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Number statistics of ultracold bosons in an optical lattice

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Abstract

We study the number statistics of ultracold bosons in an optical lattice by performing quantum Monte Carlo simulations for a 1D Bose–Hubbard model with an external harmonic trap. We calculate the density profile of the system and observe the formation of a Mott plateau as the total number of atoms increases. We also calculate the average probability P_α for a particle to occupy the Fock state $|\alpha\rangle$ ($\alpha = 1, 2, 3,$ and 4), and confirm that the evolution of P_2 is a signature of the formation of a Mott insulator plateau in an ultracold atomic system. Our numerical result agrees qualitatively with the experiment and the mean field calculation.

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

1. Introduction

Ultracold atoms in optical lattices have opened new windows to investigating the strongly correlated systems with highly tunable parameters [1]. The basic physics of these ultracold atoms is captured by the Bose Hubbard model, whose most fundamental feature is the existence of a superfluid to Mott insulator phase transition at zero temperature [2, 3]. In a very shallow optical lattice, the ultracold bosons are in superfluid phase and can be well described by a macroscopic wavefunction with long-range phase coherence [4]. In this case, the phase fluctuation is zero and the on-site number fluctuation is large. When the optical lattice is very deep, the bosons enter the Mott insulating phase with fixed number of atoms per site and without phase coherence, i.e., the on-site number fluctuation is zero and the phase fluctuation is large [4, 5]. The physics of the MI phase is such that, when the repulsive interaction between the atoms is large enough, the number fluctuation becomes energetically unfavorable and the system enters a number-squeezed state. This interaction induced MI phase plays an important role in strongly correlated systems, as well as in various quantum information processing schemes [6].

In the past, some ultracold atom experiments have been performed to detect the number-squeezed MI phase through the observation of increased phase fluctuations [4, 5, 7] or through an increased timescale for phase diffusion [8]. Recently, the continuous suppression of on-site number fluctuations was directly observed by Gerbier *et al* by monitoring the suppression of spin-changing collisions across the superfluid/Mott insulator transition [9]. By using a far off-resonant microwave field, the spin oscillations for doubly occupied sites can be tuned into resonance and the amplitude of the spin oscillation is directly related to the probability of finding atom pairs per lattice site. It was shown by Gerbier *et al* that, for small atom number, the oscillation amplitude is increasingly suppressed with increasing lattice depths and completely vanishes for large lattice depths. In the MI region, this suppression persists up to some threshold number of atoms. The authors also compared their experimental results with the prediction of the Bose Hubbard model within a mean field approximation at zero temperature. In a recent paper [10], two of us extended mean field theory to include temperature and find a better fitting between the experimental data and the finite-temperature curves.

In this paper, we step out of the mean field theory area and perform quantum Monte Carlo (QMC) simulations for the 1D Bose–Hubbard model with an external harmonic trap. In the past, many authors have used quantum Monte Carlo simulations to study the Bose–Hubbard model [11]. However, the number statistics of the Bose–Hubbard model has not been studied in detail yet; this will be the major topic of this paper. A qualitative comparison of our numerical results with the experimental data and the mean field calculation will be performed.

This paper is organized as follows. In section 2, we will briefly introduce the Bose–Hubbard model, which can be used to describe ultracold bosons in an optical lattice. In section 3, we will perform quantum Monte Carlo simulations for the 1D Bose–Hubbard model with an external harmonic trap. In section 4, we will give our conclusions.

2. Ultracold bosons in an optical lattice: the Bose–Hubbard model

We consider an ultracold atomic gas trapped in a three-dimensional optical lattice potential, $V_0(\mathbf{r}) = V_0 \sum_{j=1}^{3} \sin^2(kr_j)$, with $k = 2\pi/\lambda$ being wavevectors and λ the laser wavelength. In real experiments, an additional harmonic trap V_i is superimposed on the lattice potential. If the optical lattice is deep enough, the above system can be well described by the following inhomogeneous Bose–Hubbard Hamiltonian [3]:

$$H = -t \sum_{\langle ij \rangle} a_i^\dagger a_j + \sum_i (V_i - \mu) n_i + \frac{U}{2} \sum_i n_i(n_i - 1). \quad (1)$$

Here $a_i^\dagger$ is the creation operator at site i, $n_i = a_i^\dagger a_i$ is the particle number operator, and $\langle ij \rangle$ denotes the sum over nearest neighbor sites. t and U are the hopping amplitude and on-site interaction, respectively:

$$t = \int \mathrm{d}\mathbf{r}\, w^*(\mathbf{r} - \mathbf{r}_i) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_0(\mathbf{r}) \right) w(\mathbf{r} - \mathbf{r}_j),$$
$$U = \frac{4\pi a_s \hbar^2}{m} \int \mathrm{d}\mathbf{r} |w(\mathbf{r})|^4, \quad (2)$$

where a_s is the s-wave scattering length and $w(\mathbf{r})$ is the Wannier function. For a given optical lattice potential, t and U can be evaluated numerically [3].

