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Двостанова модель Бозе-Хаббарда в границі жорстких бозонів

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TWO-STATE BOSE-HUBBARD MODEL IN THE HARD-CORE BOSON LIMIT

ЛЬВІВ

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Двостанова модель Бозе-Хаббарда в границі жорстких бозонів

І.В.Стасюк, О.В.Величко

Анотація. Проведено дослідження переходу у фазу з бозе-конденсатом (БК-фазу) у гратковому бозе-газі у випадку, коли квантові перескоки частинок відбуваються між збудженими локальними станами. В основу покладено модель Бозе-Хаббарда (яка застосовується у теорії оптичних граток з ультрахолодними атомами та іонних провідників, а також при описі квантової делокалізації адсорбованих частинок) у границі жорстких бозонів. Показано, що рід фазового переходу може змінюватися з другого на перший, залежно від значень енергії збудження, хімічного потенціалу частинок та температури. Встановлено умови, при яких відбувається розшарування на нормальну та БК фази.

Two-state Bose-Hubbard model in the hard-core boson limit

I.V.Stasyuk, O.V.Velychko

Abstract. Appearance of the Bose-Einstein condensate (BEC) in the lattice Bose gas is investigated for the case of particle quantum hopping between the local excited states. The present study is performed on the basis of the Bose-Hubbard model (widely used in the theory of optical lattices with ultracold atoms and ionic conductors as well as for description of quantum delocalization of adsorbed particles) in the hard-core boson limit. It has been proved that the order of the phase transition can change from the second to the first one depending on values of the excitation energy, the particle chemical potential and temperature. Conditions of the phase separation into normal and BEC phases have been also established.

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1. Introduction

During the recent years Bose-Hubbard model (BHM) is proved to be a valuable tool in the theory of systems of strongly correlated particles. The model achieves a wide recognition due to a successful description of thermodynamics and dynamics of ultracold Bose atoms in optical lattices where a phase transition to the phase with the Bose-Einstein (BE) condensate (so called Mott insulator (MI) – superfluid state (SF) transition) occurs at very low temperatures. Experimental evidences of BE condensation in optical lattices were found for the first time in works [1,2] while theoretical predictions of such an effect were given earlier [3]. Starting from the 90-ies of the past century a series of papers was devoted to the theory of this phenomenon. Among the first key articles on the subject one should mention the work [4] where BHM was studied in the mean field approximation. Calculated thereat phase diagrams demonstrate that in the simplest case (hopping of Bose particles in the presence of a single-site Hubbard repulsion) the MI-SF transition is of the second order. Therewith it is supposed that particles reside in the ground state of local potential wells in the lattice. Forthcoming theoretical investigations in this field were performed with the use of various techniques, e.g. the random phase approximation (RPA) in the Green function method [5,6], a strong-coupling perturbation theory [7,8], the dynamical mean field theory (Bose-DMFT) [9,10] as well as quantum Monte-Carlo calculations [11,12] and other numerical methods.

The Bose-Hubbard model is also intensively used for a theoretical description of a wide range of phenomena: quantum delocalization of hydrogen atoms adsorbed on the surface of transition metals [13, 14], quantum diffusion of light particles on the surface or in the bulk [15,16], thermodynamics of the impurity ion intercalation into semiconductors [17,18].

In the last mentioned applications, there is usually a restriction on the position occupation number ($n_i \leqslant 1$), what for the considered model corresponds to the limit of an infinite Hubbard repulsion. Such a model of hard-core ions (where particles are described by the Pauli statistics) is known also as the fundamental one for investigation of a wide range of problems, e.g. superconductivity due to a local electron pairing [19] or ionic hopping in ionic (superionic) conductors [20, 21].

Study of a quantum delocalization or diffusion reveals an important role of excited vibrational states of particles (ions) in localized (interstitial) positions with a much higher probability of ion hopping between them [15, 22, 23]. A similar issue of a possible BE condensation in the

excited bands in optical lattices is also considered but the condition of their sufficient occupation due to the optical pumping (see, e.g. [24]) is imposed. An orbital degeneration of the excited p-state is accompanied by anisotropy of hopping parameters and results in the appearance of variously polarized bands in the one-particle spectrum. Such bands correspond by convention to different sorts (so called "flavours") of bosons and their number correlates with the lattice dimensionality. In the framework of the necessary generalization of the Bose-Hubbard model a possibility of the MI-SF transition to the phase with BE condensate in the pumping-induced quasi-equilibrium long-living state of the system has been established [25].

In the equilibrium case, the issue of BE condensation involving the excited states in the framework of ordinary Bose-Hubbard model was not considered in practice. The exception is the system of spin-1 bosons [26, 27] where a hyperfine splitting gives rise to multiplets of local states resulting in closely-spaced excited levels. As demonstrated in [28, 29], the MI-SF phase transition could be of the first order when a single-site spin interaction is of the "antiferromagnetic" type. A similar change of the phase transition order takes place also for multicomponent Bose systems in the optical lattices [30].

In the present work we consider an equilibrium thermodynamics of the Bose-Hubbard model taking into account only one nondegenerated excited state on the lattice site besides the ground one. On the one hand, such a model corresponds to 1D or strongly anisotropic (quasi-1D) optical lattice, and on the other, it is close to situation that is characteristic of system of light particles adsorbed on the metal surface. For example, excited states of hydrogen atoms on the Ni(111) surface are sufficiently distant [22] so only the lowest one could be taken into account. We shall investigate a condition of instability of a normal state of the Bose system with respect to BE condensation considering a criterion of divergence of the susceptibility ($\chi \sim \langle\langle c_l | c_p^+ \rangle\rangle_\omega |_{q=0,\omega=0}$) characterizing the system response with respect to the field related to a spontaneous creation or annihilation of particles. We shall also study the behaviour of the order parameter $\langle c_0 \rangle$ ($\langle c_0^+ \rangle$) as well as the grand canonical potential in the region of the MI-SF transition and shall build relevant phase diagrams. Special attention will be given to a change of the phase transition order and localization of tricritical points at different values of excitation energy, particle hopping parameter and temperature.

We shall limit ourselves to the hard-core boson (HCB) limit where a limitation on occupation numbers is present: no more than one particle per site regardless of state (excited or ground) which it occupies. Thus

the single-site problem is a three-level one (contrary to the two-level ordinary HCB case). For this reason, it is convenient to use the formalism of Hubbard operators [31] (standard basis operators [32]).

