Mott-Hubbard transition of bosons in optical lattices with two-body interactions

YAN Hua-Hua(燕花花)[1] MA Qing-Shan(马青山)[2,1] ZHANG Jun(张军)[1;1)]

[1] College of Physics Science and Technology, Xinjiang University, Urumqi 830046, China
[2] Department of Physics, Xi'an Jiaotong University, Xi'an 710049, China

Abstract: In this paper, based on the Bose-Hubbard model with two-body on-site interactions, we study the quantum phase transition between the superfluid state and the Mott-insulator state. With the decoupling approximation, we get the relation between the weak superfluidity and dimensionless chemical potential with different particle number and different dimensionless interaction strength, and the relation between the weak superfluidity and the reciprocal of dimensionless interaction strength with different particle number. We also calculate the corresponding experimental parameters.

Key words: Bose-Hubbard model, two-body interaction, the weak superfluidity, dimensionless interaction strength, dimensionless chemical potential

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1 Introduction

Using the interference pattern of intersecting laser beams, one can create a periodic potential for atoms, which is known as an optical lattice [1, 2]. The optical lattice - initially from a cooling experiment on atoms - can now be widely used to confine ultracold atoms [3–8]. Impressive developments in the manipulation of ultracold atoms [Bose-Einstein condensates (BEC)] in optical lattices provide one of the best environments for the search for exotic quantum phases [9, 10], and an example of quantum phase transition is the Mott-insulator-superfluid transition [11–16]. The Bose-Hubbard model is introduced as the starting point of the theoretical studies, which can well describe the behavior of the BEC in the optical lattices [17–20].

Strongly correlated systems studied in condensed matter physics or in atomic physics are usually dominated by two-body interactions. However, it has been an intriguing question of pursuing some exotic phases associated with Hamiltonians with three- or more-body terms [21], while the two-body term can be tuned as external fields. This may lead to some interesting quantum phases when generalized to more complicated situations.

This paper is organized as follows. In Sec. 2, using the single bind approximation, we derive the Bose-Hubbard model for atoms in an optical lattice with two-body repulsive interaction. In Sec. 3, applying the decoupling approximation developed in Ref. [22, 23], we derive an effective on-site Hamiltonian in the strong-coupling limit. We also calculate the energy of this Hamiltonian applying perturbation theory and discuss the decoupling-Landau order parameter expansion. In Sec. 4, we calculate some experimental parameters and suggest some practical ways to confirm our results. In Sec. 5, we summarize our results.

2 The mode

The ultracold atoms interact through s-wave scattering in the general case. Then the Hamiltonian of the system reads [24]

$$\hat{H} = \int \mathrm{d}\boldsymbol{r}\hat{\Psi}^{\dagger}(\boldsymbol{r})\left[\frac{p^2}{2m}+V_{\mathrm{ext}}(\boldsymbol{r})-\mu\right]\hat{\Psi}(\boldsymbol{r}) + \frac{c}{2}\int \mathrm{d}\boldsymbol{r}\hat{\Psi}^{\dagger}(\boldsymbol{r})\hat{\Psi}^{\dagger}(\boldsymbol{r})\hat{\Psi}(\boldsymbol{r})\hat{\Psi}(\boldsymbol{r}), \quad (1)$$

where $\hat{\Psi}(\boldsymbol{r})$ is the boson field operator, $c=\dfrac{4\pi\hbar^2 a_{\mathrm{s}}}{m}$

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1) Corresponding author. E-mail: zhj@xju.edu.cn

the interaction strength with $a_{\rm s}$ the s-wave scattering length, μ the chemical potential introduced here to keep the conservation of the number of atoms in the grand-canonical ensemble, $V_{\rm ext}(\boldsymbol{r})$ the trapping potential often expressed as follows in the case of an optical lattice,

$$V_{\rm ext}(\boldsymbol{r}) = \sum_{d=x,y,z} V_d^{\rm opt} \sin^2(\pi x_d/L_d), \tag{2}$$

where L_d is the width of the lattice in the d-th direction with d running over the dimensions of the lattice, and $L_d = \lambda/2$ for the lattices created by counter-propagating laser beams of wavelength λ, $V_d^{\rm opt}$ is the depth of the lattice potential, which depends on the strength of the laser light.

For a single atom in the periodic potential, the energy eigenstates are Bloch states. Appropriate superposition of the Bloch states can produce a set of Wannier functions $\omega_i(\boldsymbol{r})$, and in the limit of tight-banding, $\omega_i(\boldsymbol{r})$ is well localized in the ith lattice site. So it is convenient to apply the Wannier description.

