

Superfluid to Mott Insulator transition in an optical lattice

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## BOSE HUBBARD MODEL

The Hubbard model was originally proposed to describe the motion of electrons in metals with the motivation of understanding their magnetic properties. Specific aim was to yield both band like and localized electron levels. This original model remains a very active subject of research today.

We examine a simpler Bose Hubbard model. The elementary degrees of freedom are spin zero bosons, which take the place of spin-1/2 electrons in the original model. Importance of this model lies in providing one of the simplest realizations of quantum phase transition.

Let us define the degrees of freedom of the model of interest. In  $d$  dimensions we have a lattice of  $M$  sites and we introduce the  $N$  boson operators each of which annihilates boson on the site  $i$ ,  $c_i$ . These operators obey the usual bosonic commutation relationship. We also introduce the boson number operator  $n_i = c_i^\dagger c_i$ , which counts the number of bosons on each site. The number of bosons on each site can be arbitrary.

The Hamiltonian for the Bose Hubbard model (BHM) is

$$H = -J \sum_{\langle i,j \rangle} c_i^\dagger c_j - \sum_i \mu_i n_i + U \sum_i n_i (n_i - 1)$$

The first term allows hopping of bosons from site to site (nearest neighbor pairs).

The second term represents the chemical potential of the bosons. It is the same as the energy offset due to the harmonic trapping in case of an optical lattice. A change in the value of  $\mu_i$  changes the number of bosons at that site.

The third term represents the simplest possible repulsive ( $U > 0$ ) interaction between bosons. Just the onsite repulsion is taken into account. Off-site and longer range repulsion is important in realistic systems.

Hamiltonian having the first term in the absence of the third can be shown to lead to the many body condensate wave function with long range phase coherence. It's analogous to the conventional band spectrum and one electron Bloch levels in which each electron is distributed throughout the entire lattice (original Hubbard model). On the other hand just the third term without the first in the Hamiltonian leads to tighter localization of the wave functions at the lattice sites and it can be shown that the ground state energy is minimized when each lattice is filled with the same (integer) number of bosons. Local magnetic moments in case of the original Hubbard model.

To get exact results when both the terms are present in the Hamiltonian is a difficult task. Next section shows some of the theoretical results in this case.

## THEORETICAL METHODS

### Analytical

As discussed above the system we are dealing with covers regimes which show very different qualitative behaviour. When the atoms are delocalized the system is weakly correlated. As the strength of the lattice potential increases the atoms become localized and the system becomes strongly correlated. One interesting point in case of the later regime is

*The existence of a mean field in the system depends on the number of atoms per site being integer or not.*

When the number of atoms per site is integral there is no mean field (the state of the system is product of localized states at each site) – commensurate filling of lattice

When the number of atoms per site is non integral there is non zero mean field – incommensurate filling of lattice.

Hence if we start with a integral average site filling then the transition between MI and SF is noticed when one passes from no mean field to finite mean field.

Now we discuss some analytical theories[4].

Bogoliubov approximation:

First we transform the Hamiltonian to momentum space by introducing creation and annihilation operators  $c_k^{\dagger}, c_k$ .

The Hamiltonian becomes

$$H = \sum_k (-\varepsilon_k - \mu) a_k^{\dagger} a_k + \frac{1}{2} \frac{U}{M} \sum_{k_1} \sum_{k_2} \sum_{k_3} \sum_{k_4} a_{k_1}^{\dagger} a_{k_2}^{\dagger} a_{k_3} a_{k_4} \delta_{k_1+k_2} \delta_{k_3+k_4}$$

where  $\varepsilon_k = 2t \sum_j \cos(k_j a)$ ,  $j$  running from 1 to  $d$  (dimension).

As in other cases here also we replace the creation and annihilation operators of the ground momentum state by the average  $\sqrt{N_0}$  and a fluctuation.

Calculating the effective Hamiltonian and then finding the condensate density we find that as  $U/t$  goes to infinity the condensate density doesn't go to zero. Hence the bogoliubov theory doesn't predict the phase transition.

Mean Field Theory:

To have a mean field approach which can correctly describe the mott insulator state, we must decouple the tunneling term (treated as a perturbation) to effectively decouple the total Hamiltonian into single site energies. We first make the substitution

$$c_i^\dagger c_j = \langle c_i^\dagger \rangle c_j + c_i^\dagger \langle c_j \rangle - \langle c_i^\dagger \rangle \langle c_j \rangle = \psi(c_i^\dagger + c_j) - \psi^2,$$

The effective Hamiltonian then becomes

$$H^{\text{eff}} = -zt\psi \sum_i (c_i^\dagger + c_i) + zt\psi^2 N_s + \frac{1}{2}U \sum_i c_i^\dagger c_i^\dagger c_i c_i - \mu \sum_i c_i^\dagger c_i,$$

where  $z$  is the number of nearest neighbors,  $z=2d$ .

The critical value of  $U$  for which condensate density becomes zero can now be found analytically by using the second order perturbation theory. The value for  $U_c$  is found to be 5.83.