2. Two-state Bose-Hubbard model in RPA: normal phase

The Bose-Hubbard model is used for description of the system of Bose particles which are located in a periodic field and can reside in lattice sites. Taking into account only the ground and the first excited vibrational levels in the potential well on the site one can express the model Hamiltonian as:

$$\begin{aligned}\hat{H} = {} & (\varepsilon - \mu) \sum_i b_i^+ b_i + (\varepsilon' - \mu) \sum_i c_i^+ c_i + U_{bc} \sum_i n_i^b n_i^c \\ & + \frac{U_b}{2} \sum_i n_i^b (n_i^b - 1) + \frac{U_c}{2} \sum_i n_i^c (n_i^c - 1) \\ & + \sum_{ij} t_{ij}^b b_i^+ b_j + \sum_{ij} t_{ij}^c c_i^+ c_j + \sum_{ij} t_{ij}^{bc} (b_i^+ c_j + c_i^+ b_j), \end{aligned} \tag{2.1}$$

where b_i and b_i^+ (c_i and c_i^+) are Bose operators of annihilation and creation of particles in the ground (excited) state, ε and ε' are respective energies of state and μ is the chemical potential of particles. Such a Hamiltonian includes the single-site Hubbard repulsions with energies U_b, U_c and U_{bc} as well as the particle hopping between ground (t^b), excited (t^c) and different (t^{bc}) states. Hereinafter we assume $U_b = U_c = U_{bc}$ for simplicity.

Let us define a single-site basis $|n_i^b, n_i^c\rangle \equiv |i; n_i^b, n_i^c\rangle$ (which is formed by particle occupation numbers in the ground and the excited states, i.e. eigenvalues of operators $n_i^b = b_i^+ b_i$ and $n_i^c = c_i^+ c_i$) as well as introduce Hubbard operators (standard basis operators)

$$X_i^{n,m;n',m'} \equiv |i; n, m\rangle\langle i; n', m'|. \tag{2.2}$$

Annihilation and creation Bose operators may be written as

$$\begin{aligned} b_i &= \sum_n \sum_m \sqrt{n+1}\, X_i^{n,m;n+1,m}, \quad b_i^+ = \sum_n \sum_m \sqrt{n+1}\, X_i^{n+1,m;n,m}; \\ c_i &= \sum_n \sum_m \sqrt{m+1}\, X_i^{n,m;n,m+1}, \quad c_i^+ = \sum_n \sum_m \sqrt{m+1}\, X_i^{n,m+1;n,m}. \end{aligned} \tag{2.3}$$

Corresponding occupation numbers look as follows

$$n_i^b = \sum_n \sum_m n X_i^{n,m;n,m}, \qquad n_i^c = \sum_n \sum_m m X_i^{n,m;n,m}, \tag{2.4}$$

where summation indices $n, m = 0, \ldots, \infty$ in both (2.3) and (2.4) formulae.

In the X-operator representation the single-site part of Hamiltonian (2.1) can be written as

$$\hat{H}_0 = \sum_i \sum_n \sum_m \lambda_{nm} X_i^{n,m;n,m}, \tag{2.5}$$

where

$$\lambda_{nm} = n(\varepsilon - \mu) + m(\varepsilon' - \mu) + \frac{U}{2}(n+m)(n+m-1). \tag{2.6}$$

Terms describing an inter-site transfer in Hamiltonian (2.1) are transformed in the similar way.

Our primary goal is to calculate the two-time temperature boson Green's functions $\langle\langle b|b^+\rangle\rangle$ and $\langle\langle c|c^+\rangle\rangle$, which describe an excitation spectrum and give a possibility to investigate the conditions of the system instability with respect to the spontaneous symmetry breaking and the appearance of a BE condensate. As follows from definitions (2.3)

$$\begin{aligned}
\langle\langle b_l|b_p^+\rangle\rangle_\omega &= \sum_{nm}\sum_{rs} \sqrt{n+1}\,\sqrt{r+1}\,\langle\langle X_l^{n,m;n+1,m}|X_p^{r+1,s;r,s}\rangle\rangle_\omega\,, \\
\langle\langle c_l|c_p^+\rangle\rangle_\omega &= \sum_{nm}\sum_{rs} \sqrt{m+1}\,\sqrt{s+1}\,\langle\langle X_l^{n,m;n,m+1}|X_p^{r,s+1;r,s}\rangle\rangle_\omega\,.
\end{aligned} \tag{2.7}$$

We will use the equation-of-motion method for the evaluation of X-operator Green's functions. For the first one from relations (2.7) one could write

$$\begin{aligned}
\hbar\omega\langle\langle X_l^{n,m;n+1,m}|X_p^{r+1,s;r,s}\rangle\rangle_\omega = \frac{\hbar}{2\pi}\langle X_l^{n,m;n,m} - X_l^{n+1,m;n+1,m}\rangle\delta_{lp}\delta_{nr}\delta_{ms} \\
+ \langle\langle [X_l^{n,m;n+1,m}, \hat{H}]|X_p^{r+1,s;r,s}\rangle\rangle_\omega\,.
\end{aligned} \tag{2.8}$$

Let us write the commutators

$$[X_l^{n,m;n+1,m}, \hat{H}_0] = (\lambda_{n+1,m} - \lambda_{n,m}) X_l^{n,m;n+1,m}, \tag{2.9}$$

$$[X_l^{n,m;n+1,m}, b_i^+] = \delta_{li}\sqrt{n+1}\left(X_l^{n,m;n,m} - X_l^{n+1,m;n+1,m}\right), \tag{2.10a}$$

$$[X_l^{n,m;n+1,m}, b_i] = \delta_{li}\left(\sqrt{n+2}\,X_l^{n,m;n+2,m} - \sqrt{n}\,X_l^{n-1,m;n+1,m}\right), \tag{2.10b}$$

$$[X_l^{n,m;n+1,m}, c_i^+] = \delta_{li}\left(\sqrt{m}\,X_l^{n,m;n+1,m-1} - \sqrt{m+1}\,X_l^{n,m+1;n+1,m}\right), \tag{2.10c}$$

$$[X_l^{n,m;n+1,m}, c_i] = \delta_{li}\left(\sqrt{m+1}\,X_l^{n,m;n+1,m+1} - \sqrt{m}\,X_l^{n,m-1;n+1,m}\right). \tag{2.10d}$$

The latter are originated from the commutation of an initial X-operator with the inter-site transfer terms of the Hamiltonian thus producing the higher-order Green's functions

$$\langle\langle X_l^{\cdots} b_j|X_p^{r+1,s;r,s}\rangle\rangle_\omega\,, \quad \langle\langle X_l^{\cdots} b_j^+|X_p^{r+1,s;r,s}\rangle\rangle_\omega\,, \ldots, \tag{2.11}$$

where $X_l^{\cdots}$ stands for operators on the right-hand side of expressions (2.10a)–(2.10d).

