Effects of finite temperature on the robustness of the Mott insulator phase in a pseudo-two-dimensional Bose–Hubbard model

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Received 29 April 2011, in final form 27 June 2011
Published 25 July 2011
Online at stacks.iop.org/JPhysB/44/165303

Abstract
We study the superfluid-Mott insulator (SF-MI) transition in a two-dimensional optical lattice system and employ the Bose–Hubbard model in three dimensions with a combined potential of an optical lattice in two directions and a confining harmonic trap in the other direction, which we refer to as the pseudo-two-dimensional Bose–Hubbard model. Some excited states with respect to the harmonic trap are taken into account in this paper. The Mott lobes shrink in the \( \mu \) and \( J \) directions of the \( \mu-J \) phase diagram. The shrinkage occurs because the interactions involving the excited states become weaker than that between particles in the ground state. The dispersion of the in-site particle number increases because the energy spacing between the eigenstates of the Hamiltonian decreases at finite temperature. The presence of the excited states significantly affects the robustness of the MI phase at finite temperature.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
Since the realization of Bose–Einstein condensates in cold atomic systems [1], many studies both from theoretical and experimental sides have been performed. Various parameters, say the strength of the inter-atomic interaction and the configuration of the confinement potential, are experimentally well controllable in the cold atomic systems [2], which offer many intriguing phenomena such as the superfluid-Mott insulator (SF-MI) transition. Moreover, it is possible to realize a low-dimensional system simply by tightening the confinement potential in one or two directions, and it provides a good testing field to study low-dimensional physics.

Experimentally, the SF-MI transition in this system, which is the quantum phase transition, has been observed when the depth of the lattice potential is increased [3], and was followed by observations in several systems such as the multi-component one [4], the multi-band one [5] and the low-dimensional ones [6–8]. Theoretically, the strongly correlated bosonic system in an optical lattice is well described by the Bose–Hubbard model [9], according to which the possibility of the SF-MI transition was expected before its experimental observation [10]. This model has been analysed in various situations, i.e. at finite temperature [11–15], for the multi-component systems [15–19], for the multi-band ones [20, 21] and for the low-dimensional one [15, 22].

The two-dimensional optical lattice system is realized experimentally in a combined potential of a two-dimensional optical lattice and a harmonic trap. When the harmonic trap is tight in the direction perpendicular to the optical lattice and the optical lattice itself is deep, the system can be described in a good approximation by the two-dimensional (2D) Bose–Hubbard model, restricted to the first band, for which the features of the low-dimensional SF-MI transition [6, 7, 22] have been revealed and which has been used to describe the dynamics of cold atomic systems [23]. Bose–Hubbard models without higher bands for the low-dimensional systems and the superlattice ones have been investigated in some detail both at
zero and finite temperatures, since the experimental parameters are well controllable [12–14]. The strength of the confinement potential is an important control parameter in the model. When the confinement potential is not tight enough and the transitions to excited states become possible, the model is similar to the multiband Bose–Hubbard one. To control the energy-level spacing in this model is easier than that in the multiband model. Moreover, it is reported that the contributions of the higher excitations of the harmonic trap cannot be neglected for the one-dimensional system with Bose–Einstein condensates at finite temperature [24]. The effects of the confinement potential to realize the low-dimensional system have not been clarified yet at finite temperature. In this paper, our results at finite temperature indicate that the effects of the excitations cannot be neglected for the 2D SF-MI transition, either.

Our aim in this paper is to investigate the temperature dependence of the SF-MI transition in a low-dimensional optical lattice system. To this end, we concentrate on a cold atomic system in three dimensions with a combined potential of an optical lattice in the $x$- and $y$-directions and a confining harmonic trap in the $z$-direction, and suppose that the optical lattice is so deep that the 2D Bose–Hubbard Hamiltonian without higher bands describes the dynamics in the $x$- and $y$-directions, but that some excited states in the $z$-direction have to be taken into account because the harmonic potential is not tight enough to forbid transitions into the excited states absolutely. We refer to this model as the pseudo-two-dimensional (P2D) Bose–Hubbard model throughout this paper. The reason for analysing the P2D model here is that while it is simple and easy to analyse, it can be realized experimentally with a merit that the strength of the harmonic trap is variable. It is also pointed out that the structure of the transition terms in the P2D Bose–Hubbard Hamiltonian is similar to that in the spin transition [18, 19] or the one between the Bloch bands [20, 21], implying that our model serves as a prototype to understand the physics of the low-dimensional SF-MI transition in more general situations.

