Quantum phase transition from a Mott insulator to a superfluid in bosons

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(Dated: May 5, 2008)

Abstract

Bose Hubbard model is presented and basic natures of Mott insulating phase and superfluid phase are studied in this essay. Also how and when this quantum phase transition occurs is discussed. Experimental supports from ultracold atoms physics are explained, while some miscellaneous topics are touched in the end.

1. Introduction and background

For many decades physicists focused on the phenomena of metal-insulator transition in Fermi systems, yet "the understanding of it remained fragmented" [1]. Instead M.Fisher *et.al.* [1] studied the possible similar transitions in Bose systems. Analogous to currents of charged Fermions they proposed the onset of supercurrent of Bosons at zero temperature as a new quantum phase transition. In this original paper, they wrote out the Bose Hubbard model and discussed the phase transition between two possible states: Mott insulating phase (MI) in which supercurrent is absent and excitation energy gap exists, and superfluid phase (SF) which possesses supercurrent and global coherence with no energy gap. Ever since then, the studies on such a peculiar phase transition in Bose systems have been carried out with great progress mainly due to two reasons: 1) Unlike Fermi analog, Bosons can have natural order parameter in form of off-diagonal long-ranged order in superfluid phase, which were studied with mature techniques to some extent compared with the less well-understood metal-insulator transitions; 2) experimentally optical lattice technique was widely available in late 90' last century. Due to the excellent control over nearly all relevant parameters in the Hamiltonian, optical lattice is a perfect platform for observing this MI-SF phase transition and testing the predictions of theoretical work. Many interesting phenomena predicted such as the exotic interference pattern due to coherence, non-dissipative flow, particle-hole excitations etc. were observed in recent years. More over, the recent progress in experiment on supersolidty [2] is widely accepted to be associated with the disorder in Bose systems. The study on Bose Hubbard model with disorder analytically and numerically might shed light on the explanation of this peculiar yet elusive phenomenon. Therefore the research on MI-SF phase transition remains important nowadays. In this essay, I plan to introduce the theory in Bose Hubbard model mainly in frame work of mean field theory (MFT) and showed the corresponding experimental results. Also some interesting topic for Bose Hubbard model would be mentioned.

2. Bose Hubbard model

Consider spinless Bosonic particles in a uniform lattice. The system is strongly correlated in that there's a strong repulsive onsite interaction U analogous to that in common Hubbard model. Also due to virtual quantum exchange effect the energy of the system could be lowered by J, which we call hopping energy (or kinetic energy less rigorously, as in some paper). For theoretical convenience we choose to fix chemical potential (grand canonical ensemble) instead of total particle number (micro canonical ensemble). The latter is preferred in experiment and we shall return to this later. Therefore Bose Hubbard model has the following form:

$$\hat{H} = -J\sum_{<i,j>}(\hat{a}_i^{+}\hat{a}_j + c.c) + \sum_i(\varepsilon_i - \mu)\hat{n}_i + \sum_i \frac{1}{2}U\hat{n}_i(\hat{n}_i - 1) \quad (2.1)$$

The first term corresponds to hopping term and last term is interaction term, where particle number operator:

$$n_i = a_i^{+}a_i \qquad (2.2)$$

is assumed. The middle term is chemical potential term with external potential ε_i, which could be for example, the trapping potential in optical lattice.

Now let's take a closer observation on the Hamiltonian in limiting cases heuristically.
a) *U/J* >>1
Notice that in the limit of U/J >>1, onsite interaction is dominated. Any hopping would bring an extra particle on one site and one particle loss on another. Since the interaction is quadratic this leads to a net increase in energy and the small negative hopping energy cannot compensate it, therefore hopping is energetically disfavored and particle number is pinned with certain integer on every site. Due to this lack of mobility we identify it as Mott insulating phase.

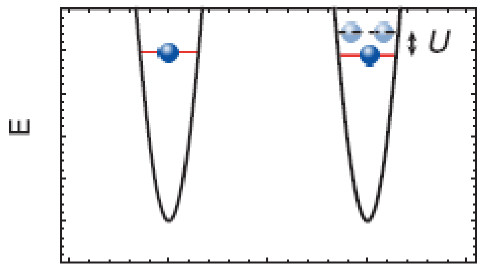

Fig.1. Onsite interaction can raise total energy, so even distribution is preferred [3].

