From Mott Insulating to Superfluid in Optical Lattices

Phys 569 ESM Term Paper

Shu Chen

ABSTRACT

This essay introduces the Bose-Hubbard model (BHM), which describes the behavior of bosonic atoms in optical lattices with strong interactions. Then this model is applied to describe two phases: superfluid and Mott insulator. The phase diagram and experiments concerning this are also discussed in this essay.

1. Introduction

Since the realization of Bose-Einstein condensation in ultra cold dilute gases, atomic and molecular physics has stepped into a whole new chapter [1]. During the recent decade, using atoms confined in optical lattice to simulate strongly correlated electrons and to explore the physics nature has grasped great attention. With the ability to tune interaction between atoms through Feshbach resonances [2], and to generate strong optical periodic potential [3], we can achieve this goal. In this essay, I first develop Bose-Hubbard model (BHM) describing ultra-cold atoms in optical lattices, then two novel phases, superfluid and Mott insulating phases, coming from different limits are discussed based on BHM and simulations. Besides, experimental results are also presented.

2. Theoretical Approach

1) Bose-Hubbard Model

At the beginning, I'll first introduce the Hamiltonian operator using spatial operators, which describes the behavior of bosonic atoms in an optical lattice with external trapping potential [4],

$$H = \int d^3x\, \psi^\dagger(x)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(\boldsymbol{x}) + V_T(\boldsymbol{x})\right)\psi(\boldsymbol{x}) + \frac{1}{2}\frac{4\pi a_s \hbar^2}{m}\int d^3x\ \psi^\dagger(x)\,\psi^\dagger(x)\psi(\boldsymbol{x})\psi(\boldsymbol{x}). \tag{1}$$

In this first term, $\psi(\boldsymbol{x})$ is a boson field operator for atoms in a given internal atomic state; $V_0(\boldsymbol{x})$ is the optical lattice potential; and $V_T(\boldsymbol{x})$ describes an additional external trapping potential (varying very slowly over space). As the simplest example, $V_0(\boldsymbol{x})$ has harmonic form: $V_0(x) = \sum_{j=1}^{3} \sin^2(kx_j)$ with wave vector $k = 2\pi/\lambda$ and λ the wavelength of laser light. This harmonic lattice has a period of $a = \lambda/2$. The magnitude of V_0, which is induced by the Stark effect of interfering laser beams, is related to the polarizability of dynamic atoms times the laser intensity.

The second term of the Hamiltonian approximates the interaction between bosonic atoms by a short-range pseudo-potential with a_s the s-wave scattering length and m the mass of the atoms.

Obviously, this "bosonic" Hamiltonian has the same form with that describing electrons in solid, so they should have the same set of solutions. Therefore, the energy eigenstates are Bloch wave functions. To move forward, we can transform these Bloch wave states to a set of Wannier functions, which are well localized on each site.

Then we can expand field operator $\psi(x)$ in Wannier basis and only keep the lowest vibrational states, $\psi(x) = \sum_i b_i w(x - x_i)$. An important assumption here is that the energies involved in the system dynamics are small compared to excitation energies to the first excited band. We will then obtain the Bose-Hubbard model (BHM) Hamiltonian

$$H = -J \sum_{<i,j>} b_i^+ b_j + \sum_i \epsilon_i \hat{n}_i + \frac{1}{2} U \sum_i \hat{n}_i(\hat{n}_i - 1), \tag{2}$$

where the operators $\hat{n}_i = b_i^+ b_i$ represent the number of bosonic atoms at lattice site i; the annihilation and creation operators b_i and b_i^+ obey the canonical commutation relations $[b_i, b_j^+] = \delta_{ij}$. The parameters U corresponds to the strength of the on site repulsion of two atoms on a same lattice site; J is hopping matrix element between nearest neighbor sites i, j; ϵ_i is related to the trapping potential.