We study the P2D Bose–Hubbard model in this paper, both analytically and numerically, and show how the transition terms affect the SF-MI phase diagram at zero and finite temperatures. The main result at zero temperature is the shrinkage of the Mott lobes, which originates from a decrease in the effective on-site interaction due to the transitions between the harmonic states in the $z$-direction. One may expect that such deformations of the Mott lobes can be fitted simply by adjusting an effective on-site interaction in the 2D model, but it is not true, and they reflect the complex structure of the interactions in the P2D model. Although the phase diagram for the P2D model reduces to that for the 2D model in the tight confinement limit, we note that the shrinkage is non-negligible even for comparatively tight confinement. The contributions of the transition in the $z$-direction are enhanced more at a higher temperature. The Mott lobes disappear gradually with an increase in temperature due to the thermal fluctuation. While the disappearance in the 2D model occurs independently of the value of the chemical potential, it is not so in the P2D model. This is explained as follows: the effective on-site interaction becomes weaker for particles in the excited states, and the fraction of the excited particles becomes larger as the chemical potential increases, which implies that the hopping term becomes relatively significant for the larger chemical potential. This way we have the dependence of the chemical potential in the phase diagram, calculated from the P2D model. We have confirmed through our analysis that it is only at very low density and temperature that the 2D Bose–Hubbard model without higher bands and the P2D one give almost the same results, and therefore that the validity of the 2D model is restrictive.

This paper is organized as follows. In section 2, we introduce the P2D Bose–Hubbard model. The phase diagram in the zero hopping limit is obtained analytically. In section 3, we show the phase diagram for non-zero hopping both at zero and finite temperatures by employing the mean-field approximation. Section 4 is devoted to summary and discussion.

2. P2D Bose–Hubbard model

We start with the following Hamiltonian to describe the cold Bose atomic gas system in three dimensions with a combined potential of an optical lattice in the $x$- and $y$-direction and a confining harmonic trap in the $z$-direction as follows:

$$\hat{H} = \int \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{opt}}(x) + V_{\text{opt}}(y) \right] \psi(x, y, z) \frac{1}{2} \left( \psi(x, y, z) + \psi(x, y, z)^\dagger \right) \psi(x, y, z)$$

$$+ \frac{g}{2} \psi(x, y, z)^\dagger \psi(x, y, z)^\dagger \psi(x, y, z)^\dagger \psi(x, y, z).$$

(1)

where $V_{\text{opt}}(x), V_{\text{opt}}(y), V_{\text{har}}(z) = m \omega^2 z^2 / 2$, $\mu$ and $g$ represent the optical lattice potentials, the harmonic potential, the chemical potential, and the coupling constant, respectively. We assume that the optical lattice potentials, $V_{\text{opt}}(x)$ and $V_{\text{opt}}(y)$, are the same functions. Note that no harmonic potential in the $x$-direction and $y$-direction is considered.

The field operator $\psi(x, y, z)$ is expanded as

$$\psi(x, y, z) = \sum_i \psi_i(x, y) u_i(z).$$

(2)

in the complete set of the wavefunctions of harmonic oscillation:

$$\left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{har}}(z) \right) u_i(z) = E_i u_i(z),$$

(3)

where $E_i = \hbar \omega_i (\ell + 1/2)$ ($\ell = 0, 1, 2, \ldots$). Then we expand the field operator $\psi_i(x, y)$ in the complete set of the Wannier functions $w_i(x, y)$ with site index $i$ as

$$\psi_i(x, y) = \sum_j \hat{a}_{i,j} w_i(x, y).$$

(4)