Quantitatively we can determine the on-site particle number by minimizing energy when J is exactly zero. We introduce on-site energy $E(n)$:

$$E(n) = -\mu n + \frac{1}{2}Un(n-1) \qquad (2.3)$$

Notice that the system is homogeneous so we abandon the index for each site. By differentiating the on-site energy with respect to particle number, we find that for fixed chemical potential, the on-site particle number n_0 which minimizes energy must satisfy:

$$n_0 = [\mu / U] \qquad (2.4)$$

where "[ ]" denotes floor function which gives the maximum integer smaller than argument. We immediately see that on-site particle number is a step function of chemical potential. As hopping energy J increases slightly from zero, but still small, as we stated above, energy gain in J can not balance the energy cost in hopping, so we expect the ground state still characterizes by this fixed integer. As we can see clearly in phase diagram Fig 2.

b) *U/J* <<1

In the opposite limit *U/J* <<1, hopping process can effectively lowered total energy which blurs on site particle number and makes phases on different sites coherent (notice the conjugation of particle number and phase), which we identify as superfluid phase. Hence we assume there would be a quantum phase transition in between these two limits due to the quantum fluctuations at zero temperature [4].

Calculations based on MFT indeed show such a phase transition exists. We start from tight binding limit in which we treat hopping terms perturbatively and assume the infinite-range hopping [1]. We divided the Hamiltonian in two parts: H_1 corresponds to hopping terms and H_0 corresponds to the rest part. Hence we get partition function in the following way:

$$Z = Tr\exp(-\beta H_0)\left\{T\exp[-\int_0^\beta d\tau H_1(\tau)]\right\} \qquad (2.5)$$

where all Hamiltonians are in the interaction representation and T is the ordering operator. Notice that all terms in H_1 are quadratic, we need to decouple them via introducing complex field ψ_i on each site. This is the standard Hubbard-Stratonovich transformation. In the end we obtained effective action:

$$S = \sum_{i,j}\int d\tau (J^{-1})_{ij}\psi_i(\tau)\psi_j(\tau) - \sum_i \ln\left\langle T\exp[\int d\tau \psi_i(\tau)a^+_i + c.c.]\right\rangle \quad (2.6)$$

We seek the lowest energy saddle point solution by assuming the filed is independent of time, and use cumulant expansion, we can transform the effective action in Landau energy form:

$$S(\psi) = \beta N[\frac{1}{2}r(\mu, J)|\psi|^2 + u|\psi|^4 + O(|\psi|^6)] \qquad (2.7)$$

Notice that change in sign of coefficient r in quadratic term leads to the phase transition in Landau theory. So by setting r=0, we can determine the phase boundary. This corresponds to the condition that:

$$\frac{1}{zJ} = \frac{n_0+1}{Un_0-\mu} + \frac{n_0}{\mu - U[n_0-1]} \qquad (2.8)$$

Notice that n_0 is a step function of chemical potential and U. Therefore we obtained phase diagram. From the diagram, we can see those “Mott lobes” in which is MI phase and the SF phase is outside. This is reasonable because if we start from very small J, as J/U increases, the probability of hopping increases, which makes the particle-hole excitation energy gap decrease but still finite, until eventually it reaches zero, indicating the onset of SF phase. The energy gap can be directly obtained by measuring the distance from the upper Mott lobe boundary to the lower Mott lobe boundary for a certain value of J. And since according to eqn.2.5, the top of Mott lobe is parabolic, based on scaling we conclude that:

$$\Delta \sim ((J/U)_C - (J/U))^{z\nu}, z\nu = 1/2 \qquad (2.9)$$

The dynamical critical exponent being 1/2 is what we expect in MFT. More rigorous calculation based on Pade analysis of series gives a slightly larger value of critical exponent around 0.69 [5].   See Fig. 3.

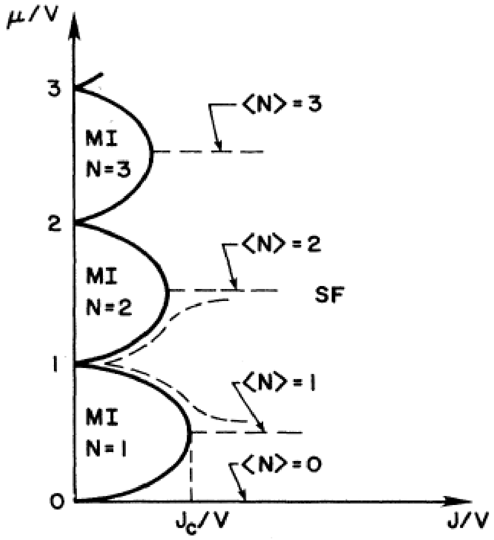

Fig.2. Phase diagram for homogeneous Bose lattice [1].