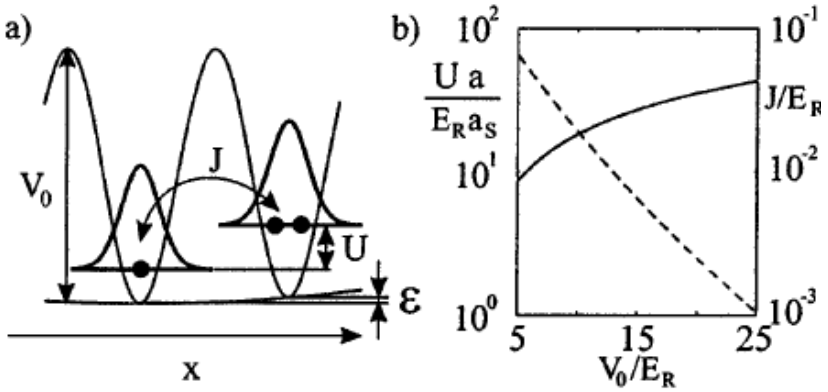

Fig. 1. (a) BHM in an optical lattice. Flat bottom curve is the external trapping potential. (b) Relation between $Ua/E_R a_S$ and well depth V_0.

Before moving on, let us recall the Hubbard model for electrons (fermions).

2) Hubbard Model for Fermions

This model is well known as a paradigm of strong electron correlation in condensed matter [5],

$$H = -t \sum_{<ij>} a_{i\sigma}^{+} a_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \tag{3}$$

where t is the hopping term, and U represents the on-site interaction.

Besides the dimensionality, the behavior of this Hubbard Hamiltonian is characterized by three dimensionless parameters: the ratio of Coulomb interaction to the bandwidth U/t, average number of electrons per site n, and the temperature T/t.

Let us consider a special case, half-filled system ($n = 1$) under zero temperature. In the limit $U/t \ll 1$, the interaction is weak, the Hamiltonian turns to $H = -t\sum a_{i\sigma}^{+} a_{j\sigma}$. Therefore we can expect that electrons could hop freely from one site to another to gain kinetic energy. In this case, this model describes a weakly interacting electron system. In the opposite limit $U/t \gg 1$, hopping is inhibited between sites, so filling number $n = 1$ is "pinned" on each site and this makes a special insulator called Mott insulator.

3) Superfluid Phase in Optical Lattices

Now, we come back to Mott-Hubbard model. When $U = 0$, just like I mention in the second section, the BHM Hamiltonian $H = -J\sum b_i^{+} b_j = \sum \epsilon_k a_k^{+} a_k$. All N atoms stay in the ground state, which is $\boldsymbol{k} = 0$ Bloch state of the lowest band. In a lattice with N_L sites, at zero temperature, this state could be written as [1]

$$|\Psi_N\rangle(U = 0) = \frac{1}{\sqrt{N!}} {a_{k=0}^{+}}^{N} |0\rangle = \frac{1}{\sqrt{N!}} \left(\frac{1}{\sqrt{N_L}} \sum_{i} b_i^{+} \right)^{N} |0\rangle. \tag{4}$$

The simplest excitation state is

$$|\Psi\rangle = a_k^+ |\Psi_N\rangle (U = 0).$$

(5)

When U is non-zero, in the limit of $U/t \ll 1$, (1) can be reduced to a Gross-Pitaevskii equation

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V_0(\boldsymbol{x}) + V_T(\boldsymbol{x}) + \frac{4\pi a_s \hbar^2}{m}|\psi(\boldsymbol{x})|^2$$

(6)

Then, the ground state is the Gross-Pitaevskii-type superfluid with a condensate fraction, which is equal to 1.

If the filling number N/N_L is not an integer, but a finite number, the ground state can be written in coherent state form [1]

$$\exp\left(\sqrt{N}a_{k=0}^+\right)|0\rangle = \prod_i \left[\exp\left(\sqrt{\frac{N}{N_L}}b_i^+\right)|0\rangle_i\right].$$

(7)

From the left side, we can see that the average total atom number is N (all with $\boldsymbol{k} = 0$). The right side means that there are $\bar{n} = N/N_L$ atoms at each site. We can expand the exponential operator on each site (I assume $N/N\_L = 1$ here)

$$\exp\left(\sqrt{\frac{N}{N_L}}b_i^+\right) = 1 + b_i^+ + \frac{1}{2!}{b_i^+}^2 + \frac{1}{3!}{b_i^+}^3 + \cdots.$$

(8)

The probability that there are more than one particle on each site is $(e - 1 - 1)/e = 1 - 2/e = 0.27$. So if U/t were finite, this state would not be energetic favorable, which will lead to the next state: Mott insulating phase.