We assume in this paper that the optical lattice is so deep that only the states in the lowest band contribute but take account of the excited states ($\ell \neq 0$) of the harmonic oscillation in the $z$-direction. Under the tight-binding approximation, we obtain the Hamiltonian, which we refer to as the P2D Bose–Hubbard Hamiltonian,

$$\hat{H} = \hat{H}_{\text{hop}} + \hat{H}_{\text{on-site}},$$

(5)
with
\[
\hat{H}_{\text{hop}} = -J \sum_{\ell, i} \hat{a}_{\ell,i}^\dagger \hat{a}_{\ell+1,i}.
\]
\[
\hat{H}_{\text{on-site}} = \sum_i \epsilon_i \hat{c}_i^\dagger \hat{c}_i,
\]
\[
\hat{h}_i = \sum_{\ell} (E_\ell - \mu) \hat{a}_{\ell,i}^\dagger \hat{a}_{\ell,i} + \frac{1}{2} \sum_{\ell \neq \ell'} U_{\ell,\ell',i} \hat{a}_{\ell,i}^\dagger \hat{a}_{\ell',i} \hat{a}_{\ell',i}^\dagger \hat{a}_{\ell,i},
\]
where
\[
J = -\int dx \, dy \, w^*_i(x,y) \left\{ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + V_{\text{opt}}(x) + V_{\text{opt}}(y) \right\} w_i(x,y),
\]
the site index \(i'\) is the nearest neighbour site to the site \(i\),
\[
g_{\ell,\ell',i} = g \int dz w^*_i(z) u^*_\ell(z) u_{\ell'}(z),
\]
\[
U_{\ell,\ell',i} = g \int dx |w_i(x,y)|^4,
\]
and \(\sum_{\ell, i, f}\) denotes the sum over nearest neighbour sites. Note that the on-site interaction coefficient \(U_{\ell,\ell',i}\) depends on \(\ell\) (the quantum number of the harmonic oscillation) while the hopping coefficient \(J\) is independent of \(\ell\). In Table 1, the ratios of the on-site interaction coefficients to the ground state interaction are listed. All on-site interaction coefficients involving the excited states are smaller than the interaction coefficient \(U_{0000}\).

The harmonic frequency \(\omega_z\) representing the strength of the harmonic potential comes into the dynamics of our model in two ways, namely through the energy-level spacing \(\Delta E_z = E_{\ell+1} - E_\ell = \hbar \omega_z\) and the on-site interaction \(U_{\ell,\ell',i}\). The latter dependence is expressed as \(U_{\ell,\ell',i} \sim \sqrt{\Delta E_z}\) universally for any \(\ell\), and is absorbed into rescaling the phase diagram by using the parameters \(\mu, U_{0000}\) and \(J/\sqrt{\Delta E_z}\). Note that it does not mean that the P2D model reduces to the 2D model by such rescaling. We pay little attention to this trivial dependence but focus on the nontrivial effect of the transitions between the harmonic states, which is absent in the 2D model.

We assume that the confinement harmonic potential is relatively tight but is not so tight as all of the excited states can be neglected. Then, the infinite sum over \(\ell\) can be approximated by a finite sum of some lower energy states. Because of the even–odd selection rule for the on-site interaction coefficient \(U_{\ell,\ell',i}\), the transition of one particle from the ground state to the first excited one is forbidden. The transition with the lowest energy from the ground state is either the simultaneous one of two particles to the first excited state or the one of one particle to the second excited state. Hence, in order to estimate the effects of the excited states at a minimum, we have to sum up the states not with \(\ell = 0\) but with \(\ell = 1, 2\) at least, and will take this minimal sum throughout this paper.

Before full numerical calculations, let us turn to the zero hopping limit, \(J = 0\). Then the hopping Hamiltonian \(\hat{H}_{\text{hop}}\) in (5) is absent, and the total Hamiltonian \(\hat{H} = \hat{H}_{\text{on-site}}\) is entirely separable with respect to the site index \(i\). Note that \(\hat{h}_i\) in \(\hat{H}_{\text{on-site}}\) commutes with the in-site particle number operator at the \(i\)-site, \(\hat{h}_i = \sum_a \hat{a}_a^\dagger \hat{a}_a\), and hence the ground state of the total system is obtained simply by the diagonalization with a fixed in-site particle number. Hereafter, the trivial subscript \(i\) is omitted.