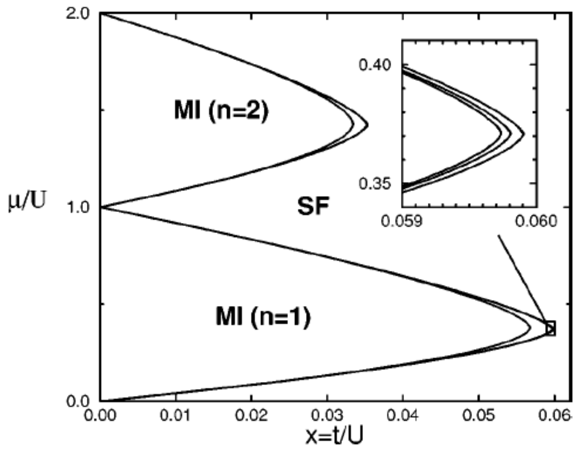

Fig. 3. Local shape at near the top of Mott lobe. The left curve corresponds to lowest order of Pade approximant(4^{th} order series), and right curves correspond to higher order of Pade approximant [5]. Notice that it gives sharper top of Mott lobes than the one from MFT.

3. Observation the onset of phase transition in optical lattice

Modern techniques in manipulating ultra-cold atoms in vacuum make the optical lattice available. Specifically we let two identical laser beams counter-propagating to set up a optical standing wave in direction. If we use six beams in x,y,z directions, 3D optical lattice can be realized. By carefully detuning the frequency of laser with respect to the resonant frequency of alkali atoms, we can exert attractive force on atoms in the direction of more-intense-field region. Therefore it is possible to control the effective potential on atoms by modulating the electromagnetic fields in laser beams arbitrarily and trap those cold atoms for a considerably long time. This brings a great advantage in studying condensed matter system in optical lattice.

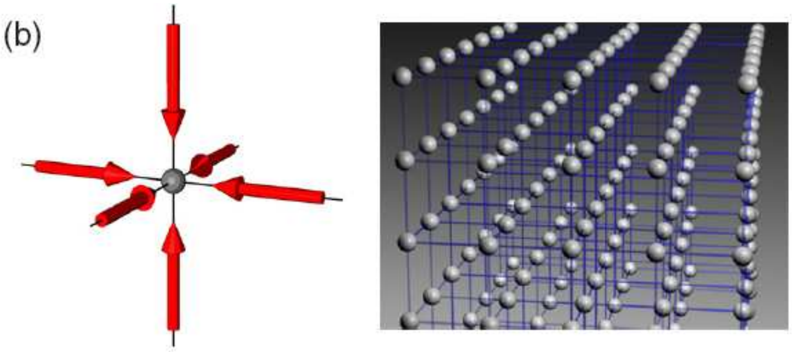

Fig 4. Illustration of optical lattice [3]

Detailed calculations on cold atoms show that values of J and U in Bose Hubbard Hamiltonian can be determined:

$$J_{ij} = -\int w(x-x_i)[-\frac{h^2}{2m}\nabla^2 + V(x)]w(x-x_j)d^3x \quad (3.1)$$

$$U = (4\pi h^2 a / m)\int |w(x)|^4 d^3x \quad (3.2)$$

Where *w(x)* is the single particle wannier function localized on one site, *V* is lattice potential and *a* is the scattering length of cold atoms. Therefore the ratio *J/U* is obtained as following:

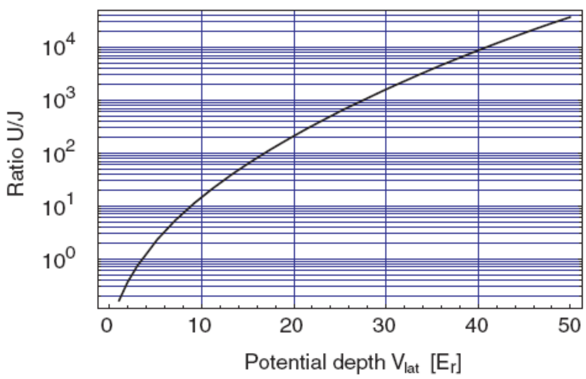

Fig 5. Relation between optical well depth *V* and ratio *U/J*. The energy is scaled by recoil energy E_r

