# Quantum phase transition of condensed bosons in optical lattices 

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#### Abstract

In this paper we study the superfluid-Mott-insulator phase transition of ultracold dilute gas of bosonic atoms in an optical lattice by means of Green function method and Bogliubov transformation as well. The superfluid-Mott-insulator phase transition condition is determined by the energy-band structure with an obvious interpretation of the transition mechanism. Moreover the superfluid phase is explained explicitly from the energy spectrum derived in terms of Bogliubov approach.


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## I. INTRODUCTION

Ultracold bosons in an optical lattice provide a tunable quantum system with variance of the potential depth and lattice constant which can be achieved by adjusting the parameters of the configuration of laser beams. Various quantum phenomena, for instance, Bloch oscillations, WannierStack ladders [1], have been investigated in such a system which shares spatial periodicity with crystal lattice in solidstate physics, however is immune from scattering of impurities or phonons. The superfluid-Mott-insulator (SMI) phase transition is one of the most significant quantum phenomena of condensate bosons in the optical lattice. A known analogous system exhibiting the SMI phase transition is liquid helium with short-range repulsive interaction in periodic potential [2]. The atomic gas in Bose-Einstein condensate (BEC) subjected to the lattice potential which is turned on smoothly can be kept in the superfluid phase (SFP) as long as the repulsive interaction between atoms is small with respect to the tunnel coupling. With increase in the potential depth of the optical lattice it is getting more and more difficult for bosons to tunnel from one site to the other, and finally the system attends an insulator phase above a critical value of the potential depth. Considerable attention has been paid to theoretical researches for understanding of the phase transition and determining of the transition condition [3-8], in which the Bose-Hubbard model is introduced as the starting point of the theoretical studies [3]. The phase transition phenomena have also been observed experimentally in BEC loaded in a three-dimensional optical lattice [3]. Using a strong-coupling expansion in terms of the hopping term called the decoupling approximation, which is as a matter of fact based on the mean-field method, van Oosten et al. have obtained an analytic phase transition condition [see Eq. (27)]. From an alternative viewpoint the phase transition condition can also be determined from the energy spectrum of the system since the excitation spectrum is necessarily gapless for the SFP while it has a finite gap for the Mott insulator phase (MIP). We in the present paper use both the Green function method and Bogliubov approach to obtain the explicit excitation energy spectrum and hence to investi-

[^0]gate the SMI phase transition.
We begin with the following second-quantized Hamiltonian operator [3] for the system of bosonic atoms in the optical lattice:
\[

$$
\begin{align*}
\hat{H}= & \int d \mathbf{x} \hat{\psi}^{\dagger}(\mathbf{x})\left(-\frac{\hbar^{2}}{2 m} \nabla^{2}+V_{0}(\mathbf{x})+V_{T}(\mathbf{x})\right) \hat{\psi}(\mathbf{x}) \\
& +\frac{g}{2} \int d \mathbf{x} \hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}(\mathbf{x}) \hat{\psi}(\mathbf{x}) \tag{1}
\end{align*}
$$
\]

where $\hat{\psi}(\mathbf{x})$ and $\hat{\psi}^{\dagger}(\mathbf{x})$ denote the boson field operators which obey the boson commutation relation

$$
\begin{equation*}
\left[\hat{\psi}(\mathbf{x}), \hat{\psi}^{\dagger}\left(\mathbf{x}^{\prime}\right)\right]=\delta\left(\mathbf{x}-\mathbf{x}^{\prime}\right) \tag{2}
\end{equation*}
$$

Here $V_{0}(\mathbf{x})=\sum_{j=1}^{3} V_{j 0}(\mathbf{x}) \sin ^{2}\left(2 \pi x_{j} / \lambda\right)$ is the potential of the optical lattice formed by the laser light of wavelength $\lambda$, and hence the lattice constant is $d=\lambda / 2 . V_{T}(\mathbf{x})$ denotes an external trap potential, and the interparticle interaction is approximated by the short-range potential $g \delta\left(\mathbf{x}-\mathbf{x}^{\prime}\right)$, where $g$ $=4 \pi a_{s} \hbar^{2} / m$ is the coupling constant with $a_{s}$ the s-wave scattering length. Expanding the field operator $\hat{\psi}(\mathbf{x})$ in the Wannier basis such that $\hat{\psi}(\mathbf{x})=\sum_{i} \hat{a}_{i} w\left(\mathbf{x}-\mathbf{x}_{i}\right)$, we obtain the Bose-Hubbard model