In the single bind approximation, the field operator $\hat{\Psi}(\boldsymbol{r})$ can be replaced by its single-mode expansion,

$$\hat{\Psi}(\boldsymbol{r}) = \sum_i \omega_i(\boldsymbol{r})\hat{b}_i, \tag{3}$$

and Eq. (1) reduces to the Bose-Hubbard model,

$$\hat{H} = -J\sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{1}{2}U\sum_i \hat{b}_i^\dagger \hat{b}_i^\dagger \hat{b}_i \hat{b}_i - \mu \sum_i \hat{b}_i^\dagger \hat{b}_i, \tag{4}$$

where $\langle i,j\rangle$ sums for all of the sets of nearest neighbor sites, and $\hat{b}_i^\dagger$ and $\hat{b}_i$ are the bosonic creation and destruction operators for the atom at site i. J is the hopping matrix element between the neighboring sites i and j, defined as

$$J = -\int {\rm d}\boldsymbol{r}\omega_i(\boldsymbol{r}) \left[\frac{p^2}{2m} + V_{\rm ext}(\boldsymbol{r})\right] \omega_j(\boldsymbol{r}), \tag{5}$$

the parameter U is the two-body repulsive interaction strength between bosons on the lattice site i, defined as

$$U = c\int {\rm d}\boldsymbol{r}|\omega_i(\boldsymbol{r})|^4. \tag{6}$$

The density operator on the site i is $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$, and $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$. Therefore, Eq. (4) can be rewritten as

$$\hat{H} = -J\sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i. \tag{7}$$

3 Decoupling approximation

In order to study the SF-MI transition, we use the decoupling approximation as follows,

$$\begin{aligned}\hat{b}_i^\dagger \hat{b}_j \;=\; & (\hat{b}_i^\dagger - \langle \hat{b}_i^\dagger\rangle)(\hat{b}_j - \langle \hat{b}_j\rangle) + \langle \hat{b}_i^\dagger\rangle \hat{b}_j \\ & + \hat{b}_i^\dagger \langle \hat{b}_j\rangle - \langle \hat{b}_i^\dagger\rangle\langle \hat{b}_j\rangle. \end{aligned} \tag{8}$$

Ignoring the second order fluctuation, this can be reduced to

$$\hat{b}_i^\dagger \hat{b}_j \sim \langle \hat{b}_i^\dagger\rangle \hat{b}_j + \hat{b}_i^\dagger \langle \hat{b}_j\rangle - \langle \hat{b}_i^\dagger\rangle\langle \hat{b}_j\rangle, \tag{9}$$

As we look forward to the superfluid phase, in the strong-coupling limit, $t \ll U_{\rm min}$. Therefore, the introduction of the superfluid order parameter is very convenient,

$$\psi = \sqrt{\hat{n}_i} = \langle \hat{b}_i^\dagger\rangle = \langle \hat{b}_i\rangle, \tag{10}$$

and the hopping term in Eq. (7) can be rewritten as

$$\hat{b}_i^\dagger \hat{b}_j \sim \psi(\hat{b}_i^\dagger + \hat{b}_j) - \psi^2. \tag{11}$$

Then Eq. (7) becomes the effective Hamiltonian,

$$\begin{aligned}\hat{H}^{\rm eff} \;=\; & -zJ\sum_i (\hat{b}_i^\dagger + \hat{b}_i) + zJ\psi^2 N_{\rm s} \\ & + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i, \end{aligned} \tag{12}$$

where z is the coordination number of a D-dimensional optical lattice ($z = 2D$), and $N_{\rm s}$ is the total number of the lattice sites. With regard to the site index i, this Hamiltonian is diagonal. If we introduce $\overline{U} = U/zJ$ and $\overline{\mu} = \mu/zJ$, Eq. (12) can be rewritten as

$$\hat{H}_i^{\rm eff} = \frac{\overline{U}}{2}\hat{n}_i(\hat{n}_i - 1) - \overline{\mu}\hat{n}_i + \psi^2 - \psi(\hat{b}_i^\dagger + \hat{b}_i), \tag{13}$$

where $\overline{U}$ is the dimensionless interaction strength and $\overline{\mu}$ is the dimensionless chemical potential. This on-site Hamiltonian is effective on every site i, so we will drop the index i in the follow discussions.