Explicitly, we set up the following eigenvalue equation for each fixed in-site particle number \(n\) and seek the lowest energy eigenstate:
\[
\hat{h}_i |\Psi_n\rangle = E_n |\Psi_n\rangle,
\]
where the state \(|\Psi_n\rangle\) is expanded as
\[
|\Psi_n\rangle = \sum_{n_{01}, n_{22}} \delta_{n_{01}, n_{22}} g(n_{00}, n_{11}, n_{22}) |n_{00}, n_{11}, n_{22}\rangle,
\]
with the direct product of the particle number states \(|n_i\rangle\) with \(\ell = 0, 1, 2\). For illustration, we write down the matrix eigenvalue equations for \(n = 1\) and \(n = 2\):
\[
\begin{pmatrix}
-\mu & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 2\Delta E_z
\end{pmatrix}
\begin{pmatrix}
g_1 \\
g_2
\end{pmatrix}
= E_1 \begin{pmatrix}
g_1 \\
g_2
\end{pmatrix},
\]
with
\[
g_1 = \begin{pmatrix}
g(1, 0, 0) \\
g(0, 1, 0) \\
g(0, 0, 1)
\end{pmatrix},
\]
and
\[
\begin{pmatrix}
-2\mu + \begin{pmatrix} M_1 & O \\ O & M_2 \end{pmatrix}
\end{pmatrix}
\begin{pmatrix}
g_1 \\
g_2
\end{pmatrix}
= E_2 \begin{pmatrix}
g_1 \\
g_2
\end{pmatrix},
\]
with
\[
M_1 = \begin{pmatrix}
U_{0000} & \sqrt{\Delta E_z}U_{0002} & U_{0022} & U_{0011} \\
\sqrt{\Delta E_z}U_{0002} & 2\Delta E_z + 2U_{0022} & \sqrt{\Delta E_z}U_{1122} & \sqrt{\Delta E_z}U_{0112} \\
U_{0022} & \sqrt{\Delta E_z}U_{1122} & 4\Delta E_z + 2U_{2222} & U_{1122} \\
U_{0011} & \sqrt{\Delta E_z}U_{0112} & U_{1122} & 2\Delta E_z + U_{1111}
\end{pmatrix},
\]
\[
M_2 = \begin{pmatrix}
\Delta E_z + U_{0011} & 2U_{0112} \\
2U_{0112} & 3\Delta E_z + 2U_{1112}
\end{pmatrix}.
\]
and

and

\[ g_2 = \begin{pmatrix} g(2, 0, 0) \\ g(1, 0, 1) \\ g(0, 0, 2) \\ g(0, 2, 0) \\ g(1, 1, 0) \\ g(0, 0, 1) \end{pmatrix}. \]  

Equation (15) implies that the lowest eigenvalue of \( E_1 \) is equal to \( E_{1, \text{min}} = -\mu \). One can calculate the lowest eigenvalue of \( E_2 \), denoted by \( E_{2, \text{min}} \), from (17). Similarly, the lowest energy and its eigenstate for each \( n \) can be obtained. The results allow us to draw the phase diagram as indicated in figure 1. There the boundary between the \( n = 1 \) and \( n = 2 \) regions, for example, is a line on which \( E_{1, \text{min}} = E_{2, \text{min}} \).

Obviously, the dispersion of the in-site particle number is equal to zero as a result of its conservation, and the state of the whole system is in a Mott phase. However, the particle number in each \( \ell \)-state can fluctuate. The dispersions of the particle number in some \( \ell \)-states (\( \ell = 0, 1, 2 \)) are shown in figure 2, where they vary stepwise as a function of \( \mu \). For comparison, we recall the corresponding 2D Bose–Hubbard model:

\[ H_{2D} = H_{\text{hop}, 2D} + H_{\text{on-site}, 2D} \]  

\[ H_{\text{hop}, 2D} = -\mu \sum_i \hat{a}_i^\dagger \hat{a}_i, \]  

\[ H_{\text{on-site}, 2D} = \sum_i \hat{h}_{i, 2D}. \]  

### Table 2.

The squared coefficients \( |g(n_0, n_1, n_2)|^2 \) for \( \Delta E_e/U_{0000} = 3.0 \).