$$
\begin{equation*}
\hat{H}=-J \sum_{\langle i, j\rangle} \hat{a}_{i}^{\dagger} \hat{a}_{j}+\sum_{i} \varepsilon_{i} \hat{n}_{i}+\frac{1}{2} U \sum_{i} \hat{n}_{i}\left(\hat{n}_{i}-1\right), \tag{3}
\end{equation*}
$$

where $\hat{a}_{i}$ is the annihilation operator of a particle at the lattice site $i$, which is assumed as being in a state described by the Wannier function $w\left(\mathbf{x}-\mathbf{x}_{i}\right)$ of the lowest energy band localized on $i t h$ site. This leads to the assumption that the energy involved in the system is small compared to the excitation energies of the second band. $\mathbf{x}_{i}$ denotes the position of the ith local minimum of the optical potential and $\hat{n}_{i}$ $=\hat{a}_{i}^{\dagger} \hat{a}_{i}$ is the number operator. The annihilation and creation operators $\hat{a}_{i}$ and $\hat{a}_{i}^{\dagger}$ obey the canonical commutation relations $\left[\hat{a}_{i}, \hat{a}_{i}^{\dagger}\right]=\delta_{i j}$. The parameter $J$ is the hopping matrix element between adjacent sites $i$ and $j$, and is evaluated as

$$
\begin{equation*}
J=-\int d \mathbf{x} w^{*}\left(\mathbf{x}-\mathbf{x}_{i}\right)\left[-\frac{\hbar^{2}}{2 m} \nabla^{2}+V_{0}(\mathbf{x})\right] w\left(\mathbf{x}-\mathbf{x}_{j}\right) \tag{4}
\end{equation*}
$$

The energy offset of each lattice site, $\varepsilon_{i}=\int d \mathbf{x} V_{T}(\mathbf{x}) \mid w(\mathbf{x}$ $\left.-\mathbf{x}_{i}\right)\left.\right|^{2} \approx V_{T}\left(\mathbf{x}_{i}\right)$, is assumed to be of the same value $\varepsilon$ in the present paper. The interparticle interaction is characterized by the parameter

$$
\begin{equation*}
U=g \int d \mathbf{x}|w(\mathbf{x})|^{4} \tag{5}
\end{equation*}
$$

For the sake of convenience we rewrite Hamiltonian (3) in the following form:

$$
\begin{equation*}
\hat{H}=\hat{H}_{0}+\frac{1}{2} U \sum_{i} \hat{n}_{i}\left(\hat{n}_{i}-1\right), \quad \hat{H}_{0}=\sum_{i, j} T_{i j} \hat{a}_{i}^{\dagger} \hat{a}_{j}, \tag{6}
\end{equation*}
$$

where

$$
T_{i j}=\left\{\begin{array}{cc}
\varepsilon & \text { for } i=j \\
-J & i, j \\
\text { are nearest neighbors, } \\
0 & \text { otherwise }
\end{array}\right.
$$

We see that the first part in Hamiltonian (6), $\hat{H}_{0}$, is the same as that of a simple lattice under tight-binding approximation (TBA) in solid-state physics, so we can rewrite $T_{i j}$ as

$$
\begin{equation*}
T_{i j}=N_{s}^{-1} \sum_{k} \varepsilon(k) \exp \left[i \mathbf{k} \cdot\left(\mathbf{x}_{i}-\mathbf{x}_{j}\right)\right] \tag{7}
\end{equation*}
$$

where $\mathbf{k}$ is the wave vector in the first Brillouin zone, $N_{s}$ is the total number of the lattice sites, and $\varepsilon(k)$ is the energy spectrum of the Hamiltonian $\hat{H}_{0}$. The inverse transformation is written as

$$
\begin{equation*}
\varepsilon(k)=N_{s}^{-1} \sum_{i, j} T_{i j} \exp \left[-i \mathbf{k} \cdot\left(\mathbf{x}_{i}-\mathbf{x}_{j}\right)\right] \tag{8}
\end{equation*}
$$

and can be approximated by $\varepsilon(k) \approx \varepsilon-\left(J / N_{s}\right) \sum_{\langle i j\rangle} \exp$ $\left[-i \mathbf{k} \cdot\left(\mathbf{x}_{i}-\mathbf{x}_{j}\right)\right]$ (TBA energy band) in simple cubic lattice. The explicit energy spectrum is seen to be

$$
\begin{equation*}
\varepsilon(k)=\varepsilon-J z \cos \left(\frac{k \lambda}{2}\right) \tag{9}
\end{equation*}
$$

where $z$ is the number of nearest neighbors of each site.
The existence of a finite gap in the excitation spectrum is the characteristic of the MIP. In Sec. II we attempt to determine the SMI phase transition condition from the energyband structure of the ultracold bosonic atoms in optical lattice in terms of Green function method. In Sec. III the Bogliubov transformation is used to obtain exact energy spectrum with which the superfluid phase is explained explicitly.