Now we can dynamically change the values of *J/U* in a wide range, which is essential in observing the MI-SF phase transition. In 2002, Greiner *et.al*. [6] observed such a phase transition for the first time. They prepared cold atoms in condensate and transferred them adiabatically into optical lattice. They changed lattice potential *V* so as to control the values of *J/U* hence sampled different points in phase diagram. As they found, in small *U/J* region which theory gives superfluid phase, interference pattern due to the coherence among particles on all sites shows up. As *U/J* was tuned large enough, such an interference pattern disappears. This marks the onset of MI-SF phase transition.

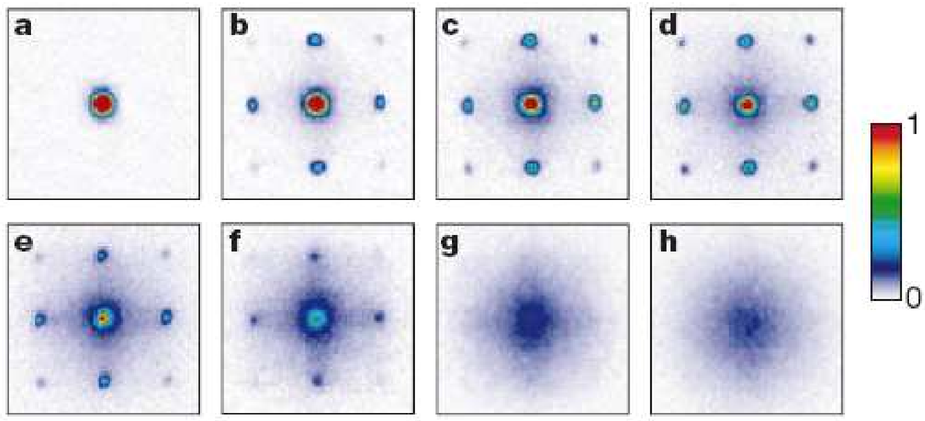

Fig 6. Without lattice potential only one central peak in momentum space is observable. As *U/J* is tuned up from a to h, we can see that the interference pattern will gradually disappear. Different colors represent different values of visibility [6].

Also in their experiment, they found such a transition is reversible as long as they crossed the phase boundary. They increased U/J to let system transform from SF phase to MI phase, kept the system in MI phase for a considerable long time and decreased *U/J*, and they found the interference pattern was recovered almost immediately on the time scale of h/J which is the tunneling time between two adjacent sites. They concluded the phase coherence over the entire lattice was restored with speed which is determined intrinsically by quantum mechanics, since all particles are identical and they act collectively. It makes no sense to tell which particle tunneled.

4. More on Mott insulating phase

a) particle-hole excitation

In M.Greiner *et.al.*' paper [6], the excitation spectrum was also tested experimentally. They applied perturbations which could either be potential gradient or shaking the system by modulating the optical well to excite the system. They noticed that in the MI region the system is robust against perturbations because phase coherence could be readily reestablished when the lattice depth decreased so that the system came into SF phase. This can be well explained by the Mott gap. As perturbations increase to a certain value, particle-hole excitation sets in and MI phase is destroyed to some extent. This can be seen from the fact that as the system goes back into SF phase the width of central peak increases enormously which means a broader distribution of momenta or coherence is less well kept. Higher order of particle-hole excitations also show up if the perturbations are even larger. See Fig. 7.