## THE EXPERIMENT

Experimentalists have realized the superfluid to Mott insulator transition in an ultracold gas of rubidium atoms with repulsive interactions trapped in an optical lattice. The experimental technique and set up is described below. [3]

### Set up

A spherically symmetric bose condensate of Rb atoms is created in a magnetic trapping potential with equal radial and axial trapping frequencies.

A three dimensional optical lattice is formed by six criss-cross laser beam with their crossing point positioned at the center of the bose condensate. By controlling the intensity of the laser beams the periodic potential height is controlled. The depth of the potential is

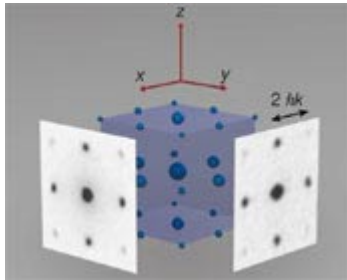
measured in terms of the recoil energy  $E = \frac{\hbar^2 k^2}{2m}$ . The form of the periodic potential looks like

$$V(x, y, z) = V_0(\sin^2 kx + \sin^2 ky + \sin^2 kz)$$

Where  $k$  is the wavevector of the laser light and  $V_0$  is the maximum potential depth.

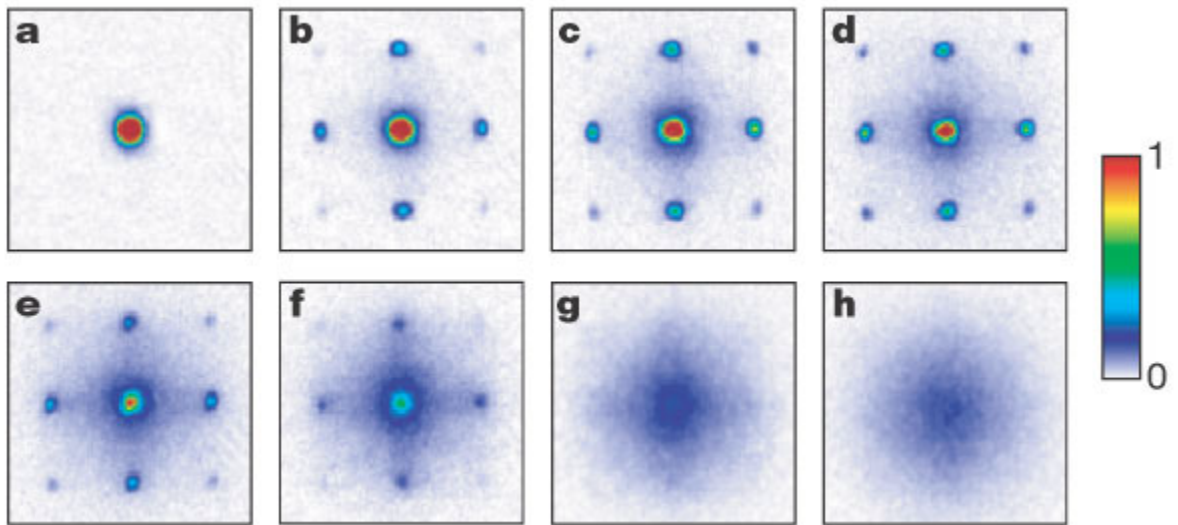
The magnetically trapped condensate is transferred into the optical lattice potential by slowly increasing the intensity of the laser beams. The slow ramp speed ensures that the condensate always remained in the many body ground state of combined magnetic and optical trapping potential.

After raising the lattice potential the condensate has been distributed over more than 150000 lattice sites with an average number of 2.5 atoms per lattice site. In order to test whether the system is still superfluid the combined trapping potential is suddenly turned off and the atomic wavefunctions are allowed to interfere. A high contrast 3-D interference pattern is observed. Each time the lattice depth is changed the same procedure is repeated.



### The transition

As the lattice depth is increased, the strength of higher order maxima increases. This is due to increased localization of the atomic wavefunctions at a single site. Remembering that this was a SF phase owing to the fact that atoms could tunnel through easily, increasing the lattice depth would lead to freezing of atoms in one lattice site. This would deplete the condensate fraction and the definite phase between that lattice site would be accompanied by finite fluctuations. This leads to the broadening of interference maxima. But as the depth of around 13  $E$  ( $E$  being the recoil energy) is reached the interference maxima no longer increase in strength. Instead, an incoherent wave pattern comes up, getting more prominent as the potential is further increased. Eventually at 22  $E$  no interference pattern is visible.