## II. GREEN FUNCTION APPROACH

We begin with the operators $\hat{a}_{i}(t), \hat{a}_{j}^{\dagger}\left(t^{\prime}\right)$ in Heisenberg picture, i.e., $\hat{a}_{i}(t)=e^{i \hat{H} t} \hat{a}_{i} e^{-i \hat{H} t}$ and $\hat{a}_{j}^{\dagger}\left(t^{\prime}\right)=e^{i \hat{H} t^{\prime}} \hat{a}_{j}^{\dagger} e^{-i \hat{H} t^{\prime}}$
(in the unit of $\hbar=1$ ). The retarded single-particle Green function at zero temperature [9] is defined by

$$
\begin{align*}
\left\langle\left\langle\hat{a}_{i}(t) ; \hat{a}_{j}^{\dagger}\left(t^{\prime}\right)\right\rangle\right\rangle= & -i \theta\left(t-t^{\prime}\right)\left\langle\left[\hat{a}_{i}(t), \hat{a}_{j}^{\dagger}\left(t^{\prime}\right)\right]\right\rangle \\
= & -i \theta\left(t-t^{\prime}\right)\left\{\left\langle\hat{a}_{i}(t) \hat{a}_{j}^{\dagger}\left(t^{\prime}\right)\right\rangle\right. \\
& \left.-\left\langle\hat{a}_{j}^{\dagger}\left(t^{\prime}\right) \hat{a}_{i}(t)\right\rangle\right\} \tag{10}
\end{align*}
$$

where $\theta\left(t-t^{\prime}\right)$ is the step function:

$$
\theta\left(t-t^{\prime}\right)=\left\{\begin{array}{lc}
1, & t>t^{\prime} \\
0, & t<t^{\prime}
\end{array}\right.
$$

The Green function $\left\langle\left\langle\hat{a}_{i}(t) ; \hat{a}_{j}^{\dagger}\left(t^{\prime}\right)\right\rangle\right\rangle$ depends only on the time difference $\left(t-t^{\prime}\right)$. The Fourier transformation of the retarded Green function $\left\langle\left\langle\hat{a}_{i}(t) ; \hat{a}_{j}^{\dagger}(0)\right\rangle\right\rangle$ is seen to be

$$
\begin{aligned}
G_{i j}(\omega) \equiv & \left\langle\left\langle\hat{a}_{i} \mid \hat{a}_{j}^{\dagger}\right\rangle\right\rangle_{\omega}=\frac{1}{2 \pi} \int_{-\infty}^{\infty} d t\left\langle\left\langle\hat{a}_{i}(t) ; \hat{a}_{j}^{\dagger}(0)\right\rangle\right\rangle \exp [i(\omega \\
& +i \eta)], \quad \eta=+0
\end{aligned}
$$

for a real frequency $\omega$. Using Heisenberg equation, we obtain

$$
\begin{equation*}
\omega G_{i j}(\omega)=\left\langle\left[\hat{a}_{i}, \hat{a}_{j}^{\dagger}\right]\right\rangle+\left\langle\left\langle\left[\hat{a}_{i}, H\right] \mid \hat{a}_{j}^{\dagger}\right\rangle\right\rangle_{\omega}, \tag{11}
\end{equation*}
$$

which can be evaluated in terms of the commutation relation

$$
\begin{equation*}
\left[\hat{a}_{i}, \hat{H}\right]=\sum_{j} T_{i j} \hat{a}_{j}+U \hat{n}_{i} \hat{a}_{i} \tag{12}
\end{equation*}
$$

where $\rangle$ denotes the ground-state expectation value. The result is

$$
\begin{equation*}
\omega G_{i j}(\omega)=\delta_{i j}+\sum_{m} T_{i m} G_{m j}(\omega)+U \Gamma_{i j}(\omega) \tag{13}
\end{equation*}
$$

where

$$
\Gamma_{i j}(\omega) \equiv\left\langle\left\langle\hat{n}_{i} \hat{a}_{i} \mid \hat{a}_{j}^{\dagger}\right\rangle\right\rangle_{\omega}
$$

is the higher-order Green function which satisfies the following equation

$$
\begin{equation*}
\omega \Gamma_{i j}(\omega)=\left\langle\left[\hat{n}_{i} \hat{a}_{i}, \hat{a}_{j}^{\dagger}\right]\right\rangle+\left\langle\left\langle\left[\hat{n}_{i} \hat{a}_{i}, \hat{H}\right] \mid \hat{a}_{j}^{\dagger}\right\rangle\right\rangle_{\omega} \tag{14}
\end{equation*}
$$