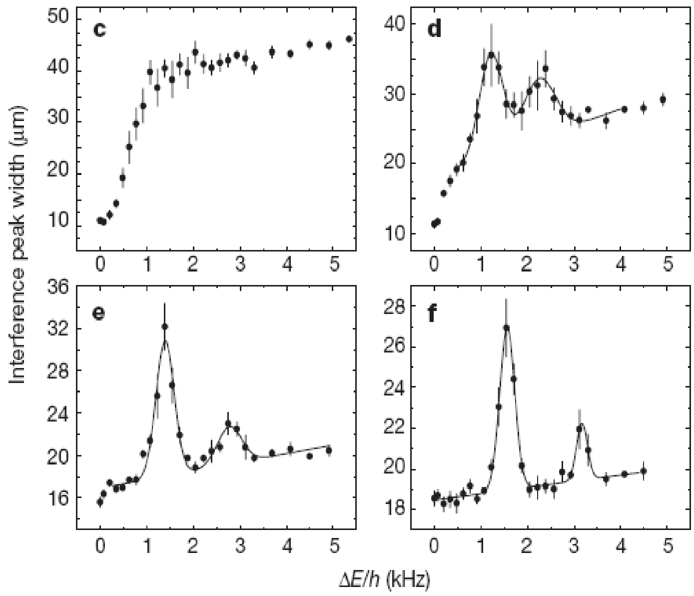

Fig. 7. Excitation spectra under external perturbations [6]. These peaks correspond to particle-hole excitations in MI phase and the background signal is from SF component which will be mentioned later.

b) Ground state of MI phase

In Guzwiller approximation [7] the many-body wavefuction is the product of single particle states. Hence the ground state of MI phase can be expressed as:

$$\left|\Psi_{MF}\right\rangle \sim \prod_i (\hat{a}_i^+)^n \left|0\right\rangle \qquad (4.1)$$

Since it is the eigenstate of local particle number operator, we see immediately there's the order parameter of superfluid (condensate fraction) is zero:

$$\psi = \left\langle \Psi_{MF} \left| a_i \right| \Psi_{MF} \right\rangle \psi_i = \left\langle \Psi_{MF} \left| a_i \right| \Psi_{MF} \right\rangle = 0 \qquad (4.2)$$

As we stated above that in MI region the onsite particle number is fixed while phase coherence is destroyed. Hence we shall expect interference vanishes immediately as we enter the Mott lobe. However close observation [8] indicates coherence may maintain even in MI phase.

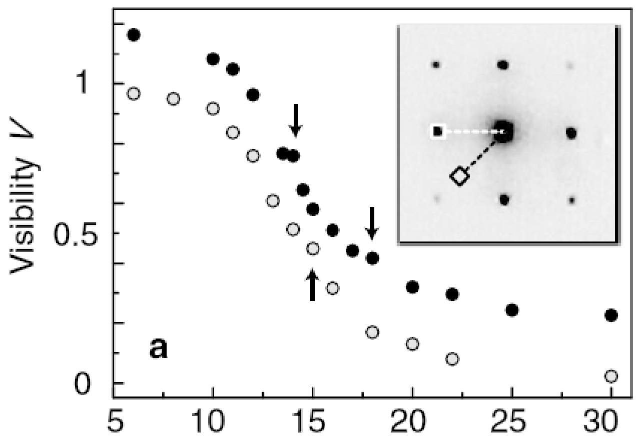

Fig. 8. Detailed detection on visibility of interference pattern shows that phase coherence does not vanish abruptly on the phase boundary of MI and SF phases. Visibility is one when there's perfect SF and zero when there's no SF component [8].

This can be explained beyond Guzwiller's approximation which is exact only when J= 0. Instead we have better guess of ground state in J/U expansion in the 1st order:

$$\left|\Psi^{(1)}\right\rangle \sim \left|\Psi_{MF}\right\rangle + \frac{J}{U}\sum_{<ij>}\hat{a}_i^{+}\hat{a}_j\left|\Psi_{MF}\right\rangle \quad (4.3)$$

Thus the ground state is not a pure eigenstate of onsite particle number and superfluid component is nonzero. Hence we conclude that in the Mott lobe the short ranged phasse coherence still persists while global phase coherence is destroyed. We can regard the ground state of MI with nonzero J as the mixture of mainly pure "Mott state" and additionally small amount of particle-hole excitations due to nonzero hopping. More detailed calculations based on this approximation can reproduce the visibility of interference which agrees with experiment quite well [9].