| Particle number | \( |g(n, 0, 0)|^2 \) | \( |g(n - 1, 0, 1)|^2 \) | \( |g(n - 2, 2, 0)|^2 \) | Others |
|----------------|------------------|------------------|------------------|-------|
| \( n = 2 \)    | \( 9.84 \times 10^{-1} \) | \( 7.88 \times 10^{-1} \) | \( 7.47 \times 10^{-3} \) | \( 8.37 \times 10^{-4} \) |
| \( n = 3 \)    | \( 9.35 \times 10^{-1} \) | \( 4.23 \times 10^{-2} \) | \( 2.11 \times 10^{-2} \) | \( 1.49 \times 10^{-3} \) |
| \( n = 4 \)    | \( 8.57 \times 10^{-1} \) | \( 1.07 \times 10^{-1} \) | \( 3.48 \times 10^{-2} \) | \( 1.15 \times 10^{-3} \) |
include the hopping Hamiltonian, we resort to the mean-field approximation [12, 13]. The mean-field approximation describes the SF-MI transition for the 2D (P2D) model well [26].

Let us introduce the order parameter
\[
\Phi_{\ell,i} \equiv \langle \hat{a}_{\ell,i} \rangle = \frac{\text{Tr}[\hat{a}_{\ell,i}e^{-\beta \hat{H}}]}{\text{Tr}[e^{-\beta \hat{H}}]},
\]
where \( \beta = 1/k_B T \) with the Boltzmann constant \( k_B \). Neglecting the fluctuation terms of the second order, we have an approximate expression of
\[
\hat{a}_{\ell,i}^\dagger \hat{a}_{\ell,i} \approx \Phi_{\ell,i}^* \hat{a}_{\ell,i} + \Phi_{\ell,i} \hat{a}_{\ell,i}^\dagger - \Phi_{\ell,i}^* \Phi_{\ell,i}.
\]

Then, the approximate hopping Hamiltonian becomes
\[
\hat{H}_{\text{hop}}^{(M)} = - J \sum_{\ell} \sum_{i,i'} [\Phi_{\ell,i}^* \Phi_{\ell,i'} - \Phi_{\ell,i} \Phi_{\ell,i'}^*].
\]

The total Hamiltonian under the mean-field approximation is given by \( \hat{H}^{(M)} = \hat{H}_{\text{hop}}^{(M)} + \hat{H}_{\text{on-site}} \). We calculate the lowest energy state, determining the order parameter \( \Phi_{\ell,i} \) self-consistently in such a way that the total energy expectation is minimized at zero temperature or the free energy,
\[
F = -\beta^{-1} \ln Z(\beta),
\]
\[
Z(\beta) = \text{Tr}[e^{-\beta \hat{H}^{(M)}}],
\]
is so at finite temperature. In this calculation, we consider the excited states up to the second excited state, as was stated in section 2, and the site index \( i \) is omitted, and the system is assumed to be homogeneous in both \( x \)- and \( y \)-directions. The physical quantities (e.g. the dispersion of the in-site particle number and the order parameter) can be calculated with the eigenstates of the eigenvalue
\[
\hat{H}^{(M)}|\Psi_M^{(M)}\rangle = E_M|\Psi_M^{(M)}\rangle.
\]
The expectation value of the physical quantity \( \hat{A} \) at zero temperature is \( \langle \Psi_M^{(M)}| \hat{A} |\Psi_M^{(M)}\rangle \), where \( |\Psi_M^{(M)}\rangle \) is the eigenstate belonging to the lowest eigenvalue, and the expectation \( \langle \hat{A} \rangle \) at finite temperature is
\[
\langle \hat{A} \rangle = \frac{\text{Tr}[\hat{A} e^{-\beta \hat{H}^{(M)}}]}{\text{Tr}[e^{-\beta \hat{H}^{(M)}}]} = \frac{\sum_m \langle \Psi_m^{(M)} | \hat{A} e^{-\beta \hat{H}^{(M)}} | \Psi_m^{(M)} \rangle |\Psi_m^{(M)}\rangle}{\sum_m |\Psi_m^{(M)}\rangle |\Psi_m^{(M)}\rangle}.
\]