3. Numerical results: quantum Monte Carlo simulations in one dimension

Although mean field theory is applicable in three dimensions, its application in 1D is questionable due to the large quantum fluctuations. In this section, we will come to the numerical calculation and focus our study on the Bose–Hubbard model (1) in a harmonic trapped potential. The trapped potential that we use is

$$V_i = V_t i (i - L/2)^2 \quad (3)$$

where L is the chain length and $V_t = 0.02t$. The method that we use is quantum Monte Carlo (QMC) simulation using the stochastic series expansion (SSE) technique [12, 13]. In the simulations, the lattice is set large enough to allow neglect of the boundary effects and the inverse of temperature is chosen to be $\beta = 100t$ which is low enough to reach the ground state properties.

The density profile of the 1D Bose–Hubbard model in a harmonic trapped potential is shown in figure 1 with various chemical potentials. We can see that there is one $n = 1$ Mott plateau in the middle region of the trapped potential when the chemical potential μ is small (e.g. the curve with $\mu = 4t$). On both sides of the Mott plateau there are superfluid regions. As we increase the chemical potential, the total number of particles is increasing. Then a new superfluid region with density larger than 1 emerges (e.g. the curve with $\mu = 8t$). This superfluid region splits the Mott plateau into two parts and pushes them to the edges of the trapped potential. If the chemical potential is increased further, the $n = 2$ Mott plateaus will come out in the middle region of the trapped potential (see the curves with $\mu > 14$). In the density profile, the Mott plateaus and superfluid regions appear alternately to form a so-called 'wedding-cake' structure. Our calculations are consistent with the previous QMC work [11].

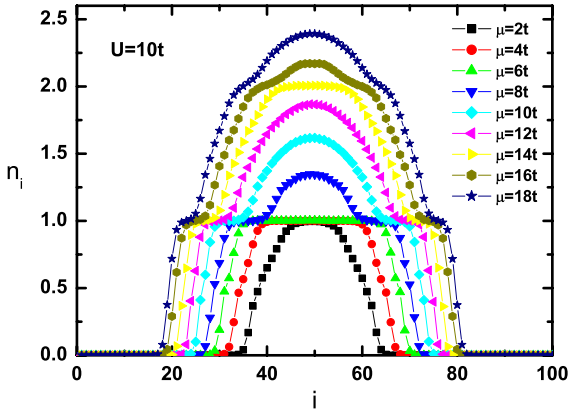

Figure 1. The particle density n_i at each lattice site i of a 1D inhomogeneous Bose–Hubbard model for various chemical potentials μ. The chain length is $L = 100$, the parameter of the trapped potential is $V_t = 0.02t$, and the interaction is $U = 10t$.

The local particle density n_i plotted in figure 1 can be decomposed into

$$n_i = \sum_{\alpha=1}^{\infty} n_{\alpha i}, \quad (4)$$

where $n_{\alpha i}$ is the density of particles occupying the Fock state $|\alpha\rangle$ at lattice site i. In order to study the number statistics of the bosonic gas in a harmonic trap, we plot $n_{\alpha i}$ ($\alpha = 1$, 2, 3, and 4) in figure 2 for various chemical potentials. When the chemical potential is small, the average particle density of the system is small. Most particles are in $|\alpha = 1\rangle$ state and the probability for the particle to occupy the $|\alpha > 1\rangle$ state is very small (see the curves with $\mu = 6t$). In this case, n_{1i} forms a plateau in the center of the trap, which corresponds to the $n = 1$ Mott plateau in figure 1. On increasing the chemical potential, a new superfluid region with average density $n > 1$ develops in the middle of the $n = 1$ Mott plateau as shown in figure 1. In this superfluid region, n_{1i} decreases, but n_{2i} and n_{3i} increase. Although n_{1i} drops in the center, there are still two shoulders on either side corresponding to the two small $n = 1$ Mott plateaus (see, e.g., the curve with $\mu = 10t$). The whole n_{1i} curve forms a 'U' shape. As the chemical potential increases further, the two legs of the 'U' shape are pushed to the edges of the trap. The evolution of the n_{2i} curve as the chemical potential increases is qualitatively the same as that of the n_{1i} curve. n_{2i} initially develops a peak as the chemical