It is easy to find

$$
\begin{align*}
{\left[\hat{n}_{i} \hat{a}_{i}, \hat{H}\right]=} & \varepsilon \hat{n}_{i} \hat{a}_{i}+\sum_{j(\neq i)} T_{i j} \hat{n}_{i} \hat{a}_{j}+\sum_{j} T_{i j( } \underline{\left.\hat{a}_{i}^{\dagger} \hat{a}_{j}-\hat{a}_{j}^{\dagger} \hat{a}_{i}\right)} \hat{a}_{i} \\
& +U{\underline{n_{i}}}_{i} \hat{n}_{i} \hat{a}_{i} \tag{15}
\end{align*}
$$

Substituting Eq. (15) into Eq. (14), we see that the obtained equation is not closed, because more higher order Green functions appear in the formula of $\Gamma_{i j}(\omega)$. We in this stage
use mean-field approximation for the underlined operators in Eq. (15), i.e., the number operator $\hat{n}_{i}$ is replaced by its expectation value $\left\langle\hat{n}_{i}\right\rangle$ :

$$
\begin{equation*}
\sum_{j} T_{i j} \hat{n}_{i} \hat{a}_{j} \approx \sum_{j} T_{i j}\left\langle\hat{n}_{i}\right\rangle \hat{a}_{j} \approx n_{0} \sum_{j} T_{i j} \hat{a}_{j} \tag{16}
\end{equation*}
$$

In the above approximation we have assumed that the average occupation number of Bose atoms condensed on ground state in each site of the optical lattice is the same, i.e., $\left\langle\hat{n}_{i}\right\rangle$ $\equiv n_{0}$ 。

Since the obvious symmetry of $\varepsilon(k)=\varepsilon(-k)$, we have the equality $T_{i j}=T_{j i}$ according to Eq. (8). Utilizing translation symmetry of the Bose system we moreover obtain

$$
\begin{equation*}
\sum_{j} T_{i j}\left(\left\langle\hat{a}_{i}^{\dagger} \hat{a}_{j}\right\rangle-\left\langle\hat{a}_{j}^{\dagger} \hat{a}_{i}\right\rangle\right)=0 . \tag{17}
\end{equation*}
$$

Equation (15) is then simplified as

$$
\left[\hat{n}_{i} \hat{a}_{i}, \hat{H}\right] \approx\left(\varepsilon+U n_{0}\right) \hat{n}_{i} \hat{a}_{i}+n_{0} \sum_{j(\neq i)} T_{i j} \hat{a}_{j} .
$$

A closed equation for the Green function is seen to be

$$
\begin{equation*}
\omega \Gamma_{i j}(\omega)=2 n_{0} \delta_{i j}+n_{0} \sum_{m} T_{i m} G_{i j}(\omega)+\left(\varepsilon+U n_{0}\right) \Gamma_{i j}(\omega) \tag{18}
\end{equation*}
$$

from which we find

$$
\begin{equation*}
\Gamma_{i j}(\omega)=\frac{n_{0}}{\omega-\varepsilon-U n_{0}}\left(2 \delta_{i j}+\sum_{m(\neq i)} T_{i m} G_{m j}(\omega)\right) . \tag{19}
\end{equation*}
$$