3.1. Zero temperature results

In figure 3, we show the phase diagrams in the 2D model and in the P2D one with the energy-level spacing \( \Delta E_z/U_{0000} = 3.0 \) at zero temperature, respectively. Comparing the result for the P2D model with that for the 2D model in figure 3(a), one can find the following two features. First, the Mott lobes of the P2D model shrink in the \( \mu \) direction, as in figure 3(b). The rate of the shrinkage of the Mott lobes of the P2D model increases as the in-site particle number does. Second, in the P2D model, the dispersion of the ground state particle number in the Mott lobes is nonzero and also increases as the in-site particle number increases, as in figure 3(c). The order parameter does not necessarily become nonzero even in the nonzero dispersion region of the ground state particle number in the Mott lobes, as in figures 3(c) and (d). The nonzero dispersion of the ground state particle number shows that the particle number of each state is not fixed and can fluctuate, but only the in-site particle number is fixed. This is attributed to the decrease of the effective on-site interaction because the on-site interaction coefficients are smaller than the ground state
interaction coefficient $U_{0000}$. The numerical results show that the results in section 2 can be applied even to the case of $J \neq 0$.

We see from figures 3(a) and (b) that the Mott lobes also shrink in the $J$ direction in the P2D model. The reason for this shrinkage is as follows: the system is favourable to the SF-phase when the ratio of the hopping to the on-site interaction is large. The effective interaction is smaller than that of the ground state particles, which means that the particles in the excited states tend to be in the SF-phase more easily than those in the ground state, because then the effect of the hopping is relatively large, compared to the on-site interaction. As a result, in comparison with the system of the 2D model, the system of the P2D model is favourable to the SF-phase.

We remark that both of the excited state particle numbers $\langle \Psi_{0}^{M}|\hat{n}_{1}\rangle|\Psi_{0}^{M}\rangle$ and the order parameters $\langle \Psi_{\ell}^{M}|\hat{a}_{1}\rangle|\Psi_{\ell}^{M}\rangle \ (\ell = 1, 2)$ are very small because the energy spacing is much larger than the interaction energy in our analysis. This is the reason why the quantities only with $\ell = 0$ are shown in figure 3.

We emphasize that the P2D model is essential in the above considerations since the particles in the excited states play a crucial role.

3.2. Finite temperature results

In the previous subsection, we found that the effects of the excited states become more conspicuous for larger in-site particle numbers. It is therefore anticipated that the excited state is more important at finite temperature. In this subsection, we analyse the effect of finite temperature in the P2D model. Recall that the expectation value of the physical quantity at finite temperature is $\langle \hat{A} \rangle = \text{Tr}[\hat{A} e^{-\beta \hat{H}}]/\text{Tr}[e^{-\beta \hat{H}}]$.

In figure 4, we show the dispersions of the in-site particle number $\langle \hat{n}_{0}^{2} \rangle - \langle \hat{n} \rangle^{2}$ and the absolute square of order parameter of the ground state particles $|\Phi_{0}^{1}\rangle^{2} = |\langle \hat{a}_{0} \rangle^{2}|$ in the 2D model with $\beta U_{0000} = 20.0$. (c), (d) Those with $\beta U_{0000} = 8.0$.

Figure 4. (a) The dispersion of the in-site particle number $\langle \hat{n}_{0}^{2} \rangle - \langle \hat{n} \rangle^{2}$ and (b) the absolute square of the order parameter of the ground state particles $|\Phi_{0}^{1}\rangle^{2} = |\langle \hat{a}_{0} \rangle^{2}|$ in the 2D model with $\beta U_{0000} = 20.0$. (c), (d) Those with $\beta U_{0000} = 8.0$.

not fit the region of the vanishing order parameter, the latter is wider than the former. We have some regions where the dispersion is non-vanishing but the order parameter vanishes, $\Phi_{0} = 0$, and interpret that they represent the normal-liquid phase, and the results correspond to those in [12, 13].

The phase diagram of the P2D model is shown in figure 5. There the order parameter is that for the ground state. As in the 2D model, the vanishing order parameter region covers the vanishing dispersion one. The normal-liquid region expands as the temperature goes up. In a fashion similar to the zero temperature case, the shrinkage of the Mott lobes is also seen at finite temperature in the P2D model. The shape of the lobes for the order parameter in figures 5(b) and (d) is lost at finite temperature more clearly than in figures 4(b) and (d) for the 2D model.