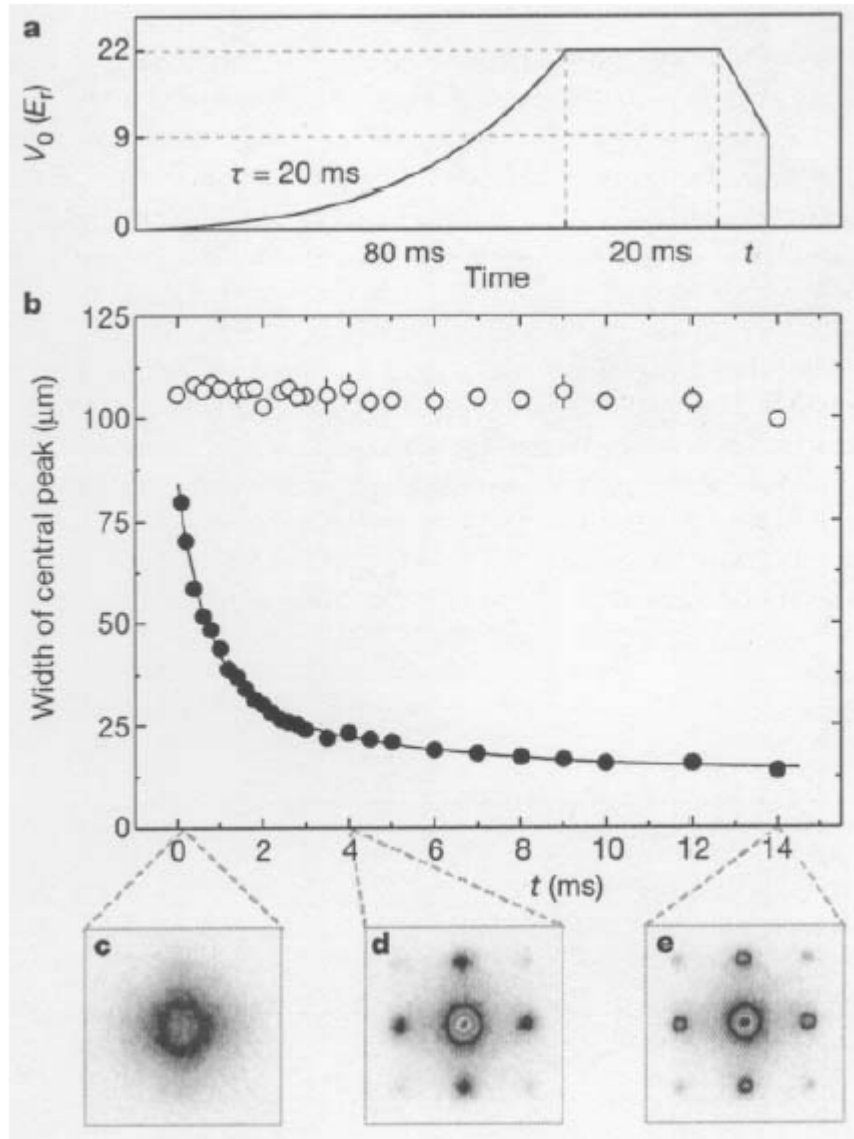
### Restoring Phase Coherence:

How do we make sure that the state we are getting is a state having perfect number correlation between sites and not just a dephased condensate. Two more sets of experiments confirm that there indeed is a transition to a Mott insulator state.

A notable property of the Mott Insulator is that phase coherence can be restored within order of tunneling time when the optical potential is lowered again to a value for which the ground state is a superfluid. This rapid restoration of coherence from a Mott Insulator can be compared to that of a phase incoherent state where random phases are present between neighboring sites. It is observed that while the width of the central interference peak exponentially goes down with time for a Mott Insulator, it remains constant for a dephased condensate.

Now to restore coherence potential is ramped down suddenly to  $9E$  where the ground state is a superfluid. After this the combined trapping and periodic potential is turned off and subsequent interference patterns are observed and analysed. It should be noted that the perfect number correlation characteristic of the Mott insulator strictly depends on the lattice potential (the controlling parameter in the quantum phase transition) and once below the critical value there are high fluctuations which lead to phase coherence. Hence with time any fluctuation in the number of atoms per lattice site leads to a stabilization of the phase because there is no other alternative owing to the reduced periodic potential.

A dephased condensate is created by 22 E by introducing non linear interactions in the system during the ramp up period. Even after the potential is ramped down to 9E these interactions remain and prevent the system to become a superfluid.



The second way to know that we indeed have a new state is to probe into the excitation spectrum. Mott insulator is characterized by a gap in the excitation spectrum.

Conclusion:

Mott insulator is an emergent state of matter. Temperature is an important factor for a convincing demonstration of a controllable Quantum phase transition. Thermal fluctuations can completely wash out the effect of their quantum counterparts. Future study in this field could be the experimental demonstration of finite T effects. This transition has been successfully realized in 1, 2 and 3 dimensions. Here the transition is realized by reducing the tunneling. Increasing U or the basically the scattering length (Feshbach resonances) and demonstrating the transition could be some of the future experiments in this field.

References

- [1] Quantum Phase Transitions S. Sachdev
- [2] Solid State Physics Ashcroft/Mermin
- [3] Griener et al Nature, 415, 39
- [4] Stoof et al PR-A 63, 053601