Substitution of $\Gamma_{i j}(\omega)$ in Eq. (19) into Eq. (13) yields

$$
\begin{align*}
\omega G_{i j}(\omega)= & \delta_{i j}+\sum_{m} T_{i m} G_{m j}(\omega) \\
& +\frac{U n_{0}}{\omega-\varepsilon-U n_{0}}\left(2 \delta_{i j}+\sum_{m(\neq i)} T_{i m} G_{m j}(\omega)\right), \tag{20}
\end{align*}
$$

which is the equation for the site space Green function $G_{i j}(\omega)$. The Green function $G_{i j}(\omega)$ is a function of the position difference $\left(\mathbf{x}_{i}-\mathbf{x}_{j}\right)$ of two sites only for a system with translational invariance. Equation (20) for the Green function $G_{i j}(\omega)$ can be solved with the Fourier transformation. To this end we express the site space operator $\hat{a}_{i}$ in terms of the wave-vector-space operator $\hat{a}_{k}$ as

$$
\begin{gather*}
\hat{a}_{i}=\frac{1}{\sqrt{N_{s}}} \sum_{k} e^{i \mathbf{k} \cdot \mathbf{x}_{i}} \hat{a}_{k}, \\
\hat{a}_{i}^{\dagger}=\frac{1}{\sqrt{N_{s}}} \sum_{k} e^{-i \mathbf{k} \cdot \mathbf{x}_{i}} \hat{a}_{k}^{\dagger} . \tag{21}
\end{gather*}
$$



FIG. 1. Excitation spectrum and energy gap.
We can prove that the single-particle Green function in the Bloch representation is orthogonal, i.e.,

$$
\begin{aligned}
G_{k k^{\prime}}(\omega) & \equiv\left\langle\left\langle\hat{a}_{k} \mid \hat{a}_{k^{\prime}}^{\dagger}\right\rangle\right\rangle_{\omega} \\
& =\frac{1}{N} \sum_{i, j} e^{-i \mathbf{k} \cdot \mathbf{x}_{i}} e^{i \mathbf{k}^{\prime} \cdot \mathbf{x}_{j}}\left\langle\left\langle\hat{a}_{i} \mid \hat{a}_{j}^{\dagger}\right\rangle\right\rangle_{\omega} \\
& =\delta_{k k^{\prime}} G_{k}(\omega)
\end{aligned}
$$

where $G_{k}(\omega)=\left\langle\left\langle\hat{a}_{k} \mid \hat{a}_{k}^{\dagger}\right\rangle\right\rangle_{\omega}$ denotes the orthogonal Green function in Bloch representation. The Fourier transformation of the Green function $G_{i j}(\omega)$ is then seen to be

$$
\begin{equation*}
G_{i j}(\omega)=\frac{1}{N_{s}} \sum_{k} e^{i \mathbf{k} \cdot\left(\mathbf{x}_{i}-\mathbf{x}_{j}\right)} G_{k}(\omega) \tag{22}
\end{equation*}
$$

Substituting Eq. (22) into Eq. (20) the single-particle Green function in the Bloch representation is explicitly obtained as

$$
\begin{equation*}
G_{k}(\omega)=\frac{\omega-\varepsilon+U n_{0}}{[\omega-\varepsilon(k)]\left(\omega-\varepsilon-U n_{0}\right)-U n_{0}[\varepsilon(k)-\varepsilon]} . \tag{23}
\end{equation*}
$$

We can rewrite the solution in the following form:

$$
\begin{equation*}
G_{k}(\omega)=\frac{A_{k}^{(1)}}{\omega-E^{(1)}}+\frac{A_{k}^{(2)}}{\omega-E_{k}^{(2)}} \tag{24}
\end{equation*}
$$

where $E^{(1)}$ and $E_{k}^{(2)}$ denote the poles of the Green function $G_{k}(\omega)$, and it is seen that the excitation spectrum possesses a band structure such as

$$
\begin{equation*}
E^{(1)}=\varepsilon, \quad E_{k}^{(2)}=\varepsilon(k)+U n_{0} \tag{25}
\end{equation*}
$$

The lowest band shrinks to a single level of zero bandwidth (see Fig. 1). Although the energy spectrum Eq. (25) comprises two parts, they may, in a certain case depending on the relative values of the interatomic repulsion $U$ and the tunnel coupling $J$, be merged into the same energy band. The energy gap between the two bands is (Fig. 1)

$$
\Delta=\left.E_{k}^{(2)}\right|_{k=0}-E^{(1)}=U n_{0}-J z
$$

When the constant of the interatomic repulsion $U$ is large with respect to the tunnel coupling $J$ such that $\Delta>0$, a gap exists implying the MIP. With increase in tunnel coupling $J$ the gap width $\Delta$ decreases and finally the two energy bands in the excitation spectrum overlap and the gap disappears, indicating the SFP. We then obtain the condition of SMI phase transition that

$$
\begin{equation*}
\Delta=0 \tag{26}
\end{equation*}
$$

namely,

$$
\begin{equation*}
\frac{U}{z J}=\frac{1}{n_{0}} \tag{27}
\end{equation*}
$$

which agrees with the result in Refs. [2,8,10,11].
To see the SFP more closely we take the zero wave-vector limit of the energy band $E_{k}^{(2)}(k \rightarrow 0)$,

$$
E_{k}^{(2)} \sim \varepsilon-J z+U n_{0}+\frac{1}{2^{3}} J z \lambda^{2} k^{2}
$$