3.1 Perturbation theory

In this section, we use perturbation theory to calculate the energy of Eq. (13) in the strong-coupling regime. To achieve this, we will treat the last term in Eq. (13) as a perturbation $-\psi(\hat{b}_i^\dagger + \hat{b}_i) = -\psi\hat{V}$ with $\hat{V} = -(\hat{b}_i^\dagger + \hat{b}_i)$ the perturbation term. We separate Eq. (13) in two parts,

$$\hat{H}^{\rm eff} = \hat{H}^{(\rm o)} + \psi\hat{V}, \tag{14}$$

with the unperturbed Hamiltonian $\hat{H}^{(\rm o)} = \dfrac{\overline{U}}{2}\hat{n}(\hat{n} - 1) - \overline{\mu}\hat{n} + \psi^2$. The corresponding ground-state energy is

$$E_g^{(0)} = \{E_n^{(0)}|_{n=0,1,2,\cdots}\}_{\rm min} = \frac{\overline{U}}{2}g(g-1) - \overline{\mu}g, \tag{15}$$

where $E_n^{(0)}$ means the unperturbed energy of states with integer fillings, and g is an integer specifying the average number of particles on a lattice site.

In the occupation number basis, the odd powers of the extension of Eq. (14) with regard to ψ disappear. Hence, we only calculate the second- and fourth-order corrections to the ground-state energy,

$$E_g^{(2)} = \sum_{n\neq g}\frac{|\langle n|\hat{V}|g\rangle|^2}{E_g^{(0)}-E_n^{(0)}} = \sum_{n=g+1}\frac{|\langle n|\hat{b}_i^{\dagger}|g\rangle|^2}{E_g^{(0)}-E_n^{(0)}}\psi^2 + \sum_{n=g-1}\frac{|\langle n|\hat{b}_i|g\rangle|^2}{E_g^{(0)}-E_n^{(0)}}\psi^2 = a_2\psi^2, \tag{16}$$

with

$$a_2 = \frac{g+1}{\overline{\mu}-g\overline{U}} + \frac{g}{(g-1)\overline{U}-\overline{\mu}}, \tag{17}$$

and

$$E_g^{(4)} = \sum_{n,p,q\neq g}|\langle n|\hat{V}|g\rangle|\left[-E_g^{(2)}\frac{|\langle n|\hat{V}|g\rangle|}{(E_g^{(0)}-E_n^{(0)})^2} + \frac{|\langle n|\hat{V}|p\rangle}{E_g^{(0)}-E_n^{(0)}}\frac{|\langle p|\hat{V}|q\rangle}{E_g^{(0)}-E_p^{(0)}}\frac{|\langle q|\hat{V}|g\rangle}{E_g^{(0)}-E_q^{(0)}}\right] = a_4\psi^4, \tag{18}$$

with

$$a_4 = \frac{g}{[(g-1)\overline{U}-\overline{\mu}]^2}\cdot\frac{g-1}{[(2g-3)\overline{U}-2\overline{\mu}]} + \frac{g+1}{(\overline{\mu}-g\overline{U})^2}\cdot\frac{g+2}{[2\overline{\mu}-(2g+1)\overline{U}]} - \left[\frac{g+1}{\overline{\mu}-g\overline{U}}+\frac{g}{(g-1)\overline{U}-\overline{\mu}}\right]\cdot\left\{\frac{g+1}{(\overline{\mu}-g\overline{U})^2} + \frac{g}{[(g-1)\overline{U}-\overline{\mu}]^2}\right\}, \tag{19}$$

and here, $|n\rangle$, $|p\rangle$, $|q\rangle$ mean the unperturbed states with n, p and q particles.

3.2 Decoupling-Landau order parameter expansion

In Section 3.1, we have calculated the second- and fourth-order corrections to the ground-state energy, so the ground-state energy modified by adding the second- and fourth-order corrections becomes $E_g(\psi) = E_g^{(0)} + E_g^{(2)} + E_g^{(4)}$. Applying perturbation theory, we find that $E_g(\psi)$ has the structure as an expansion in ψ,

$$E_g(\psi) = a_0(g,\overline{U},\overline{\mu}) + [1+a_2(g,\overline{U},\overline{\mu})]\psi^2 + a_4(g,\overline{U},\overline{\mu})\psi^4, \tag{20}$$

where a_2 can be either positive or negative, but a_4 is always positive, meaning that the SMQPT is the second order. For given particle number g, we obtain the weak superfludity,

$$\psi^2 = -\frac{1+a_2}{2a_4}. \tag{21}$$

Here, we would like to make a remark on our decoupling-Landau expansion proposal, originally introduced in Refs. [22, 23]. From Eq. (21), we get the relation between ψ^2 and $\bar{\mu}$ with different g and different $\bar{U}$, and the relation between ψ^2 and $\bar{U}^{-1}$ with different g.

