Superfluid to Mott insulator transition on an Optical Lattice

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Abstract

Quantum phase transition is studied in a Bose-Einstein condensate held in a three dimensional optical lattice potential. The system shows a superfluid to Mott insulator transition as the lattice potential is increased. But unlike the unconfined case, this system shows a Mott insulator phase even at incommensurate densities. Experimental results along with Quantum Monte Carlo studies indicate a remarkable situation where there are locally confined Mott domains in the condensate. This new feature is an outcome of translational symmetry breaking in presence of harmonic confinement. Nevertheless, the system exhibits most of the essential features of a superfluid-Mott insulator transtion observed in unconfined lattice bosons.

1 Introduction

A classical system cannot change its configuration at absolute zero temperature. But according to Heisenberg's uncertainty principle, quantum fluctuations still prevail at zero temperature and can be responsible for a loss of order and hence a different state of the system. This kind of a critical phenomenon is common in strongly interacting quantum systems. Fermionic examples of strongly correlated systems include high temperature superconductors, heavy fermion materials and a class of systems undergoing metal-insulator transitions. The bosonic counterpart includes short correlation length superconductors, granular superconductors, Josephson arrays and the dynamics of flux lattices in type II superconductors. The composite Cooper pair of electrons in granular superconductors have been described as bosonic degrees of freedom. There have been efforts to explain the problem of unconventional vortex state for high temperature superconductors through a model of interacting bosons. Other examples of strongly correlated bosonic systems include Helium-4 absorbed in porous media like Vycor or carbon black [7], 2D array of mesoscopic granules and studies of exciton lifetimes in quantum well structures. Recently, quantum phase transition has been observed in a gas of ultracold alkali atoms.[1] This experiment has opened up a new window to the world of quantum phase transition and many body physics.

Atoms in a Bose Condensate when arranged on an optical lattice have a wavefunction that spreads over the entire lattice in a wave-like manner, as described by quantum mechanics. In this state the phase of the atomic wavefunctions are coherent to each other and the system is in a superfluid state. As the tunneling of the atoms from one site to another is decreased, the interaction between the atoms become more prominent. Since the atoms interact through a hardcore repulsion, the interaction tends to freeze the atoms to their respective sites. When the atoms do not have sufficient kinetic energy to bear the cost of tunneling to an already occupied site, the system enters the Mott insulator state and the phase coherence is completely lost.

2 Bose Hubbard Hamiltonian

The relevant physics of these problems is presumed to be contained in the Bose Hubbard Hamiltonian which describes the competition between kinetic energy and potential energy effects.

$$\mathcal{H} = -J \sum_{<i,j>} \hat{a}_i^\dagger \hat{a}_j + U \sum_i \hat{n}_i(\hat{n}_i - 1) - \sum_i \mu_i \hat{n}_i, \tag{1}$$

where the symbol $< i, j >$ denotes a restricted summation over indices such that the sites i and j are nearest neighbours. The operators $\hat{a}_i$ and $\hat{a}_i^\dagger$ correspond to the annihilation and creation of a boson at the site i respectively. μ_i is the chemical potential and in the case of an optical lattice it is the energy offset of the i^{th} site and is denoted by ϵ_i [1]. The strength of the tunneling term is given by the hopping matrix element between two adjacent sites i and j.

$$J = -\int d^3x \mathbf{w}(\mathbf{x}-\mathbf{x_i})(-\frac{\hbar^2\nabla^2}{2m} + \mathbf{V_{lattice}}(\mathbf{x}))\mathbf{w}(\mathbf{x}-\mathbf{x_j}), \tag{2}$$

where $\mathbf{w}(\mathbf{x}-\mathbf{x_i})$ is the single particle wannier function localized at the i^{th} lattice site. $V_{lattice}$ is the lattice potential and the interaction matrix element

$$U = \frac{4\pi\hbar^2 a}{m}\int |\mathbf{w}(\mathbf{x})|^4 \mathbf{d^3x}, \tag{3}$$

with a being the scattering length of an atom.