To investigate the temperature dependence of the dispersion in more detail, we show the dispersions for small $J$, namely for $J = 0$ in figure 6 and for $J/U_{0000} = 0.01$ in figure 7. Comparing the results of the P2D model in figures 6(b) and 7(c) with those of the 2D model in figures 6(a) and (a), we see that the dispersion is larger in the P2D model than in the 2D model. In addition, the dispersion is independent of the chemical potential $\mu$ in the 2D model, but in the P2D model, it depends on $\mu$ in such a manner that it is larger at larger $\mu$. The order parameter of the P2D model begins to be non-vanishing in a smaller $\mu$ region than that of the 2D model, as in figures 6(b) and (d). At higher temperature, the order parameter becomes smaller and the regions in the normal-liquid phase expand equally for the 2D and P2D models in figure 7.

It is known that the compressibility, defined by $\partial n/\partial \mu$, distinguishes between the Mott and normal-liquid phases. It is vanishing in the Mott phase, while it is not in the normal-liquid one. We show the compressibility of the 2D and P2D models with $J = 0.01$ in figure 8. One can see that its increases in figures 8(a) and (b) synchronize with those of the dispersion in figures 7(a) and (c).
Figure 5. (a) The dispersion of the in-site particle number \( \langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2 \) and (b) the absolute square of the order parameter of the ground state particles \( \left| \Phi_0 \right|^2 = |\langle \hat{a}_0 \rangle|^2 \) with in the P2D model \( \beta U_{0000} = 20.0 \). (c), (d) Those with \( \beta U_{0000} = 8.0 \).

Figure 6. The dispersions of the in-site particle number \( \langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2 \) in the zero hopping limits \( J = 0 \) (a) in the 2D model and (b) in the P2D one with \( \Delta E_{1m} / U_{0000} = 3.0 \).

Table 3. In this table, \( E_{m}^{(2D)} \) and \( E_{m}^{(P2D)} \) represent the \( m \)th eigenvalues of the Hamiltonian in the 2D and P2D systems with \( \langle \hat{n} \rangle = 3 \) and \( \beta U_{0000} = 10.0 \). These values are the eigenvalues of the grand canonical Hamiltonian \( H - n \mu \), so the values can be negative. The symbol \( \Delta E_{m-1,m} \) stands for the spacing between energy levels, \( \Delta E_{m-1,m} = E_m - E_{m-1} \).

| \( m \) | \( 0 \) | \( 1 \) | \( 2 \) | \( 3 \) |
|---|---|---|---|---|
| \( E_{m}^{(2D)} / U_{0000} \) | -4.50 | -4.00 | -4.00 | -2.50 |
| \( \Delta E_{m-1,m}^{(2D)} / U_{0000} \) | 0.500 | 0.000 | 1.50 |
| \( E_{m}^{(P2D)} / U_{0000} \) | -3.54 | -3.19 | -3.19 | -2.15 |
| \( \Delta E_{m-1,m}^{(P2D)} / U_{0000} \) | 0.359 | 0.000 | 1.04 |

Figure 9(a) shows the dispersions of the various average in-site particle numbers in the case of \( J = 0 \), concretely \( \langle \hat{n} \rangle = 2, 3, 4 \). In both of the 2D and P2D models, the dispersions increase as the temperature rises, but their increasing rate depends on the average particle number \( \langle \hat{n} \rangle \) in the P2D model. We also illustrate the temperature dependence of the increasing rates of the excited particle numbers for \( \ell = 1, 2 \) in figure 9(b). One can see in figure 9 that the increase in the excited particle numbers synchronizes with that in the dispersions. This indicates that the excited particles contribute to the large dispersions in the P2D model.

To clarify the rapid increase of the dispersions in the P2D model, we investigate the eigenvalues of the Hamiltonian (31) for the 2D and P2D models. In table 3, the eigenvalues of the Hamiltonian and the energy-level spacings are shown. One finds that the energy-level spacing \( \Delta E_{m-1,m} \) in the P2D model than \( \Delta E_{m-1,m}^{(2D)} \) in the 2D model. This narrow energy-level spacing enhances the contributions of the higher energy eigenstates \( m = 1, 2, \ldots \) at finite temperature, so that the dispersions become larger then. In addition, it turns out in the case of \( \langle \hat{n} \rangle = 3 \) that the eigenstates belonging to the eigenvalues \( E_1 \) and \( E_2 \) are those with the in-site particle numbers \( n = 4 \) and \( n = 2 \), respectively, while the eigenstate belonging to \( E_0 \) is that with \( n = 3 \). The number of excited particles grows as the in-site particle number does, according to table 2. Thus the increase of excited particles in figure 8(b) reflects the contribution of the eigenstate with \( E_1 \), namely of the state of the in-site particle number \( n = 4 \).