Decoupling of functions (2.11) in the random phase approximation (RPA) is performed in the following way

$$\langle\langle X_l^{\cdots} b_j|X_p^{r+1,s;r,s}\rangle\rangle_\omega \approx \langle X_l^{\cdots}\rangle\langle\langle b_j|X_p^{r+1,s;r,s}\rangle\rangle_\omega + \langle b_j\rangle\langle\langle X_l^{\cdots}|X_p^{r+1,s;r,s}\rangle\rangle_\omega\,. \tag{2.12}$$

In the case of the normal phase (which will be studied here) $\langle b_j\rangle = \langle b_j^+\rangle = 0$. Thus, retaining only the averages $\langle X_l^{\cdots}\rangle$ of diagonal X-operators we have

$$\begin{aligned}
[X_l^{n,m;n+1,m}, \hat{H}] \approx \Delta_{nm} X_l^{n,m;n+1,m} \\
+ \sqrt{n+1}\,Q_{nm}\sum_j t_{lj} b_j + \sqrt{n+1}\,Q_{nm}\sum_j t''_{lj} c_j
\end{aligned} \tag{2.13}$$

and equation (2.8) can be rewritten as

$$\begin{aligned}
\langle\langle X_l^{n,m;n+1,m}|X_p^{r+1,s;r,s}\rangle\rangle_\omega = \frac{\hbar}{2\pi}\delta_{lp}\delta_{nr}\delta_{ms}\frac{Q_{nm}}{\hbar\omega - \Delta_{nm}} \\
+ \frac{\sqrt{n+1}\,Q_{nm}}{\hbar\omega - \Delta_{nm}}\sum_j t_{lj}\langle\langle b_j|X_p^{r+1,s;r,s}\rangle\rangle_\omega \\
+ \frac{\sqrt{n+1}\,Q_{nm}}{\hbar\omega - \Delta_{nm}}\sum_j t''_{lj}\langle\langle c_j|X_p^{r+1,s;r,s}\rangle\rangle_\omega\,.
\end{aligned} \tag{2.14}$$

The following notations are introduced

$$Q_{nm} = \langle X_l^{n,m;n,m} - X_l^{n+1,m;n+1,m} \rangle, \qquad \Delta_{nm} = \lambda_{n+1,m} - \lambda_{n,m}\,, \quad (2.15)$$

for the occupation difference of adjacent levels and the related transition energies when the number of Bose particles in the ground state (with the energy ε) on the site increases by one.

Going from X-operators in equation (2.14) to the Bose operators b and b^+ according to definition (2.3) we obtain

$$\langle\langle b_l|b_p^+\rangle\rangle_\omega = \frac{\hbar}{2\pi}\delta_{lp} g_0(\omega) + g_0(\omega)\biggl(\sum_j t_{lj}\langle\langle b_j|b_p^+\rangle\rangle_\omega + \sum_j t''_{lj}\langle\langle c_j|b_p^+\rangle\rangle_\omega\biggr), \quad (2.16)$$

where the function

$$g_0(\omega) = \sum_{nm}\frac{Q_{nm}}{\hbar\omega - \Delta_{nm}}(n+1) \quad (2.17)$$

has a meaning of the unperturbed Green's function for bosons residing in the single-site ground state.

Equations of motion for "mixed" Green's functions $\langle\langle c|b^+\rangle\rangle$ are obtained in the way similar to the described above scheme. Using decoupling (2.12) one can write

$$[X_l^{n,m;n,m+1}, \hat{H}] \approx \Delta'_{nm} X_l^{n,m;n,m+1} + \sqrt{m+1}\,Q'_{nm}\sum_j t''_{lj} b_j + \sqrt{m+1}\,Q'_{nm}\sum_j t'_{lj} c_j\,, \quad (2.18)$$

what results in the equation

$$\langle\langle c_l|b_p^+\rangle\rangle_\omega = g'_0(\omega)\biggl(\sum_j t''_{lj}\langle\langle b_j|b_p^+\rangle\rangle_\omega + \sum_j t'_{lj}\langle\langle c_j|b_p^+\rangle\rangle_\omega\biggr). \quad (2.19)$$

Here, similarly to (2.15) and (2.17)

$$Q'_{nm} = \langle X_l^{n,m;n,m} - X_l^{n,m+1;n,m+1}\rangle, \qquad \Delta'_{nm} = \lambda_{n,m+1} - \lambda_{n,m}\,,$$
$$g'_0(\omega) = \sum_{nm}\frac{Q'_{nm}}{\hbar\omega - \Delta'_{nm}}(m+1), \quad (2.20)$$

and the function $g'_0(\omega)$ is the unperturbed Green's function for bosons residing in the excited state.

By means of the Fourier transform

$$\langle\langle b_l|b_p^+\rangle\rangle_\omega = \frac{1}{N}\sum_q \mathrm{e}^{\mathbf{i}\mathbf{q}(\mathbf{R}_l - \mathbf{R}_p)}\langle\langle b|b^+\rangle\rangle_{q,\omega}\,, \quad (2.21)$$

one can pass to the momentum representation obtaining a system of equations

$$\begin{aligned}\langle\langle b|b^+\rangle\rangle_{q,\omega} &= \frac{\hbar}{2\pi}g_0(\omega) + g_0(\omega)t_q\langle\langle b|b^+\rangle\rangle_{q,\omega} + g_0(\omega)t''_q\langle\langle c|b^+\rangle\rangle_{q,\omega}\,,\\ \langle\langle c|b^+\rangle\rangle_{q,\omega} &= g'_0(\omega)t''_q\langle\langle b|b^+\rangle\rangle_{q,\omega} + g'_0(\omega)t'_q\langle\langle c|b^+\rangle\rangle_{q,\omega}\,, \end{aligned} \quad (2.22)$$

where t_q, t'_q and t''_q stand for the Fourier transforms of hopping parameters.