2.1 The Mean Field Approach

The mean-field approximation that is done here [3], aims at de-coupling the t_{ij} term so that the whole Hamiltonian is a sum over single site energies. The mean-field theory used here corresponds to the approximation

$$(a_i - < a_i >)(a_j^\dagger - < a_j^\dagger >) \approx 0 \tag{4}$$

Using equation (4) the hopping term is decoupled as

$$a_i^\dagger a_j = < a_i^\dagger > a_j + < a_j > a_i^\dagger - < a_i^\dagger >< a_j > \tag{5}$$

We now identify $< a_i >$ and $< a_i^\dagger >$ as the superfluid order parameter ψ_i. Assuming the system is *homogeneous*

$$< a_i > = < a_i^\dagger > = \psi_i = \psi \tag{6}$$

We note that for the normal state with fixed number of particles, $< a >$ or $< a_i^\dagger >$ yields zero. Now, since the superfluid phase is characterized by off-diagonal long range ordering, the value of ψ is non-zero in this phase. Hence, ψ can be taken as the order for this transition and the superfluid density as $\rho_s = |\psi|^2$. The resulting mean-field version of the Hamiltonian (1) can thus be written as a *sum over single-site terms* which are

$$\mathcal{H}_i^{MF} = \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu\hat{n}_i - \psi(a_i + a_i^\dagger) + \mid \psi \mid^2, \tag{7}$$

Hamiltonian in (7) now contains a summation over only one index.

In the strong coupling limit $U \to \infty$ this Hamiltonian can be diagonalized by truncating the basis to contain a maximum of $n = 2$ particles at each site. Then in this limit one obtains the important result [3]:

$$\frac{\rho_s}{\rho} = 1 - \rho, \tag{8}$$

where ρ_s is the superfluid density and ρ is the overall density. This result is peculiar because it says that for incommensurate densities the superfluid phase persists even when the onsite repulsion between the atoms become very large.

The critical value of U for which the superfluid density ψ_s becomes zero, is denoted by U_c. The value of U_c can be found analytically by a small ψ expansion (it is expected that the order parameter will be small near the transition) and it is found that $U_c = (3+2\sqrt{2}) \simeq 5.83$ for $\rho = 1$ [3]

The critical behavior is of two types: mean field for transitions induced by changing the density and of the $(d+1)$ dimensional XY universality class when the interaction strength is swept at fixed commensurate densities.

3 Experimental set up

The experimental set up [1]consists of a spin-polarized sample of ^{87}Rb atoms in the $(F = 2, m_F = 2)$ state held in a magnetic trap with trapping frequencies of ν_{radial} and ν_{axial} equal to 240Hz. Here F represents the total angular momentum and m_F the magnetic quantum number of the state. The resulting condensate is spherically symmetric with a Thomas-Fermi diameter of $26\mu m$. The three-dimensional optical lattice is realized by aligning three counter-propagating beams orthogonal to each other. The beams are derived from a laser diode operating at $\lambda = 852nm$ with a relative frequency difference of 30 MHz between them to avoid interference. The optical potential resulting from the standing waves has the cubic geometry of the lattice:

$$V(x, y, z) = V_0[sin^2(kx) + sin^2(ky) + sin^2(kz)] \tag{9}$$

Here k is the wavevector of the laser light and V_0 the maximum potential depth of a single standing wave laser field. The depth of the potential is measured in units of the recoil energy $E_r = \hbar^2 k^2/2m$. After the atoms are trapped, there are about 150,000 lattice sites with an average of 2.5 atoms at each site in the center. Since the radiation force experienced by the atoms is proportional to the intensity of the laser field, so increasing the intensity raises the depth of the lattice potential.

3.1 Testing Phase Coherence

To test for any existing phase coherence, the combined trap potential is suddenly turned off and the atom cloud is allowed to expand. If the atoms are in the superfluid phase, then there will be perfect phase coherence in the atomic wavefunctions and one would obtain a high-contrast three dimensional interference pattern. On the otherhand, when the system is in the insulator phase, the number fluctuation at each site is exactly zero and hence the phases of the atomic wavefunctions are completely arbitrary. In such a case, when the atom cloud is allowed to expand, no interference is observed. As the lattice potential depth is increased, the strength of higher order maxima in the interference pattern increases. This is ascribed to a higher amount of scattering which results in the formation of quasiparticles of higher wavenumber in the condensate. These higher wavenumbers contribute to the higher orders in the interference pattern. But after this, increasing the lattice potential depth lowers the amount of tunneling which causes the atoms to stick to their lattice sites. This would