4) Mott Insulating Phase in Optical Lattices

In the limit $U/t \gg 1$, with unit filling number ($N = N_L$), compared to the case for fermions, hopping of atoms between sites is negligible, so the ground state is [1]

$$|\Psi_{N=N_L}\rangle(J=0) = \left(\prod_i \hat{b}_i^+\right)|0\rangle\,. \tag{6}$$

This is just a simple product of local Fock states with precisely one atom per site.

In fact, there is a very interesting calculation result [6] to demonstrate this state in $U/t \gg 1$ regime. These results calculated the entropy vs. temperature figure of bosonic atoms on a cubic optical lattice with $N_s \approx 3\times10^4$ sites.

It should be noted that the well depth V is related to bosons interaction term parameter U as,

$$\frac{U}{J} \sim \left(\frac{a}{d}\right)\exp\left(2\sqrt{\frac{V_0}{E_R}}\right), \qquad E_R \equiv \frac{\hbar^2}{2m}k^2.$$

Therefore, $V_0 = 20E_R$ means $U/J \gg 1$, which should be Mott insulating regime.

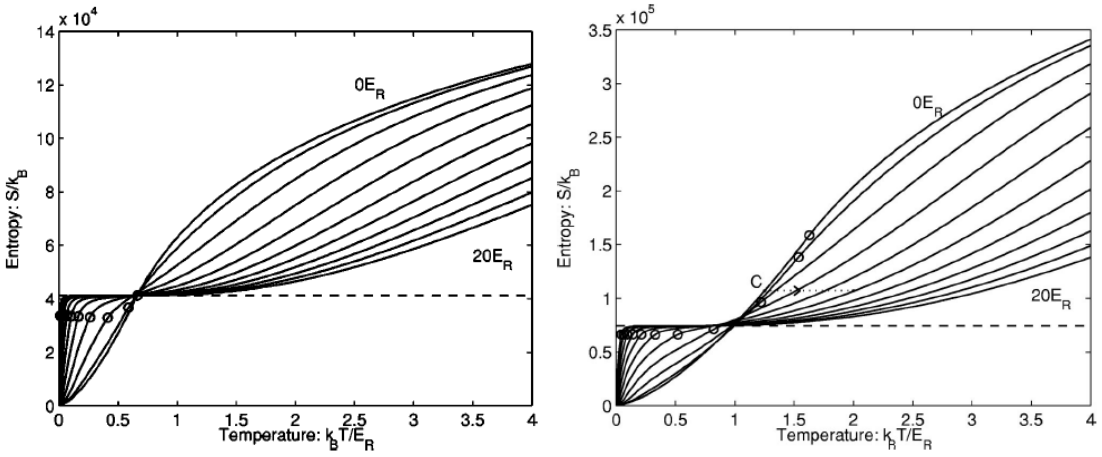

Fig. 2. Entropy vs. temperature curves for $N_s \approx 3\times10^4$ site cubic lattice, with filling fact n=1 (left) and n=4 (right). The well depth varies from V=0 to $20E_R$ (with a spacing of $2E_R$ between each curve). The entropy plateau S_0 is shown as a dashed line in each graph.

Now, I assume at low temperature, the $V_0 = 20E_R$ curve represents Mott insulating phase and calculated entropy plateau in a simple way.