A pair of equations for other Green's functions are obtained in a similar way

$$\begin{aligned}\langle\langle b|c^+\rangle\rangle_{q,\omega} &= g_0(\omega)t_q\langle\langle b|c^+\rangle\rangle_{q,\omega} + g_0(\omega)t''_q\langle\langle c|c^+\rangle\rangle_{q,\omega}\,,\\ \langle\langle c|c^+\rangle\rangle_{q,\omega} &= \frac{\hbar}{2\pi}g'_0(\omega) + g'_0(\omega)t''_q\langle\langle b|c^+\rangle\rangle_{q,\omega} + g'_0(\omega)t'_q\langle\langle c|c^+\rangle\rangle_{q,\omega}\,. \end{aligned} \quad (2.23)$$

Solutions of equations (2.22) and (2.23) look like

$$\begin{aligned}\langle\langle b|b^+\rangle\rangle_{q,\omega} &= \frac{\hbar}{2\pi}\frac{1}{D_q(\omega)}g_0(\omega)(1 - g'_0(\omega)t'_q),\\ \langle\langle c|c^+\rangle\rangle_{q,\omega} &= \frac{\hbar}{2\pi}\frac{1}{D_q(\omega)}g'_0(\omega)(1 - g'_0(\omega)t_q),\\ \langle\langle c|b^+\rangle\rangle_{q,\omega} &= \frac{\hbar}{2\pi}\frac{1}{D_q(\omega)}g_0(\omega)g'_0(\omega)t''_q = \langle\langle b|c^+\rangle\rangle_{q,\omega}\,, \end{aligned} \quad (2.24)$$

where

$$D_q(\omega) = 1 - g_0(\omega)t_q - g'_0(\omega)t'_q + g_0(\omega)g'_0(\omega)\left[t_q t'_q - (t''_q)^2\right]. \quad (2.25)$$

The equation $D_q(\omega) = 0$ gives the excitation spectrum which is obtained here in the RPA. On the other hand, the divergence of boson Green's functions (2.24) at the zero values of wave vector and frequency is a criterion of instability with respect to BE condensation [5, 33] thus giving the following condition

$$D_{q=0}(\omega = 0) = 0, \quad (2.26)$$

which can be rewritten in the explicit form

$$1 - g_0(\omega)t_q - g_0'(\omega)t_q' + g_0(\omega)g_0'(\omega)\left[t_q t_q' - (t_q'')^2\right] = 0, \qquad (2.27)$$

where

$$g_0(0) = -\sum_{nm} \frac{Q_{nm}}{(n+m)U - \mu}(n+1),$$
$$g_0'(0) = -\sum_{nm} \frac{Q'_{nm}}{(n+m)U + \delta - \mu}(m+1), \qquad (2.28)$$

and $\delta = \varepsilon' - \varepsilon$ is the excitation energy.

We should point out that divergence of the $\langle\langle b|b^+\rangle\rangle_{0,0}$ function correlates with appearance of the BE condensate in the ground state while at the divergence of the $\langle\langle c|c^+\rangle\rangle_{0,0}$ function BE condensation takes place in the excited state. In general, both condensates appear simultaneously except the case $t_q'' = 0$ (e.g. due to symmetry reasons) when these effects become independent and only the one type of condensate arises in the instability point.

Equation (2.27), relating mutually the chemical potential, hopping parameters and temperature, allows to construct spinodal surfaces (or lines) in the mentioned above coordinates and to find the temperature of the phase transition to the phase with BE condensate (so called SF phase) when such a transition is of the second order. Below, this problem (especially the issue of the phase transition order) will be investigated in more details.

3. NO phase instability in HCB limit

Let us consider now a simple special case of the HCB limit when occupation numbers in the $|n, m\rangle$ state are restricted by a condition $n + m \leqslant 1$. In the framework of the model it formally means $U \to \infty$.

In this case the model becomes a three-level one with the local energies

$$\lambda_{00} = 0, \qquad \lambda_{01} = \delta - \mu, \qquad \lambda_{10} = -\mu \qquad (3.1)$$

and the following transition energies

$$\Delta_{00} = -\mu, \qquad \Delta'_{00} = \delta - \mu. \qquad (3.2)$$

Thus, equation (2.27) can be rewritten in the form

$$1 - \frac{Q_{00}}{\mu}t_0 - \frac{Q'_{00}}{\mu - \delta}t_0' + \frac{Q_{00}Q'_{00}}{\mu(\mu - \delta)}\left[t_0 t_0' - (t_0'')^2\right] = 0, \qquad (3.3)$$

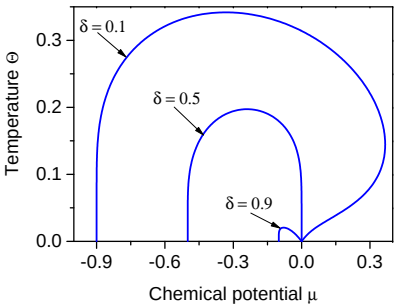


Figure 1. Lines of the NO phase instability (spinodals) with respect to the appearance of BE condensate in the (Θ, μ) plane in the HCB limit at various excitation energies ($t_0 = 0$, $|t_0'| = 1$, $t_0'' = 0$).

where

$$Q_{00} = \frac{1 - \mathrm{e}^{\beta\mu}}{1 + \mathrm{e}^{\beta\mu} + \mathrm{e}^{\beta(\mu-\delta)}},$$
$$Q'_{00} = \frac{1 - \mathrm{e}^{\beta(\mu-\delta)}}{1 + \mathrm{e}^{\beta\mu} + \mathrm{e}^{\beta(\mu-\delta)}} \qquad (3.4)$$

in the zero approximation with respect to hopping.

We take into account (according to estimations made in [15, 25]) that boson wave functions in adjacent potential wells overlap in greater extent in the excited states compared to the ground ones. Accordingly, we shall put here $t_0 = 0$. For a centrosymmetric lattice and in the case of different parity of wave functions of ground and excited states we have also $t_0'' = 0$. Finally, we follow a usual convention of the BH model for optical lattices taking $t_0' < 0$. In this way equation (3.3) can be reduced to

$$\frac{|t_0'|}{\delta - \mu}\frac{1 - \mathrm{e}^{\beta(\mu-\delta)}}{1 + \mathrm{e}^{\beta\mu} + \mathrm{e}^{\beta(\mu-\delta)}} = 1. \qquad (3.5)$$

Its solutions determine the stability region boundaries of the normal (NO) phase. Respective lines of spinodals are numerically calculated and presented in figure 1 (here and below the energy quantities are given in units of $|t_0'|$).