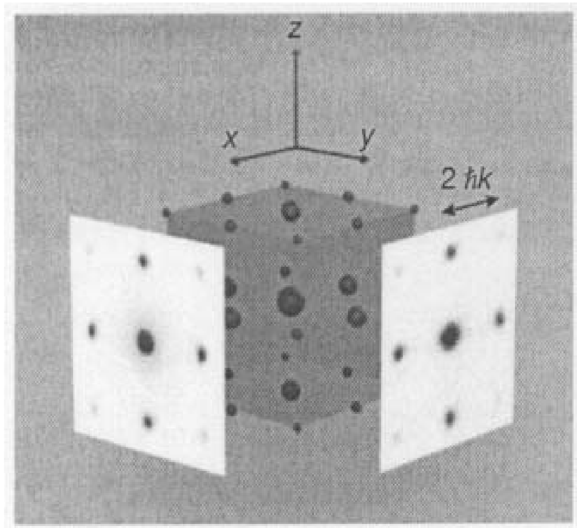

Figure 1: Schematic 3-dimensional interference pattern with measured absorption images obtain after ballistic expansion from a lattice with potential depth of $V_0 = 10E_r$ and a time of flight of 15ms.

deplete the condensate and would cause a fluctuation in the phase of the wavefunction. So one would normally expect a broadening of the interference peaks as the potential depth is increased. But what one observes is at a potential depth of $13E_r$ the interference maxima no longer increase in strength but an incoherent background of atoms starts to gain strength, until at a potential depth of $22E_r$ the interference pattern is totally lost to the background noise.

This remarkable behaviour is a signature of coexisting domains of superfluid and Mott insulator phases in the system. It is important to note here that the average density at the center of the trap is about 2.5. But according to the previous mean field calculation of the unconfined boson Hubbard model, one obtains a Mott insulator phase only for commensurate densities. This apparent paradox can be solved by noting that the external harmonic potential applied to trap the atoms actually breaks the translational invariance of the lattice. The density is no longer constant, it is maximum at the center of the trap. This inhomogenity is the cause of formation of such peculiar Mott insulator domains in the system as we shall see later.

3.2 Restoring Phase Coherence

A distinct property of the Mott insulator phase is that phase coherence is restored when the optical potential is lowered back to a value where the ground state of the system is completely superfluid. This property is shown in Fig.3. It is also interesting to contrast the behaviour of a phase incoherent state with that of the Mott insulator state undergoing same experimental sequence. The phase incoherent state shows no signs of superfluid state when the lattice potential is lowered adiabatically, in contrast to the Mott insulator state. When

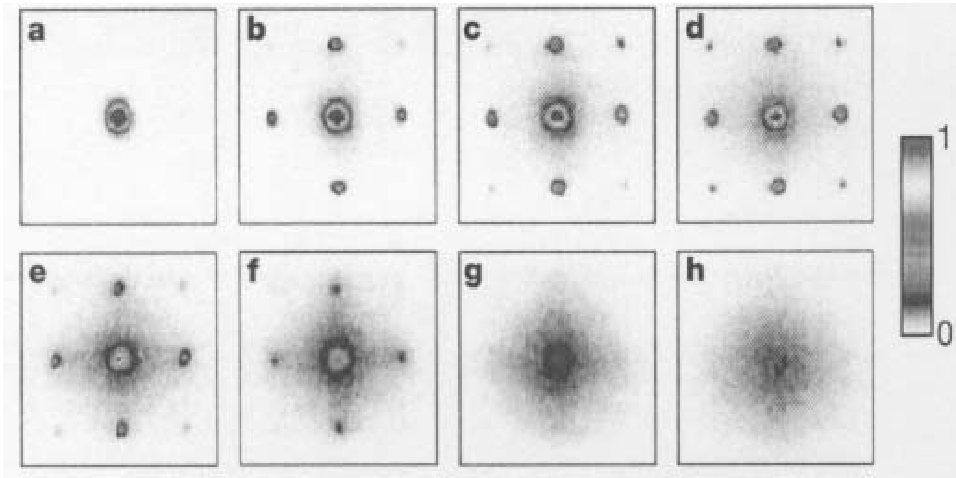

Figure 2: Absorption images of multiple matter wave interference pattern. These were obtained for different V_0 and after a time of flight of 15ms. Values of V_0 were **a. 0, b.** $3E_r$, **c.** $7E_r$, **d.** $10E_r$, **e.** $13E_r$, **f.** $14E_r$, **g.** $16E_r$, **h.** $20E_r$

the lattice potential is turned off, the phase incoherent state homogeneously populates the first Brillouin zone of the optical lattice. This means that the state is in the vibrational ground state of the system. But the relative phase difference between the adjacent sites is still random. We infer that the Mott insulator is not just a state with random phases between adjacent sites, but correlations play an important role in governing the physics of the system.