As shown in Fig. 1, Fig. 2 and Fig. 3, for the cases of the same particle number, the stronger the dimensionless interaction strength is, the larger the amplitude of superfluidity will be. When the dimensionless chemical potential reaches its maximum, ψ^2 disappears. So no matter how the dimensionless chemical potential increases, ψ^2 will not occur again. And the stronger the dimensionless interaction strength is, the larger the dimensionless chemical potential reaches its maximum will be.

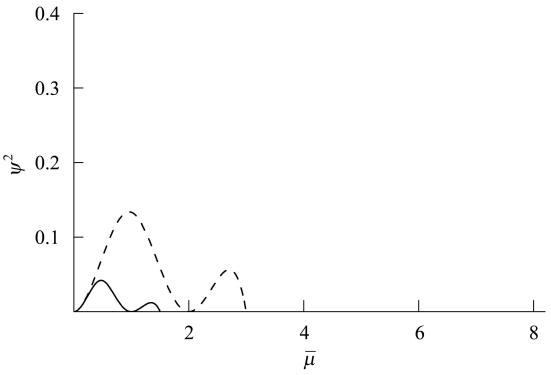

Fig. 1. g=1, with fixed $\bar{U}$ at $\bar{U}=1$, $\bar{U}=2$ and varying $\bar{\mu}$. The black line denotes $\bar{U}=1$, and the dashed line denotes $\bar{U}=2$.

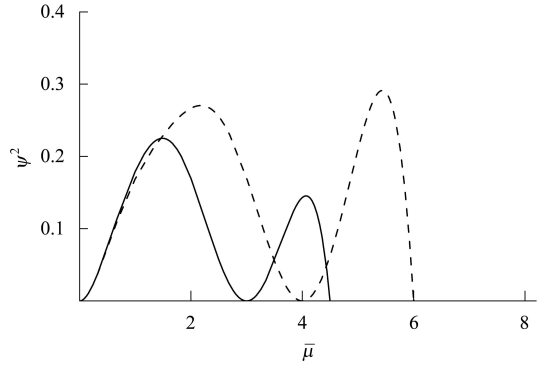

Fig. 2. g=1, with fixed $\bar{U}$ at $\bar{U}=3$, $\bar{U}=4$ and varying $\bar{\mu}$. The black line denotes $\bar{U}=3$, and the dashed line denotes $\bar{U}=4$.

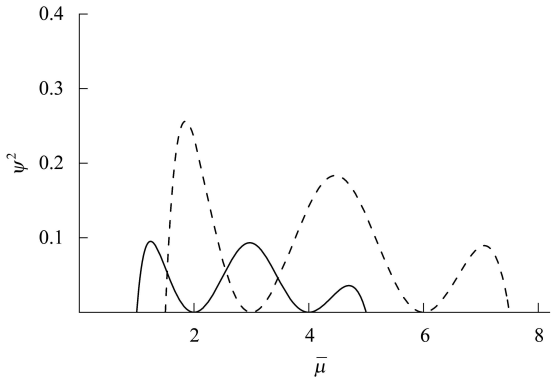

Fig. 3. g=2, with fixed $\bar{U}$ at $\bar{U}=2$, $\bar{U}=3$ and varying $\bar{\mu}$. The black line denotes $\bar{U}=2$, and the dashed line denotes $\bar{U}=3$.

As shown in Fig. 4, in the case of the same dimensionless interaction strength, the amplitude of superfluidity of g=2 is larger than that of g=1. And when ψ^2 vanishes, the dimensionless chemical potential of the critical point in the case of g=2 is larger than that of g=1.

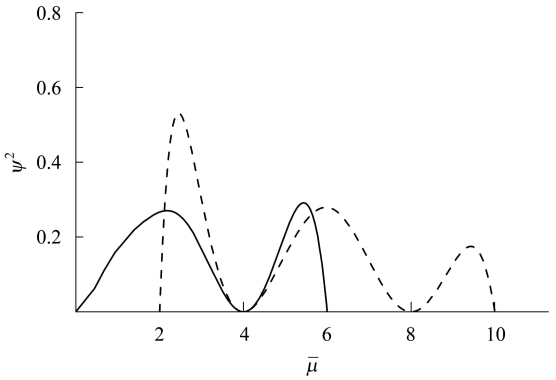

Fig. 4. $\bar{U}=4$, with fixed g at g=1, g=2 and varying $\bar{\mu}$. The black line denotes g=1, and the dashed line denotes g=2.