Under the condition (27) at which the energy gap between $E^{(1)}$ and $E_{k}^{(2)}$ disappears, we have a gapless Goldstone mode in the excitation spectrum such as

$$
\begin{equation*}
E_{\text {exc }} \sim \frac{1}{2^{3}} J z \lambda^{2} k^{2} \tag{28}
\end{equation*}
$$

which is different from the result of Bogoliubov theory for the system of weakly interacting bosons, in the absence of the periodic potential, where the wave-vector dependence of the excitation spectrum is linear in the zero wave-vector limit so that a nonvanishing velocity can exist. Strictly speaking what we obtained here is an ordinary fluid phase. The energy spectrum of Eq. (25) determined with the help of Green function method is too simple to realize the superfluid phase explicitly. This may be due to the particular procedure of the approximation used in the above derivation. It is certainly of interest to study the spectrum of bosonic atoms in the BEC trapped in the optical lattice in terms of Bogliubov method to see whether or not the system can possess a superfluid phase which we are going to discuss in the following section.

It is worthwhile to point out that when the interaction between bosons vanishes, i.e., $U=0$, the Green function (23) reduces to the well-known single band solution

$$
\begin{equation*}
\left.G_{k}(\omega)\right|_{U=0}=\frac{1}{\omega-\varepsilon(k)} \tag{29}
\end{equation*}
$$

for bosons in a periodic potential.

## III. BOGLIUBOV METHOD

Now we study the energy spectrum of boson atoms in the optical lattice by means of the Bogliubov method. Using relation(21), Hamiltonian (6) can be converted into

$$
\begin{gather*}
\hat{H}=\sum_{k} \varepsilon(k) \hat{a}_{k}^{\dagger} \hat{a}_{k}+\hat{H}_{\text {int }}, \\
\hat{H}_{\text {int }}=\frac{U}{2 N_{s}} \sum_{k, p, k, p} \delta_{k+p, k^{\prime}+p^{\prime}} \hat{a}_{k^{\prime}}^{\dagger} \hat{a}_{p^{\prime}}^{\dagger} \hat{a}_{k} \hat{a}_{p} \tag{30}
\end{gather*}
$$

Since the number of atoms condensed in the zero-momentum state is much larger than one, we have $\hat{a}_{0} \hat{a}_{0}^{\dagger}=\hat{a}_{0}^{\dagger} \hat{a}_{0}+1 \simeq N_{0}$ $\gg 1$, where $N_{0}$ is the total number of condensed atoms. Thus, we can replace the operator $\hat{a}_{0}$ and $\hat{a}_{0}^{\dagger}$ with a " $c$ " number $\sqrt{N_{0}}$. The interacting part of Hamiltonian (30) can be written as (in the order of $N_{0}$ )

$$
\hat{H}_{\text {int }}=\frac{U}{2 N_{s}} N_{0}^{2}+\frac{U N_{0}}{2 N_{s}} \sum_{k}^{\prime}\left(\hat{a}_{k} \hat{a}_{-k}+\hat{a}_{k}^{\dagger} \hat{a}_{-k}^{\dagger}+2 \hat{a}_{k}^{\dagger} \hat{a}_{k}\right)
$$

and the total Hamiltonian is

$$
\begin{align*}
\hat{H}= & \frac{U N_{0}^{2}}{2 N_{s}}+N_{0}(\varepsilon-z J)+\sum_{k}^{\prime}\left\{\frac{U n_{0}}{2}\left(\hat{a}_{k} \hat{a}_{-k}+\hat{a}_{k}^{\dagger} \hat{a}_{-k}^{\dagger}\right)\right. \\
& \left.+\left(\varepsilon(k)+U n_{0}\right) \hat{a}_{k}^{\dagger} \hat{a}_{k}\right\} \tag{31}
\end{align*}
$$

where $\Sigma_{k}^{\prime}$ denotes the sum with exclusion of the term of $k$ $=0$.