As illustrated in figure 1, at $\delta < |t_0'|$ spinodals surround an asymmetric area in the (Θ, μ) plane which is located between the points $\mu = \delta - |t_0'|$ and $\mu = 0$ of the abscissa axis. In this region the NO phase is unstable; it is connected with an appearance of BE condensate. At $\delta < |t_0'|/2$ and $\mu > 0$ the backward path of spinodal is observed and a lower temperature of the NO phase instability appears, thus suggesting a possibility of the SF phase existence in the intermediate temperature range (so called "re-entrant transition"). However, as will be shown further, in the mentioned region a real thermodynamic behaviour is even more complicated. The order of the NO-SF transition can change to the first one and the SF-phase remains stable up to the zero temperature.

4. Phase diagrams in MFA

For a more detailed treatment of the NO-SF transition issue let us study thermodynamics of the considered system in the HCB limit thus reducing the problem to a three-state model with the Hamiltonian

$$\hat{H} = \sum_{ip} \lambda_p X_i^{pp} + \sum_{ij} t_{ij} X_i^{10} X_j^{01} + \sum_{ij} t'_{ij} X_i^{20} X_j^{02} + \sum_{ij} t''_{ij} (X_i^{10} X_j^{02} + X_i^{20} X_j^{01}), \tag{4.1}$$

where the shorthand notations are used

$$|0\rangle \equiv |00\rangle,\ |1\rangle \equiv |10\rangle,\ |2\rangle \equiv |01\rangle; \qquad \lambda_0 = \lambda_{00},\ \lambda_1 = \lambda_{10},\ \lambda_2 = \lambda_{01}\,. \tag{4.2}$$

Possibility of BE condensation will be studied in the MFA. Average values of creation (annihilation) operators for Bose particles in the ground or excited local state

$$\eta = \langle X_i^{10} \rangle = \langle X_i^{01} \rangle\ (\equiv \langle b_i \rangle), \qquad \xi = \langle X_i^{20} \rangle = \langle X_i^{02} \rangle\ (\equiv \langle c_i \rangle) \tag{4.3}$$

play the roles of order parameters for the SF-phase. Hence the mean-field Hamiltonian looks like

$$\hat{H}_{\rm MF} = -N(t_0\eta^2 + t'_0\xi^2 + 2t''_0\eta\xi) + \sum_{ip} \lambda_p X_i^{pp} + \sum_i \big[t_0\eta(X_i^{10} + X_i^{01}) + t'_0\xi(X_i^{20} + X_i^{02}) + t''_0\xi(X_i^{10} + X_i^{01}) + t''_0\eta(X_i^{20} + X_i^{02})\big]\,. \tag{4.4}$$

Self-consistency equations for parameters η and ξ

$$\eta = Z^{-1}\,{\rm Sp}(X_i^{10}\exp(-\beta\hat{H}_{\rm MF})), \quad \xi = Z^{-1}\,{\rm Sp}(X_i^{20}\exp(-\beta\hat{H}_{\rm MF})) \tag{4.5}$$

are equivalent to the condition of minimum of the grand canonical potential $\Omega = -\Theta \ln Z$, where $Z = {\rm Sp}\exp(-\beta\hat{H}_{\rm MF})$.

Limiting our consideration to the case of particle hopping only through excited states ($t'_0 \neq 0$, $t_0 = t''_0 = 0$) we can diagonalize Hamiltonian (4.4) by a rotation transformation

$$\begin{pmatrix} |0\rangle \\ |1\rangle \\ |2\rangle \end{pmatrix} = \begin{pmatrix} \cos\vartheta & 0 & -\sin\vartheta \\ 0 & 1 & 0 \\ \sin\vartheta & 0 & \cos\vartheta \end{pmatrix} \begin{pmatrix} |\tilde{0}\rangle \\ |\tilde{1}\rangle \\ |\tilde{2}\rangle \end{pmatrix}, \tag{4.6}$$

where

$$\cos 2\vartheta = \frac{\lambda_2 - \lambda_0}{\sqrt{(\lambda_2 - \lambda_0)^2 + 4(t'_0\xi)^2}}, \qquad \sin 2\vartheta = \frac{2|t'_0|\xi}{\sqrt{(\lambda_2 - \lambda_0)^2 + 4(t'_0\xi)^2}} \tag{4.7}$$

and $\lambda_2 - \lambda_0 = \delta - \mu$. In terms of operators $\widetilde{X}^{rs} = |\tilde{r}\rangle\langle\tilde{s}|$

$$\hat{H}_{\rm MF} = N|t'_0|\xi^2 + \sum_{ip} \tilde{\lambda}_p \widetilde{X}_i^{pp}. \tag{4.8}$$

New energies of single-site states are

$$\tilde{\lambda}_{0,2} = \frac{\delta - \mu}{2} \mp \sqrt{\left(\frac{\delta - \mu}{2}\right)^2 + (t'_0\xi)^2}, \qquad \tilde{\lambda}_1 = -\mu. \tag{4.9}$$

In the new basis

$$X_i^{02} + X_i^{20} = -(\widetilde{X}_i^{22} - \widetilde{X}_i^{00})\sin 2\vartheta + (\widetilde{X}_i^{20} - \widetilde{X}_i^{02})\cos 2\vartheta, \tag{4.10}$$

what gives after averaging

$$\xi = \frac{1}{2}\langle \widetilde{X}^{00} - \widetilde{X}^{22} \rangle \sin 2\vartheta. \tag{4.11}$$

Taking into account that $\langle \widetilde{X}^{pp} \rangle = Z^{-1}\exp(-\beta\tilde{\lambda}_p)$, $Z = \sum_p \exp(-\beta\tilde{\lambda}_p)$ we come to the equation for the order parameter ξ:

$$\xi = \frac{1}{Z} \frac{|t'_0|\xi}{\sqrt{(\delta - \mu)^2 + 4(t'_0\xi)^2}} \left(\mathrm{e}^{-\beta\tilde{\lambda}_0} - \mathrm{e}^{-\beta\tilde{\lambda}_2}\right). \tag{4.12}$$

Solution $\xi = 0$ corresponds to the NO phase. A nonzero solution describing the BE condensate is obtained from the equation

$$\frac{1}{Z} \frac{|t'_0|}{\sqrt{(\delta - \mu)^2 + 4(t'_0\xi)^2}} \left(\mathrm{e}^{-\beta\tilde{\lambda}_0} - \mathrm{e}^{-\beta\tilde{\lambda}_2}\right) = 1. \tag{4.13}$$

In the limit $\xi \to 0$ this equation determines the line where the order parameter for the SF phase tends to zero. One can readily see that it coincides with spinodal equation (3.5) thus defining the line of the second order NO-SF phase transition (when just the transition of such an order takes place).