Then the simplified problem is what is the entropy of $N_p = nN_s$ bosons occupying N_s sites at temperature T.

$$S = k_B T \log \Omega\,, \quad \Omega = \frac{(N_p + N_s - 1)!}{N_p!\,(N_s - 1)!}$$

Apply Stirling's approximation,

$$\frac{S}{k_B T} \approx N_p \log\left(\frac{N_p + N_s}{N_p}\right) + N_s \log\left(\frac{N_p + N_s}{N_s}\right) = N_s \left(n \log\left(\frac{n+1}{n}\right) + \log(n+1)\right).$$

So for $n = 1$, $\frac{S}{k_B T} = 2 \log 2\, N_s = 4.13\times10^4$; for n=4, $\frac{S}{k_B T} = \left(\log 5 + 4 \log\frac{5}{4}\right) N_s = 7.45\times10^4$.

These two results both coincide with Fig. 2.

3. Phase Diagram and Experimental Demonstration

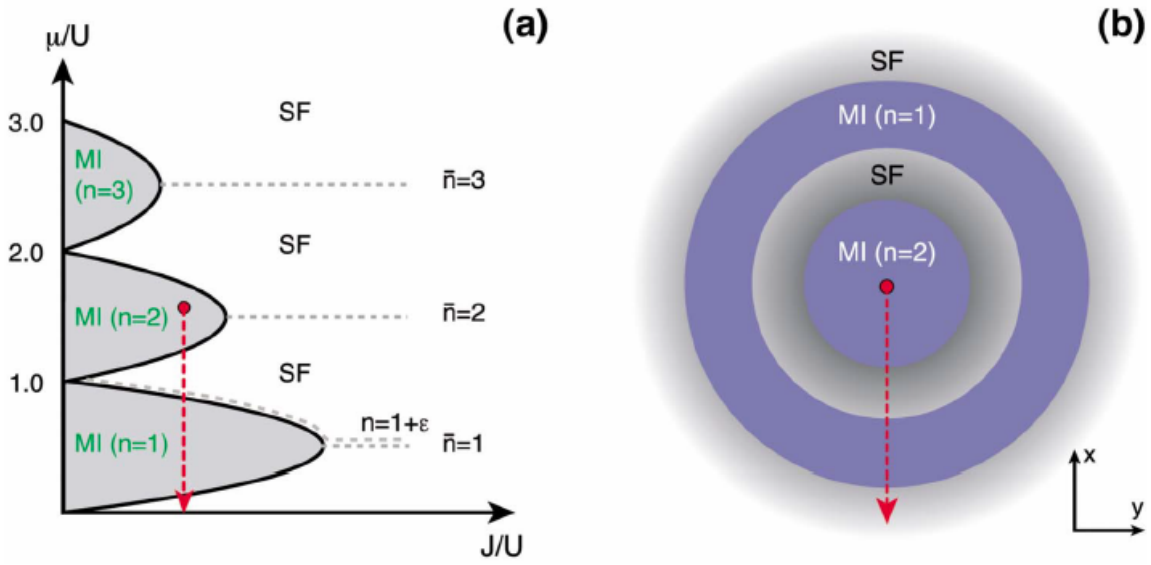

Fig. 3. (a) zero-temperature phase diagram of BHM. (b) Corresponding real space figure. [1]

The zero-temperature phase diagram of BHM is shown in Fig. 3(a). In this graph, normalized chemical potential denotes roughly the local density of atoms. At a given chemical potential, the phase is a function of the ratio of hopping and on-site interaction J/U. In fact the chemical potential is a spatially slowly varying function, $\mu_R = \mu_0 - \epsilon_R$ with $\epsilon_R = 0$ at the trap center. While at the boundary of the trap, μ_R vanishes. Fig. 3(b) assumes that μ_0 falls into filling number $n = 2$ "Mott lobe". One obtains series of Mott insulating phases and superfluid phases from the center to trap boundary [1]. Therefore, the density profile is like a wedding-cake.

It should be noted that, the compressibility $\kappa = \partial n/\partial \mu$ equals to zero in Mott insulating (MI) phase because n stays as a constant, which means that MI states are incompressible.

This very novel density profile is demonstrated numerically and experimentally as shown in Fig. 4 [7] and Fig. 5 [8].