The following Bogoliubov transformation is introduced in order to diagonalize the Hamiltonian (31):

$$
\begin{align*}
& \hat{b}_{k}=u_{k} \hat{a}_{k}+v_{k} \hat{a}_{-k}^{\dagger}, \\
& \hat{b}_{k}^{\dagger}=u_{k} \hat{a}_{k}^{\dagger}+v_{k} \hat{a}_{-k} . \tag{32}
\end{align*}
$$

We require that the quasiboson operators $\hat{b}_{k}$ and $\hat{b}_{k}^{\dagger}$ satisfy the usual commutation relation $\left[\hat{b}_{k}, \hat{b}_{k}^{\dagger}\right]=1$, which leads to the condition

$$
\begin{equation*}
u_{k}^{2}-v_{k}^{2}=1 \tag{33}
\end{equation*}
$$

for the coefficients $u_{k}$ and $v_{k}$ and then the Hamiltonian can be written as

$$
\hat{H}=E_{c}+\hat{H}_{1}+\hat{H}_{2}
$$

where

$$
\begin{equation*}
E_{c}=\frac{1}{2} U N_{0} n_{0}+N_{0}(\varepsilon-z J) \tag{34}
\end{equation*}
$$

is a constant and

$$
\begin{equation*}
\hat{H}_{1}=\sum_{k}^{\prime}\left[\left(u_{k}^{2}+v_{k}^{2}\right)\left(\bar{\varepsilon}_{k}+U n_{0}\right)-2 U n_{0} u_{k} v_{k}\right] \hat{b}_{k}^{\dagger} \hat{b}_{k} \tag{35}
\end{equation*}
$$

$$
\begin{align*}
\hat{H}_{2}= & \sum_{k}^{\prime}\left(\frac{U n_{0}}{2}\left(u_{k}^{2}+v_{k}^{2}\right)-\left(\bar{\varepsilon}_{k}+U n_{0}\right) u_{k} v_{k}\right)\left(\hat{b}_{k} \hat{b}_{-k}\right. \\
& \left.+\hat{b}_{k}^{\dagger} \hat{b}_{-k}^{\dagger}\right) \tag{36}
\end{align*}
$$

To eliminate the off-diagonal part $\hat{H}_{2}$ we require

$$
\begin{equation*}
\frac{U n_{0}}{2}\left(u_{k}^{2}+v_{k}^{2}\right)-\left(\bar{\varepsilon}_{k}+U n_{0}\right) u_{k} v_{k}=0 \tag{37}
\end{equation*}
$$

where $\bar{\varepsilon}_{k}=z J[1-\cos (k d)]$. Introducing a parameter $\phi_{k}$ such that

$$
u_{k}=\cosh \phi_{k}, \quad v_{k}=\sinh \phi_{k},
$$

conditions (33) and (37) lead to the useful relations

$$
\begin{gathered}
\tan \phi_{k}=\frac{2 u_{k} v_{k}}{u_{k}^{2}+v_{k}^{2}}=\frac{U n_{0}}{\bar{\varepsilon}_{k}+U n_{0}}, \\
u_{k}^{2}+v_{k}^{2}=\cosh \left(2 \phi_{k}\right)=\frac{\bar{\varepsilon}_{k}+U n_{0}}{E_{k}}
\end{gathered}
$$

with which the diagonalized Hamiltonian is obtained as

$$
\hat{H}=E_{c}+\sum_{k} E_{k} \hat{b}_{k}^{\dagger} \hat{b}_{k}
$$

where the energy spectrum $E_{k}$ of quasiparticle is

$$
\begin{equation*}
E_{k}=\sqrt{\bar{\varepsilon}_{k}\left(\bar{\varepsilon}_{k}+2 U n_{0}\right)} \tag{38}
\end{equation*}
$$

The energy spectrum is different from that of Eq. (25) and is typical for the superfluid. The energy gap $\Delta_{g}$ of excitation spectrum is obviously

$$
\begin{equation*}
\Delta_{g}=\frac{E_{c}-N_{0} \varepsilon}{N_{0}}=\frac{1}{2} U n_{0}-z J . \tag{39}
\end{equation*}
$$