The narrow energy-level spacing arises from the fact that the on-site interaction coefficients involving the excited particles are small. This is explained in the following way. As the fraction of the excited particle number becomes larger at the large average in-site particle number \( \langle \hat{n} \rangle \), the
Figure 7. (a) The dispersions of the in-site particle number $\langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2$ and (b) the absolute square of the order parameter of the ground state particles $|\Phi_0|^2$ in the 2D model with $J/U_{0000} = 0.01$. (c), (d) Those in the P2D model.

Figure 8. The compressibility with $J = 0.01$ (a) in the 2D model and (b) in the P2D one with $\Delta E_r/U_{0000} = 3.0$.

Figure 9. (a) The dispersions $\langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2$ of the various average in-site particle numbers, $\langle \hat{n} \rangle = 2, 3, 4$ and $\Delta E_r/U_{0000} = 3.0$ for the P2D and 2D models. The dispersion of the 2D model is independent of the average in-site particle number $\langle \hat{n} \rangle$. (b) The ratios of the excited particle numbers at finite temperature $n_i$ to those at zero temperature $n_{i,T=0}$ in the average in-site particle number $\langle \hat{n} \rangle = 3$ in the P2D model with $\Delta E_r/U_{0000} = 3.0$.

The above discussions indicate that the presence of the excited states affects the robustness of the Mott phase definitely and essentially. Although the approximation of the 2D model is valid for very low density and temperature, the effects of the excited states cannot be neglected for describing finite-density and/or temperature systems.
4. Summary and discussion

In this paper, we have analysed the SF-MI transition at zero and finite temperatures for the P2D Bose–Hubbard model. The P2D model, which differs from the 2D model, contains the transition terms, which are similar to the spin transition and the transition between the Bloch bands. Specifically, the form of the multiband Bose–Hubbard Hamiltonian corresponds to that of the P2D one, aside from the values of the on-site interaction coefficients $U_{\ell}$ and the hopping coefficient $J$. We expect that our analysis is also useful in analysing the multiband model.

In zero temperature analysis, the SF-MI phase diagram of the P2D model is different from that of the 2D model even for the relatively tight confinement. The major difference is the shrinkage of the Mott lobes in the $\mu$ direction. The effect is attributed to the small effective on-site interaction, caused by the transition between the ground and excited states. The transitions in the P2D model produce the fluctuation of the particle number in each $\ell$-state in the Mott lobes. The decrease of the on-site interaction enhances the hopping relatively, which leads to the shrinkage of the Mott lobes in the $J$ direction, as that in the $\mu$ direction. We note that the 2D model cannot take account of these effects by adjusting the parameters.

At finite temperature, the dispersion of the in-site particle number increases as the temperature becomes higher. In addition, the regions of the normal-liquid phase surrounding the Mott lobes expand. These effects occur in both of the 2D and P2D models due to the thermal fluctuation. The result in the 2D model corresponds to that in [13]. We note that the increase of the dispersion in the P2D model is enhanced more than that in the 2D model. The tendency is more noticeable at higher density and/or temperature, which leads to the shrinkage of the Mott lobes in the $\mu$ direction. We consider the excited states coming from the confinement potential and finite temperatures for the P2D Bose–Hubbard model.

In this paper, we have analysed the SF-MI transition at zero and finite temperature for the 2D Bose–Hubbard model. The 2D model, which differs from the 2D model, contains the transition terms, which are similar to the spin transition and the transition between the Bloch bands. Specifically, the form of the multiband Bose–Hubbard Hamiltonian corresponds to that of the 2D one, aside from the values of the on-site interaction coefficients $U_{\ell}$ and the hopping coefficient $J$. We expect that our analysis is also useful in analysing the multiband model.

The pseudo-one-dimensional model, or the cigar-shaped one-dimensional model which is a three-dimensional system restricted to very low density and temperature for realistic cold atomic gases. At higher density and/or temperature, one has to consider the excited states coming from the confinement potential.

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