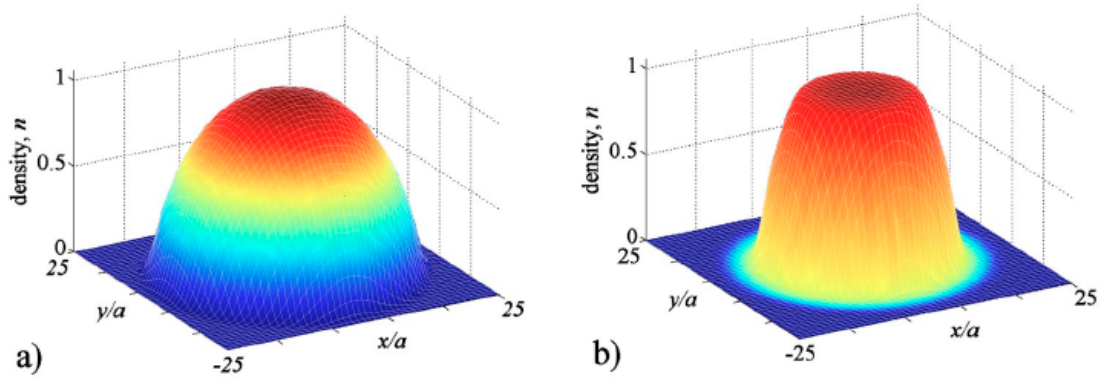

Fig. 4. Monte-Carlo results of local density vs. position relation of a 2D confined bosonic atoms system. The lattice depth of b) is stronger than that of a). a) U/t=6.7 b) U/t=25.

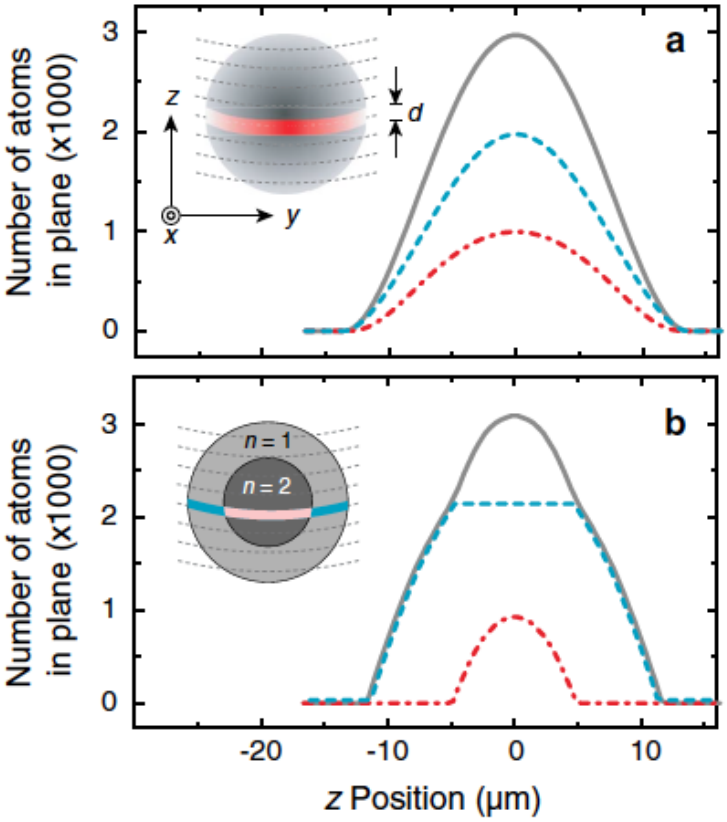

Fig. 5. Integrated distribution of (a) a superfluid and (b) a Mott insulating state of bosonic atoms in a harmonic trapped optical lattice. Grey solid line represents the total density profile over z-direction. Blue and red are for singly and doubly occupied sites. It is shown that the n=1 blue dashed line has a plateau through the core n=2 region in z-direction. Therefore this graph **indirectly** proves the **wedding-cake-like** density profile.

4. Conclusion

In this essay, I introduced Bose-Hubbard model and two novel phases coming from this. I also showed the numerical and experimental evidence to support this model. The realization of Hubbard model gives us another perspective to investigate strongly interacting condensed systems, which is very meaningful.

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