The phase transition condition determined from $\Delta_{g}=0$ is

$$
\begin{equation*}
\frac{U}{2 z J}=\frac{1}{n_{0}}, \tag{40}
\end{equation*}
$$

which shows a factor of 2 difference comparing with the condition in Eq. (27). This may be caused by the approximation itself. When the energy gap disappears, i.e., $\Delta_{g}=0$, the dispersion relation of $E_{k}(k \rightarrow 0)$ reads

$$
\begin{equation*}
E_{k} \sim\left(z J U n_{0} d^{2}\right)^{1 / 2} k \tag{41}
\end{equation*}
$$

indicating explicitly the superfluidity in agreement with the Bogliubov superfluid theory for weakly interacting bosons in the absence of the periodic potential. The linear wave-vector dependence of the excitation spectrum $E_{k}$ [unlike the ordinary fluid (28) where $E_{\text {exc }}$ is proportional to $k^{2}$ ] is the characteristic of the superfluid which gives rise to a persistent velocity of superfluid or quasiparticle found as

$$
\begin{equation*}
v_{s}=\left(\frac{\partial E_{k}}{\partial k}\right)_{k \rightarrow 0}=\left(z J U n_{0} d^{2}\right)^{1 / 2} \tag{42}
\end{equation*}
$$

For the case of boson atoms with repulsive interaction ( $a_{s}$ $>0$ ), the parameters $J$ and $U$ are positive and $v_{s}$ is a real number which implies a persistent current. The velocity $v_{s}$ can be controlled by the tuning of laser lights which result in the optical lattice. As seen from the definitions (4) and (5) for $J$ and $U$, both these parameters depend on the Wannier functions which are essentially determined by the potential of optical lattice. Therefore, $J$ and $U$ are not independently tunable by the adjusting of the laser parameters. In fact when the depth of the lattice potential increases, the hopping matrix element $J$ decreases exponentially while the matrix element of the on-site interaction, $U$, increases. We thereby expect that there exist a maximum value of the persistent velocity $v_{s}$ in some particular values of $J$ and $U$.

## IV. CONCLUSION

We have studied the Bose-Hubbard model of BEC trapped in a periodic potential in terms of Green function method and Bogliubov transformation as well. The condition of phase transition between SFP and MIP is determined by the energy-band structure of the excitation spectrum due to, obviously, the competition between the interatomic repulsion and the tunnel coupling. Our result agrees with the condition of SMI phase transition obtained in the literature. The SFP property of BEC in the optical lattice is explained explicitly from energy spectrum derived by means of the Bogliubov approach. It is shown that the persistent velocity of the quasiparticle in SFP can be tuned by the adjusting of the laser lights which result in the optical lattice.

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[1] M. Ben Dahan, E. Peik, J. Reichel, Y. Castin, and C. Salomon, Phys. Rev. Lett. 76, 4508 (1996); S.R. Wilkinson, C.F. Bharucha, K.W. Madison, Q. Niu, and M.G. Raizen, ibid. 76, 4512 (1996); M. Raizen, C. Salomon, and Q. Niu, Phys. Today $\mathbf{5 0}$ (7), 30 (1997); D.I. Choi and Q. Niu, Phys. Rev. Lett. 82, 2022 (1999); O. Morsch, J.H. Müller, M. Cristiani, D. Ciampini, and E. Arimondo, ibid. 87, 140402 (2001); W.M. Liu, B.

Wu, and Q. Niu, ibid. 84, 2294 (2000); W.M. Liu, W.B. Fan, W.M. Zheng, J.Q. Liang, and S.T. Chui, ibid. 88, 170408 (2002).
[2] M.P.A. Fisher, P.B. Weichman, G. Grinstein, and D.S. Fisher, Phys. Rev. B 40, 546 (1989).
[3] D. Jaksch, C. Bruder, J.I. Cirac, C.W. Gardiner, and P. Zoller, Phys. Rev. Lett. 81, 3108 (1998).
[4] G.H. Chen and Y.S. Wu, Phys. Rev. A 67, 013606 (2003).
[5] E. Demler and F. Zhou, Phys. Rev. Lett. 88, 163001 (2002).
[6] S. Tsuchiya, S. Kurihara, and T. Kimura, e-print cond-mat/0209676.
[7] M. Greiner, O. Mandel, T. Esslinger, T.W. Hansch, and I. Bloch, Nature (London) 415, 39 (2002).
[8] D. van Oosten, P. van der Straten, and H.T.C. Stoof, Phys. Rev.

A 63, 053601 (2001).
[9] A. L. Fetter and J. D. Walecka, Quantum Theory of ManyParticle System (McGraw-Hill, New York, 1971).
[10] J.K. Freericks and H. Monien, Europhys. Lett. 26, 545 (1994).
[11] K. Sheshadri, H.R. Krishnamurthy, R. Pandit, and T.V. Ramakrishnan, Europhys. Lett. 22, 257 (1993).


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