Numerical solutions of equation (4.13) allow to study the behavior of the order parameter ξ depending on chemical potential μ at various temperatures as illustrated in figure 2. In the main, at negative values of chemical potential the parameter ξ changes smoothly and the phase transition to the SF phase is of the second order. But at $\mu \gtrsim 0$ and low enough temperatures the $\xi(\mu)$ dependence has an S-like bend. In this case the first order phase transition with an abrupt change of the parameter ξ takes place. This phase transition occurs at a certain value of the chemical potential which could be calculated using the Maxwell rule or considering the minimum of the grand canonical potential $\Omega(\mu)$ as function of the chemical potential (see below). Obviously, the point of ξ nullification does not correspond here to the phase transition anymore.

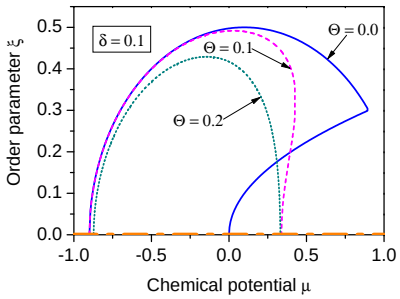


Figure 2. Dependences of the order parameter ξ on the chemical potential μ for the reduced three-level (HCB) model at various temperatures indicating the possibility of the first order phase transition at low enough temperatures ($\delta = 0.1$, $|t_0'| = 1$).

Similar behaviour of the parameter ξ holds even at zero excitation energy ($\delta = 0$) where the first order phase transition remains for nonzero temperatures whereas at $T = 0$ its order changes to the second one

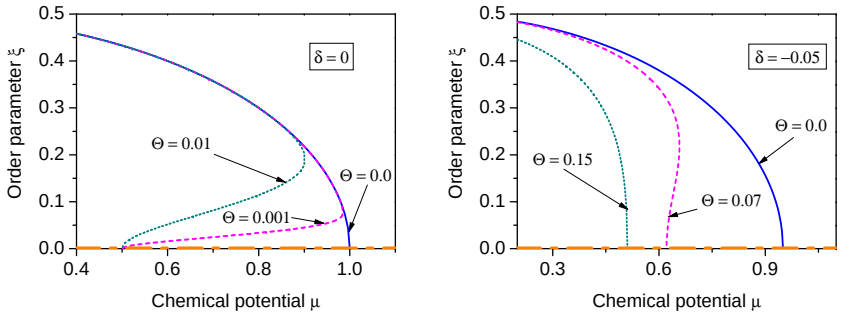


Figure 3. Low-temperature behaviour of the order parameter ξ for the reduced three-level (HCB) model at zero and negative excitation energies δ and various temperatures ($|t_0'| = 1$).

(figure 3). At negative values of δ (what corresponds to inversion of ε and ε' levels and to hopping between ground states) the second order of the transition preserves in the low-temperature region close to $T = 0$ transforming to the first order one at the temperature increase and recovering henceforth (figure 3).

Changes of the NO-SF phase transition order and localization of the corresponding tricritical points are depicted in figure 4, where phase diagrams are given for various values of the excitation energy δ. At temperatures lower than the tricritical one, spinodal lines and phase transition curves come apart as one can see comparing figures 1 and 4. At small values of δ the discrepancy is quite significant (figure 5). In the case of $\delta < 0$ two critical points appear at a certain distance; the latter tends to zero at $\delta = \delta_{\rm crit} \approx -0.12|t_0'|$ and the first order phase transitions at the further increase of δ (figure 6) is suppressed.

Phase diagrams in the $(|t_0'|, \mu)$ plane at various temperatures for $\delta > 0$ are depicted in figure 7 with indication of tricritical points. In distinction to the standard two-level HCB model [34] (where the SF phase transition is of the second order) the diagrams are asymmetric. In the limit $T \to 0$ for $\mu > 0$ the first order transition occurs at $\mu = (\sqrt{\delta} - \sqrt{|t_0'|})^2$ (see the next section) whereas for $\mu < 0$ they are of the second order on the line $\mu = \delta - |t_0'|$.

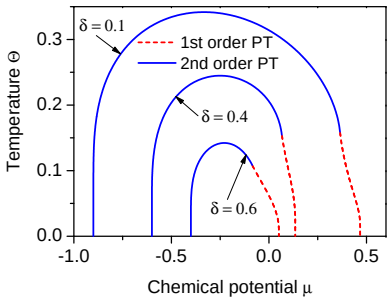


Figure 4. Lines of the NO-SF phase transition in the (Θ, μ) plane at various excitation energies δ ($|t_0'| = 1$).

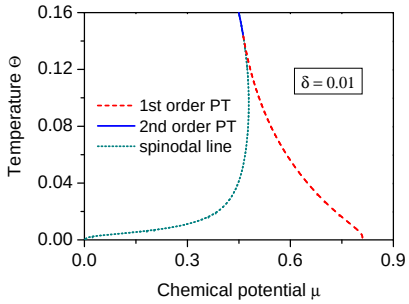


Figure 5. An illustration of discrepancy between the spinodal curve and the real line of the first order phase transition for $\delta = 0.01$ ($|t_0'| = 1$).

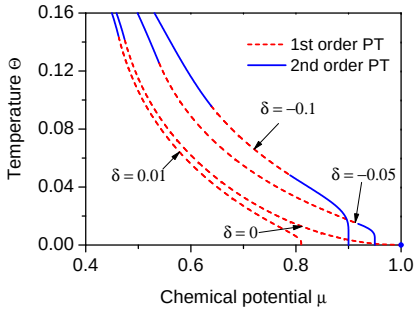


Figure 6. Appearance of two tricritical points at zero and negative values of excitation energy δ ($|t_0'| = 1$).