5. More on Superfluid phase

In Guzwiller's approximation we can write out the ground state easily:

$$\left|\Psi_{MF}\right\rangle \sim (\prod_i \hat{a}_i^{+})^N \left|0\right\rangle \quad (5.1)$$

In order to have a well defined macroscopic phase the ground state must be coherent state:

$$a\left|\alpha\right\rangle = \alpha\left|\alpha\right\rangle, \alpha = \sqrt{n}\cdot e^{i\varphi} \quad (5.2)$$

Hence the coefficients of basis in Fork space follows the Poissonian distribution:

$$\left|\Phi(t)\right\rangle = e^{-|\alpha|^2}\sum_n \frac{\alpha^n}{\sqrt{n!}}\cdot e^{iUn(n-1)t/2h}\left|n\right\rangle \quad (5.3)$$

A simple prediction from this wave function form is that each ket would evolve with different speed so initial coherence could be destroyed until after the revival time t=h/U when each number state undergoes a phase shift of integer periods. Experiment directly proved this [3].

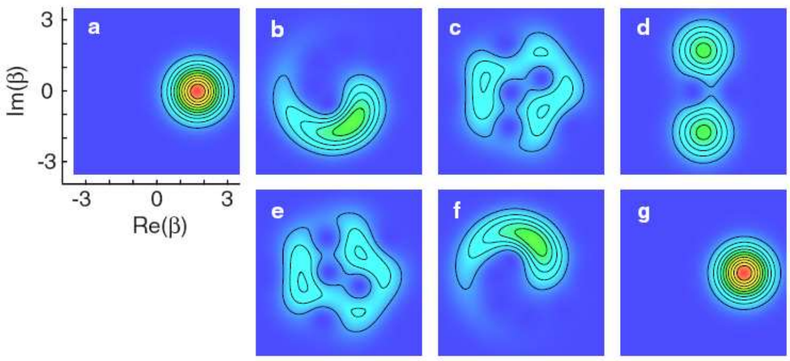

Fig. 9. Quantum dynamics of a coherent state. The macroscopic field collapsed and

fully revived as time elapses. The x,y coordinates are real and imaginary part of complex number β, similar to α in eqn. 5.2

Once the ground state of SF phase is obtained from Guzwiller's ansatz, we can calculate condensate fraction (superfluid order parameter ψ, see eqn.4.2). Detailed numerical calculations [10] based on variation method using mean field Hamiltonian yielded condensate fraction a long time ago. But only recent the accurate experimental plots were obtained from Kettle's group [11] (Fig. 10.). They studied the stability of superfluid currents in a system of ultracold Bosons in a moving optical lattice. Unlike the method of observing the onset of interference pattern, the transition point were observed quite clearly and sharply in this approach.

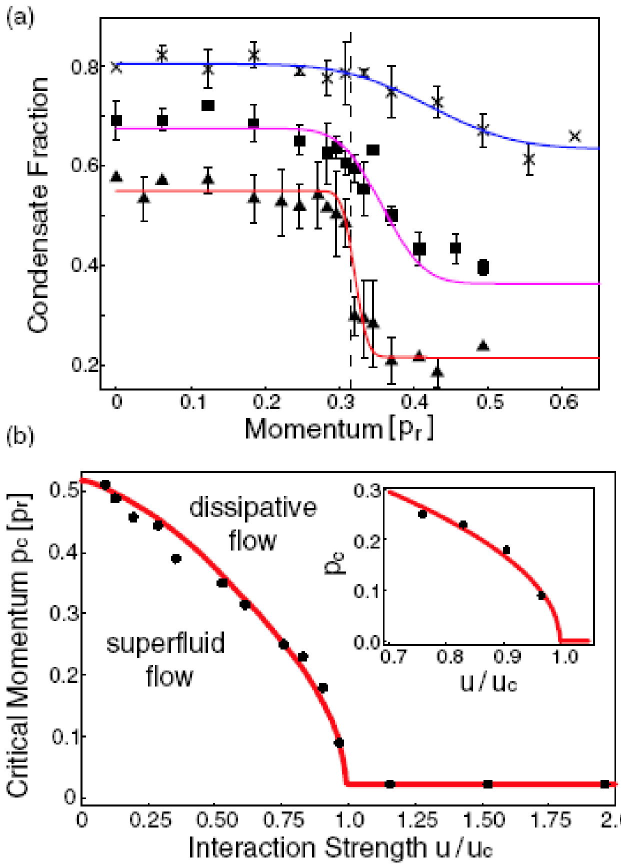

Fig. 10. a) Determination of the critical momentum of superfluid flow at U/U_C= 0.61 for a variable number of cycles of the momentum modulation (blue, purple and red lines). b) Critical momentum for a 3D condensate. Notice that theory (solid line) fits well with experimental data.

