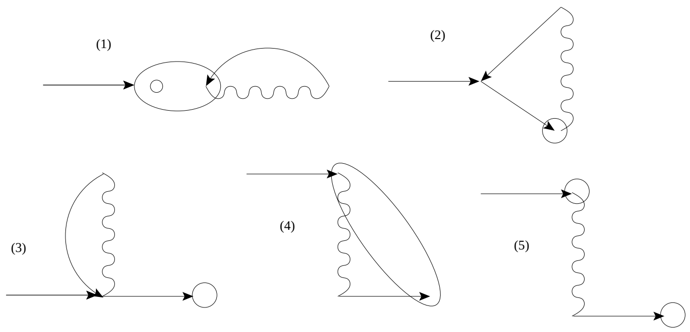

Figure 2. First order diagrams for the correlator $\langle T_\tau S^+(\tau)S^-\rangle$. The diagram notation is the same as in Fig. 1.

$$\Phi = \frac{1}{\beta N}\sum_{\omega_n \boldsymbol{q}} J(\boldsymbol{q})K_{\mathrm{RPA}}(\boldsymbol{q},\omega_n)e^{-i\omega_n(+0)} = -\frac{1}{2}\sum_{\boldsymbol{q}} J_{\boldsymbol{q}}\coth\left(\frac{\beta E_{\boldsymbol{q}}}{2}\right). \qquad (2.9)$$

Here $E_{\boldsymbol{q}} = h - J_{\boldsymbol{q}}\frac{1}{2}\tanh(\frac{\beta h}{2})$ is the bosonic energy in the random phase approximation (as it can be seen at the calculation we used the expression for the Green's function (2.6) in RPA but we consider the case when the average $\langle S^z\rangle$ in (2.6) is calculated using the Hamiltonian H_0).

To investigate the transition to the superfluid phase we take into account that mean value $\langle S^z\rangle = h/J_0$ corresponds to the MFA transition to the superfluid phase (it follows from the condition $E_0 = 0$) and this allows us to investigate corrections to the mean field approximation (when we put $\langle S^z\rangle = h/J_0$ in the left side of the expression (2.8) then we obtain equation for the h at the fixed temperature, the first term in right-hand side of the equation (2.8) corresponds to the MFA). At $h \to 0$ (symmetrical case, which corresponds to the upper point of the phase-transition curve for the hard-core boson case) we obtain the following equation

$$\frac{1}{J_0} = \frac{\beta}{4} - \sum_{\boldsymbol{q}}\frac{\beta^3 J_{\boldsymbol{q}}^2}{192} - \frac{\beta^2}{16}\sum_{\boldsymbol{q}}\frac{J_{\boldsymbol{q}}}{1-\frac{\beta J_{\boldsymbol{q}}}{4}}. \qquad (2.10)$$

The first term in the right-hand side of the equation (2.10) corresponds to the mean field approximation, and the second and third terms take into account corrections in the developed here approximations.

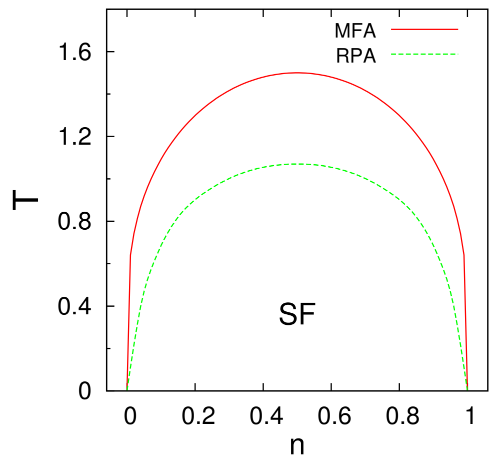

Figure 3. Phase diagram in the $T-n$ plane. Lines of the transition from the normal to the superfluid phase are shown in the mean field approximation and developed here random phase approximation for calculation of the pseudospin average value.

Now we make some numerical estimations to check the validity of our approximation. We consider three-dimensional case and perform direct summation over lattice sites at the calculation of the transition temperature using the equation (2.8). In Fig. 3, we plot the lines of phase transition from the normal to superfluid (SF) phase in the mean field approximation as well as in the developed here approximation in the plane temperature T-bosonic concentration ($n = S^z + 1/2$ and $S^z = h/J_0$ on the phase transition line), in our numerical calculations we take $J_0 = 6$ for the case of the cubic lattice as it was done in [26] to make comparison between our calculations and the results of Monte-Carlo studies [26]. The upper point of the transition to the superfluid phase (in the hard-core boson limit it is symmetrical case, $n = 0$) in our aproximation $T^c \approx 1.07$ agrees well with $T^c_{\mathrm{MC}} \approx 0.97 \pm 0.04$ obtained in [26]. As we can see from Fig. 3, the results of the mean field approximation are only qualitative ($T^c_{\mathrm{MFA}} \approx 1.5$) and can not be applied for quantitative analysis.

In conclusion, we have developed an analytical method which allows us to go beyond the mean field approximation at the investigation of the transition from the normal to superfluid phase in the Bose-Hubbard model at finite temperature. This method gives good quantitative agreement with numerical Monte-Carlo calculations and can be used to investigate in more details the thermodynamics of the Bose-Hubbard model.

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