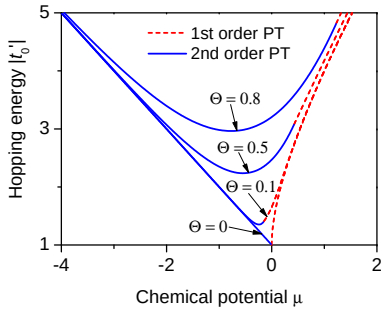


Figure 7. Lines of the NO-SF phase transition in the $(|t_0'|, \mu)$ plane at various temperatures Θ (energy quantities are given in units of δ).

5. Phase separation at fixed boson concentration

Let us consider now thermodynamics of the model at a fixed concentration of Bose particles. We will utilize a connection between the concentration and the chemical potential of bosons which can be established using its definition in such a form

$$n \equiv \langle n_i^b + n_i^c \rangle = \langle X_i^{11} + X_i^{22} \rangle \tag{5.1}$$

or basing on the relationship

$$n = -\frac{\partial(\Omega/N)}{\partial \mu}. \tag{5.2}$$

In the first case similarly to equality (4.10) one can obtain a relation

$$X_i^{11} + X_i^{22} = \widetilde{X}_i^{11} + \widetilde{X}_i^{00} \sin^2\vartheta + \widetilde{X}_i^{22} \cos^2\vartheta + (\widetilde{X}_i^{02} + \widetilde{X}_i^{20}) \sin\vartheta \cos\vartheta \tag{5.3}$$

what results in

$$\begin{aligned} n &= \langle \widetilde{X}_i^{11} \rangle + \langle \widetilde{X}_i^{00} \rangle \sin^2\vartheta + \langle \widetilde{X}_i^{22} \rangle \cos^2\vartheta = \\ &= \frac{1}{Z} \left\{ \mathrm{e}^{-\beta\tilde{\lambda}_1} + \left[\frac{1}{2} - \frac{\delta - \mu}{2\sqrt{(\delta-\mu)^2 + 4(t_0'\xi)^2}} \right] \mathrm{e}^{-\beta\tilde{\lambda}_0} \right. \\ &\quad \left. + \left[\frac{1}{2} + \frac{\delta - \mu}{2\sqrt{(\delta-\mu)^2 + 4(t_0'\xi)^2}} \right] \mathrm{e}^{-\beta\tilde{\lambda}_2} \right\}. \end{aligned} \tag{5.4}$$

In the second case, taking into account that

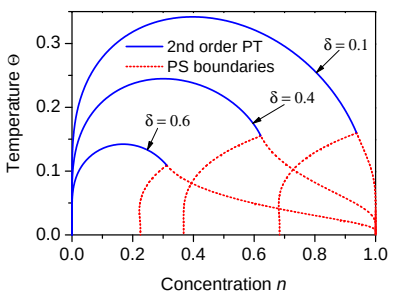
$$\begin{aligned} \Omega/N &= |t_0'|\xi^2 - \Theta \ln Z, \\ Z &= \mathrm{e}^{\beta\mu} + \mathrm{e}^{-\beta(\delta-\mu)/2} \cosh\beta \sqrt{\left(\tfrac{\delta-\mu}{2}\right)^2 + (t_0'\xi)^2}, \end{aligned} \tag{5.5}$$

and differentiating with respect to μ, one can come to (5.4).

There are different relationships between n and μ in NO and SF phases; in the last case a nonzero value of ξ (a solution of equation (4.13)) should be substituted into expression (5.4). Order parameter ξ has a jump at the first order phase transition, so a stepwise change of concentration n takes place. In the $n = \text{const}$ regime (at the value of n in the region of step) it means a phase separation into two phases with different concentrations: the NO phase ($\xi = 0$ and a larger concentration of bosons) and the SF phase ($\xi \neq 0$ and their smaller concentration).

The above-described situation is illustrated in figure 8, where the numerically calculated (Θ, n) phase diagrams are presented. At $\delta > 0$ phase separation region spans up to tricritical temperatures. When δ goes to zero and finally reverses its sign, the shape of the separation region changes in a peculiar way moving off abscissa axis (figure 8). Now the phase separation begins at nonzero temperatures and vanishes at $\delta < \delta_{\mathrm{crit}}$; the line of the second order phase transition remains only. At the further increase of $|\delta|$ (in the $\mu < 0$ region) the (Θ, n) diagram becomes more and more symmetric, approaching by its shape to the diagram known for the usual HCB model [35] (see also [36]).

Phase diagrams in the $(|t_0'|, n)$ coordinates are given in figure 9 where the regions of NO, SF and separated phases are shown at various temperatures.



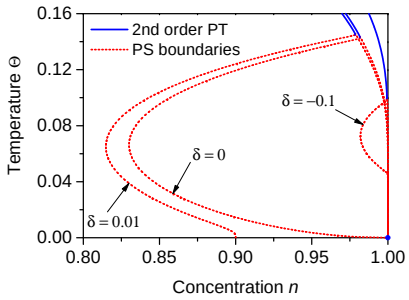


Figure 8. Lines of the NO-SF phase transition and the phase separation region in the (Θ, n) plane at various excitation energies δ including the case of small, zero and negative values of δ ($|t_0'| = 1$).

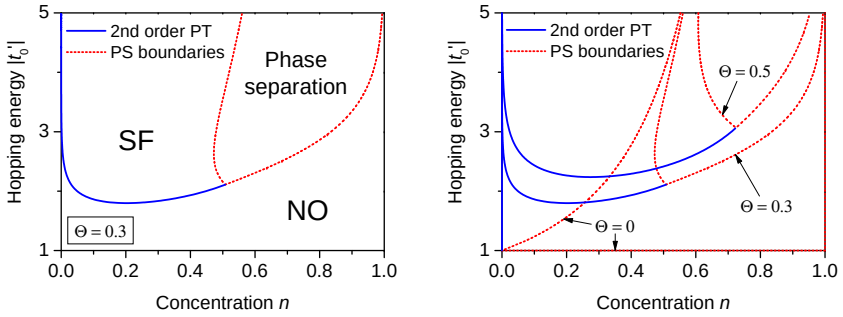


Figure 9. Phase diagram with the indication of possible phases (above) and lines of the NO-SF phase transition in the $(|t_0'|, \mu)$ plane at various temperatures Θ (energy quantities are given in units of δ).