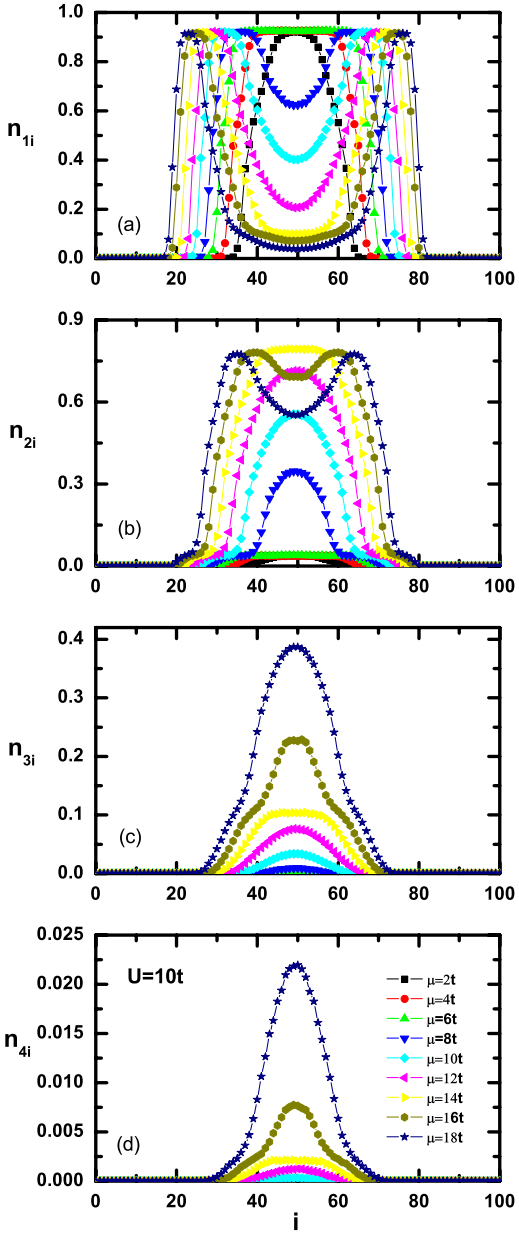

Figure 2. The density $n_{\alpha i}$ of atoms occupying the Fock state $|\alpha\rangle$ ($\alpha = 1, 2, 3$, and 4) at each lattice site i for various chemical potentials μ. The chain length is $L = 100$, the parameter of the trapped potential is $V_t = 0.02t$, and the interaction is $U = 10t$.

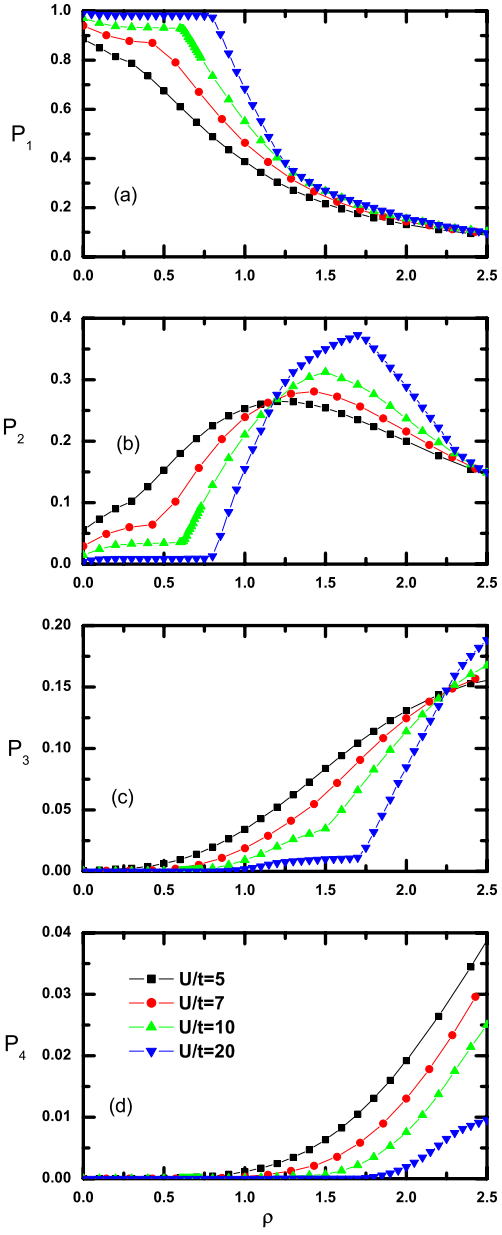

Figure 3. The probability P_α ($\alpha = 1, 2, 3$, and 4) as a function of average particle density ρ for various interactions U/t. P_α is the average probability for a particle to occupy the $|\alpha\rangle$ state over the whole lattice. The chain length is $L = 100$, and the parameter of trapped potential is $V_t = 0.02t$.

potential increases, then forms a plateau corresponding to the formation of the $n = 2$ Mott plateau. After that, n_{2i} drops in the center of the trap and forms a 'U' shape curve (see the sub-figure (b) in figure 2). The same thing happens to the n_{3i} and n_{4i} curves if the chemical potential is large enough.