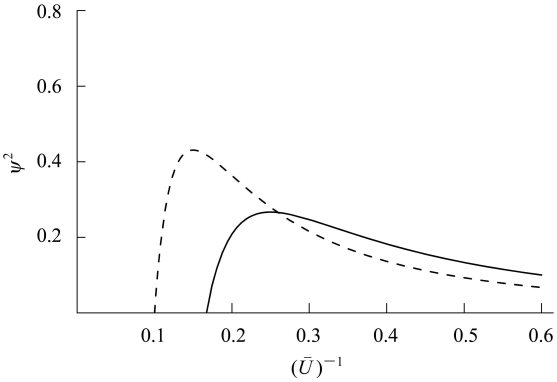

Fig. 5. $\bar{\mu}=(g-1/2)\bar{U}$, with fixed g at g=1, g=2 and varying $\bar{U}^{-1}$. The black line denotes g=1, and the dashed line denotes g=2.

As shown in Fig. 5, ψ^2 tends to decrease towards zero as the dimensionless interaction strength decreases. And ψ^2 decreases faster in the case of g=2 than that of g=1 as $\bar{U}$ decreases.

4 Calculation of experimental parameters

In the simplest case, three orthogonal, independent standing laser fields with wavevector k produce a separable 3-dimensional lattice potential,

$$\begin{aligned} V(x,y,z) &= V_0(\sin^2 kx+\sin^2 ky+\sin^2 kz) \\ &\approx V_0k^2(x^2+y^2+z^2), \end{aligned} \tag{22}$$

where $k=2\pi/\lambda$ is the wave vector of the laser light and V_0 the maximum depth of the lattice potential. In a deep optical with $V_0 \gg E_\mathrm{r}=\dfrac{\hbar^2k^2}{2m}$, and E_r is the recoil energy. The Wannier function at the lowest band in the well can be approximated as a Gaussian ground state,

$$\omega(\boldsymbol{r})=\left(\frac{\alpha^2}{\pi}\right)^{3/4}\exp\left(-\frac{1}{2}\alpha^2\boldsymbol{r}^2\right), \tag{23}$$

where

$$\alpha=\left(\frac{2mV_0k^2}{\hbar^2}\right)^{1/4}$$

is the characteristic of harmonic oscillators. Thus, Eq. (5) and Eq. (6) can be rewritten as

$$J = \frac{2}{\sqrt{\pi}}E_\mathrm{r}\left(\frac{V_0}{E_\mathrm{r}}\right)^{3/4}\exp\left[-2\left(\frac{V_0}{E_\mathrm{r}}\right)^{1/2}\right], \tag{24}$$

$$U = \sqrt{\frac{8}{\pi}}ka_\mathrm{s}E_\mathrm{r}\left(\frac{V_0}{E_\mathrm{r}}\right)^{3/4}. \tag{25}$$

Therefore, the dimensionless interaction strength $\overline{U}$ is

$$\overline{U}=\sqrt{2}ka_\mathrm{s}\exp\left[2\left(\frac{V_0}{E_\mathrm{r}}\right)^{1/2}\right]. \tag{26}$$

As we can see, in this section, the strength of two-body interaction is strong, which means that three-body effects can hardly be observed. This is consistent with the recent experiments [25] where the manipulation of two-body dimensionless interactions $\overline{U}$ is achieved by adjusting the depth of the optical potential V_0.

5 Conclusion

In conclusion, the superfluid-insulator transition with two-body interactions between optically trapped ultracold bosonic atoms is discussed. For the cases of the same particle number, the stronger the dimensionless interaction strength is, the larger the amplitude of superfluidity will be and the larger the dimensionless chemical potential reaching its maximum will be. When the dimensionless chemical potential reaches its maximum, the superfluidity disappears. And no matter how the dimensionless chemical potential increases, the superfluidity will not occur again. The phenomena are the same for the cases of the same dimensionless interaction strength with different particle number. In addition, the weak superfluidity tends to decrease towards zero as the dimensionless interaction strength decreases.

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