The case of the zero temperature can be studied in more details in a pure analytic way. In this limit there are three branches of order parameter ξ as a function of the chemical potential (see figure 2):

$$\begin{aligned} &(1)\colon \xi = \frac{1}{2|t_0'|}\sqrt{|t_0'|^2 - (\mu-\delta)^2}, \\ &(2)\colon \xi = \sqrt{\mu\delta}/|t_0'|, \\ &(3)\colon \xi = 0. \end{aligned} \tag{5.6}$$

After elimination of ξ parameter, one can obtain the grand canonical potential Ω as follows

$$\begin{aligned} &(1)\colon \Omega/N = \frac{(\mu-\delta+|t_0'|)^2}{4|t_0'|}, \\ &(2)\colon \Omega/N = (\delta/|t_0'|-1)\mu, \\ &(3)\colon \Omega/N = \begin{cases} 0, & \mu<0, \\ -\mu, & \mu>0. \end{cases} \end{aligned} \tag{5.7}$$

Differentiating expressions (5.7) with respect to μ we have

$$\begin{aligned} &(1)\colon n = \frac{1}{2} + \frac{\mu-\delta}{2|t_0'|}, \\ &(2)\colon n = 1 - \delta/|t_0'|, \\ &(3)\colon n = \begin{cases} 0, & \mu<0, \\ 1, & \mu>0. \end{cases} \end{aligned} \tag{5.8}$$

At the first order phase transition from the SF phase to the NO one order parameter ξ jumps from branch (1) to branch (3). This occurs at the $\mu = \mu^* \equiv (\sqrt{|t_0'|} - \sqrt{\delta})^2$ value given by equality of respective grand canonical potentials $\Omega_{(1)} = \Omega_{(3)}$. Boson system then separates into SF and NO phases with concentrations of bosons:

$$n_{\mathrm{SF}} = \frac{1}{2} + \frac{\mu^*-\delta}{2|t_0'|}, \qquad n_{\mathrm{NO}} = 1. \tag{5.9}$$

6. Discussion and conclusions

As was shown in this work, the transition to the SF phase (the phase with BE condensate) in the Bose-Hubbard model with two local states (the ground and excited ones) on the lattice site can be of the first order in the case, when the particle hopping takes place only in the excited band. Calculations and estimates for optical lattices give evidence of significant distinction between hopping parameters t_0 and t_1 in the ground and excited bands, respectively. It follows from estimates [25] that $t_1/t_0 \approx 30-50$ depending on depth V_0 of local potential wells (one can influence on V_0 changing the intensity of laser beams which create an optical lattice). Similar results are obtained in studies of quantum delocalization of the adsorbed hydrogen atoms. One can see from calculations [22, 23] of energy spectrum of the H-atom subsystem on the nickel surface that the ground-state band has a negligible band width. At the same time, for excited bands the band width varies in the range from 15 to 45 meV (depending on the excited state symmetry and on the crystallographic orientation of metal surface), being mostly of the order of half of corresponding excitation energy $\Delta\varepsilon_\alpha = \varepsilon_\alpha - \varepsilon_0$. There are, however, the cases of strong delocalization (e.g. H on the Ni(110) surface) when excited bands overlap, and the width of the lowest one is of the same order as $\Delta\varepsilon_\alpha$ [22].

The values of hopping parameters increase significantly at the decrease of V_0; the distance between the local energy levels becomes smaller in this case (see [37, 38]). It is one of the possible ways to change the relation between the hopping parameters and excitation energy ($|t_0'|$ and δ in our model). Another possibility (discussed in [39]) is connected with an essential reduction of energy gap between local s- and p-levels due to sufficiently strong interspecies Feshbach resonance in the presence of Fermi atoms added to the Bose system in optical lattice.

Along with investigation of BE condensation in the excited band (or bands p_x, p_y (p_x, p_y, p_z) in two- (three-) dimensional case) on condition that certain concentration of Bose-atoms has been created in the band by

optical pumping [25,38], an attempt was performed in [40] to study the influence of excited bands on physics of BE condensation in the lowest (s-) band (when the s-band hopping is taken into account). The case of finite values of the one-site interaction U was considered. The possibility of the re-entrant behaviour of the MI-SF transition was claimed. However, the order of phase transition was not investigated; the consideration was restricted to the case of zero temperature. As we show in this work, re-entrant type dependence on T or μ takes place only for spinodals and return to the initial MI phase from the SF one could be possible only in the case of the second order phase transitions. In reality, the order of phase transition changes to the first one in this region. In the HCB limit (no more than one particle per lattice site), it takes place mainly at positive values of chemical potential of particles; at $\mu < 0$ the transition remains, for the most part, of the second order. Region of existence of SF phase is restricted as a whole to the interval $-|t_0'| < \mu < |t_0'|$, while excitation energy must obey the inequality $\delta < |t_0'|$. We have constructed the corresponding phase diagrams and established localization of tricritical points, where the order of phase transition is changed. The separation on SF and NO phases at the fixed particle concentration is investigated; the conditions of appearance of phase-separated state are analyzed.

It should be mentioned that phase diagrams in figures 2–9 are close by their shape to diagrams obtained in the framework of Bose-Hubbard model for Bose atoms with spin $S = 1$ in optical lattices [29]. Excited levels are formed in that case by the higher spin single-site states and corresponding interactions of the "ferromagnetic" or "antiferromagnetic" type (the Hund-rule-like splitting), while the hopping parameter is taken the same for all bands. Similarity of the mentioned diagrams point out to the fact that the role of excited states in the change of the phase transition order in going to the phase with the BE condensate is analogous in both cases. Distinction, however, consists in another genesis of the single-site spectrum. In our model in the limiting case of HCB the effects connected with the level splitting due to interaction, are absent; the excited single-particle states are taken by us into account instead.

Consideration developed in this work can be extended on systems with the close or degenerate excited local levels. Generalization of the model by the addition of inter-site interactions is also important; it could provide a possibility to have in view another phases (density-modulated or supersolid) besides NO and SF ones.

We emphasize finally that hopping parameter t_{ij}' in the excited band can be positive; in particular, it concerns the p-bands [39]. In such a situation the condensation takes place into states with wave vector $\vec{Q}$ on the boundary of the Brillouin zone and order parameters $\langle c_Q \rangle$, $\langle c_Q^+ \rangle$ describe the p-wave condensate. Because $t_Q' = -t_0'$, the obtained in this works results are valid (with $|t_Q'|$ in place of $|t_0'|$) also in that case.

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