In the number fluctuation experiment by Gerbier *et al* [9], the total number of atoms in the doubly occupied state (that is, the $|2\rangle$ state) is measured by the so-called spin-changing collisions method. After determining the total number for the system, it is easy to obtain the average probability of finding an atom in the doubly occupied state. In the following, we will calculate the average probability of double occupation of a 1D inhomogeneous system using SSE quantum Monte Carlo simulations. For the fixed interaction U/t and chemical potential μ, we can calculate the density $n_{\alpha i}$ of atoms occupying the $|\alpha\rangle$ state at each lattice site i, as shown in figure 2 for a special case of $U = 10t$. We define the average probability P_α as

$$P_\alpha = N_\alpha/N = \sum_i n_{\alpha i}/N, \tag{5}$$

where N is the total number of the 1D system and N_α is the total number of atoms occupying the $|\alpha\rangle$ state.

In figure 3, the probability P_α ($\alpha = 1, 2, 3$, and 4) is plotted as a function of average particle density $\rho = N/L$ for

various interaction U/t values. We can see from the figure that, as the average particle density ρ increases, P_1 monotonically decreases, and P_3 and P_4 monotonically increase. However, P_2 does not change monotonically with the increasing of ρ. We first focus on the region with small average particle density ρ. When the interaction U/t is small, both P_1 and P_2 are large, P_3 is small, and P_4 is very small. That is, the number of fluctuations of the system is large and therefore the system is in a superfluid state. When we increase the interaction, P_1 increases to 1, but P_2, P_3, and P_4 drop to zero, which means that almost all the atoms are in the $|\alpha = 1\rangle$ state. In this case, the $n = 1$ Mott plateau forms in the center of the system (see figure 1). Therefore, the observation of P_2 decreasing to zero with increase in the interaction in the small ρ region can provide evidence of the system entering the Mott insulator state. This suppression of P_2 with increase in interaction has been observed in an experiment of Geiber *et al* [9].

In the following, we particularly focus on the average probability of double occupation P_2 in the sub-figure (b) of figure 3. When the interaction is large (e.g. for the curve with $U/t = 20$), P_2 is very small in the small average density ρ region. At a typical value of density ρ_{c1}, P_2 suddenly increases and P_1 decreases sharply. This is due to the appearance of a superfluid region in the middle of the $n = 1$ Mott plateau (see figure 1). At the same time, n_{i1} in figure 2(a) begins to drop in the center of the trap. As ρ increases further, P_2 reaches its maximum at ρ_{c2} and then decreases with increase of ρ. The maximum of P_2 corresponds to the formation of the widest $n = 2$ Mott plateau in the middle of the trap. The following decrease of P_2 is due to the formation of a superfluid region in the middle of the $n = 2$ Mott plateau (see figure 1). The evolution of P_2 can also be understood from figure 2(b). When the interaction U/t decreases, both ρ_{c1} and ρ_{c2} move to small values. Note that the sudden decrease of P_2 corresponds to an increase of P_3.

Comparing with the number statistics experiment and the mean field theory, we can see that the behavior of P_2 in figure 3(b) agrees well qualitatively with the experimental measurement and mean field calculation (see figure 4 of [9] and figure 7 of [10]), although our simulation is based on a 1D system. Figure 3(b) has the same important feature as the experiment: that P_2 in the small ρ region is suppressed to zero with increase of the interaction, which is regarded as a signature of the formation of a Mott insulator. When the interaction is large, P_2 in figure 3(b) increases and decreases sharply at the typical values ρ_{c1} and ρ_{c2}, respectively. These two typical values of density have been observed in the number statistics experiment [9] as well as in the mean field calculations [9, 10]. In all, our QMC simulations for the 1D system have reproduced all the main features of the experiment and the mean field theory.

4. Conclusion

We have studied the number fluctuation of ultracold bosons in optical lattices using quantum Monte Carlo simulations. The ultracold bosonic gas in an optical lattice can be described using the Bose–Hubbard model, and therefore we performed QMC simulations for the one-dimensional Bose–Hubbard model with an external harmonic trap. We obtained the density profile of the system for various chemical potentials, and showed the formation of $n = 1$ and 2 Mott plateaus with increase in the total number of atoms. In order to investigate the number fluctuation, we calculated the average probability P_α for a particle to occupy the Fock state $|\alpha\rangle$ ($\alpha = 1$, 2, 3, and 4). We found that the evolution of P_2 is a signature of the formation of a Mott insulator plateau in the ultracold atomic system. Our numerical result for P_2 agrees qualitatively with the recent experimental data [9] and a mean field calculation [9, 10].

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Note added. Recently we become aware of parallel numerical work [14] which reaches similar conclusions.

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