6. Even more on optical lattice

All the previous theoretical discussions were limited in homogeneous system. However in real practice this is not always possible. Since optical lattices are formed by Gaussian laser beams, the trapping potential is asymptotically simple harmonic potential. Hence the translational invariance of lattice is broken and we need to introduce the so called local chemical potential:

$$\tilde{\mu}(x) = \mu - V(x) \qquad (6.1)$$

Where *V(x)* is the harmonic potential. Our previous results can work again once we replace chemical potential by local counterpart. This is called local density approximation. Notice that now local chemical potential is no longer fixed, different sites correspond to different place in phase diagram, indicating a coexistence of MI and SF phases in the arrangement of wedding cake in real space. This fact gives a natural explanation of SF background signal in Fig.7.

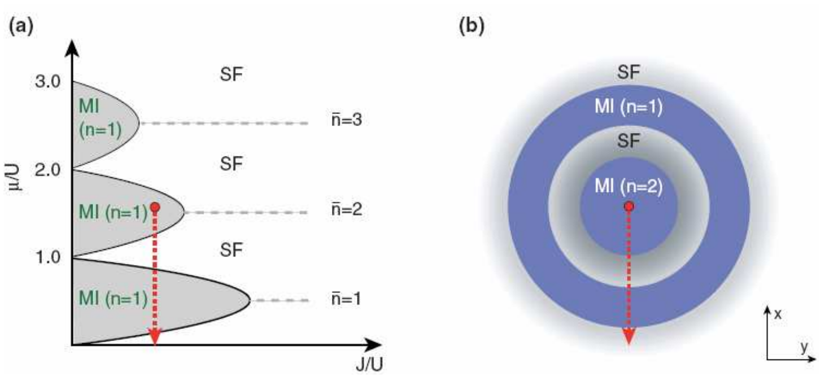

Fig. 11. a) Phase diagram of Bose Hubbard model in inhomogeneous lattice; b) arrangement of SI and MI phases correspondingly. Notice that mean particle number decreases from center towards outside with layers, so it looks like a wedding cake [3].

7. Miscellaneous topics

a) Bose Hubbard model with disorder

In M.Fisher, *et.al.*' original paper, the possibility of Bose glass phase in disordered lattice was discussed and phase diagram given based on physical argument. It is characterized as no gap, finite compressibility and yet an infinite superfluid susceptibility. Since then little progress was achieved in concrete calculations on its phase boundary. Recent work [12] using replica treatment and renormalization flow gave a possible phase boundary, which is quite different from Fisher's however. More work is needed on Bose Hubbard model with disorder since it might shed light on understanding the origin of supersolidity. A very recent work [13] on this topic is quite intriguing and worth reading.

b) Lower dimensions

Unlike MI phse which depends weakly on dimensionality, the physics of SF depends greatly on dimentsionality: in 3D it is conventional BEC; in 2D a Kosterlitz-Thouless SF; in 1D no true SF. Quantum Monte Carlo methods [14] give the most accurate results in these lower dimensions while MFT is worse. Experimentally MI-SF transitions have been observed in 3D[6] in 2002, 2D[15] in 2007, 1D[16] in 2005.

Interested readers may find details in these references.

c) Next nearest site hopping effects

Though the next nearest site hopping term is two orders of magnitude smaller than nearest site hopping term, the effects of the former was studied [17] via Bogoliubov method. The conclusion is that BEC termperature is enhanced due to this effect in sc lattice but decreases in bcc and fcc lattice.

d) Bose Hubbard model with two different Bosons

If we set the number of species of Bosons to be two instead one, we may get five stable SF and MI ground states with rich nontrivial phase diagram [18]. Interested readers may find details in this reference.

8. Conclusion

In this essay we studied Bose Hubbard Model mainly in MFT. We identified MI phase as finite gap, infinite compressibility, exact integer commensurate fillings of particles and none global phase coherence, while SF phase as gapless, arbitrary fillings of particles with phase coherence. We studied the particle-hole excitation in MI phase and condensate fraction, dissipative current in SF phase both theoretically and experimentally, pointing out the drawbacks of MFT. We mentioned some interesting topics relevant to traditional Bose Hubbard model and commented on the significance of some of them.

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