3.3 Probing the Excitation Spectrum

The Mott insulator state is characterized by a gap in the excitation spectrum. In the limit $J \ll U$, the energy gap $\Delta = U$, the on-site interaction energy. One can imagine a situation where there is one boson at each site. Now the energy cost for hopping one boson to an already occupied site is U. It can be shown that this also holds for n bosons at one site. So in a second order virtual process, it takes an energy U to create such a particle-hole pair. This is the origin of the gap in excitation spectrum of Mott insulators.

In the experiment, the Mott insulator excitation spectrum is probed by tilting the lattice potential with the application of a potential gradient. This would impart kinetic energies to atoms at a higher potential and they start tunneling. But these atoms have to overcome an excitation gap Δ before they can start tunneling. So probing the excitation spectrum one would expect a resonance in tunneling probablity versus the energy difference between the neighbouring sites. The technique used is analogous to the one used in NMR and is outlined in the figure caption. For a completely superfluid system at $10E_r$, the system is easily perturbed for small potential gradients and finally the wavefunctions get completely dephased and the peak width saturates. At about $13E_r$ two resonance peaks start appearing and finally at a potential depth of $20E_r$ we see two narrow resonance peaks on top of a flat

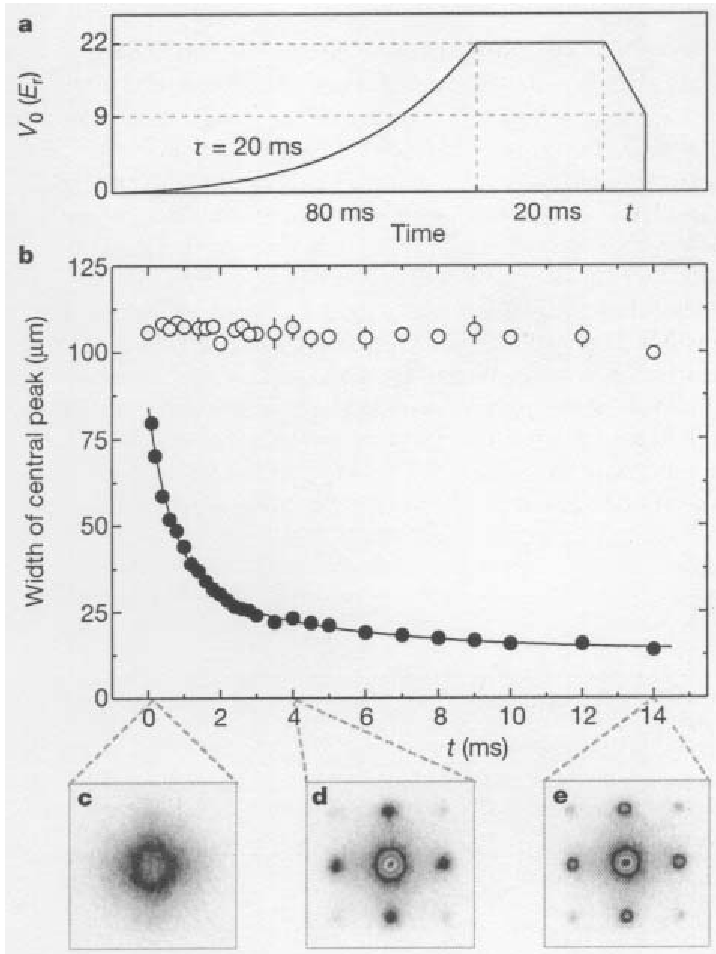

Figure 3: **a. Experimental sequence: V_0 is increased to a value of $22E_r$ in a time of 80ms. Then the atoms are held for a time of 20ms after which the potential is lowered to a value of $9E_r$ when the atoms are in the superfluid state again. The potential is then turned off and the atom cloud is let to expand. b. Width of the interference peak versus ramp time. Filled circles correspond to the Mott insulator and show restoration of coherence. Open circles correspond to a phase coherent state which shows no phase restoration. c-e Absorption images of the interference patterns from the Mott insulator phase for ramp-down times: (c) 0.1ms, (d) 4ms, (e) 14ms**

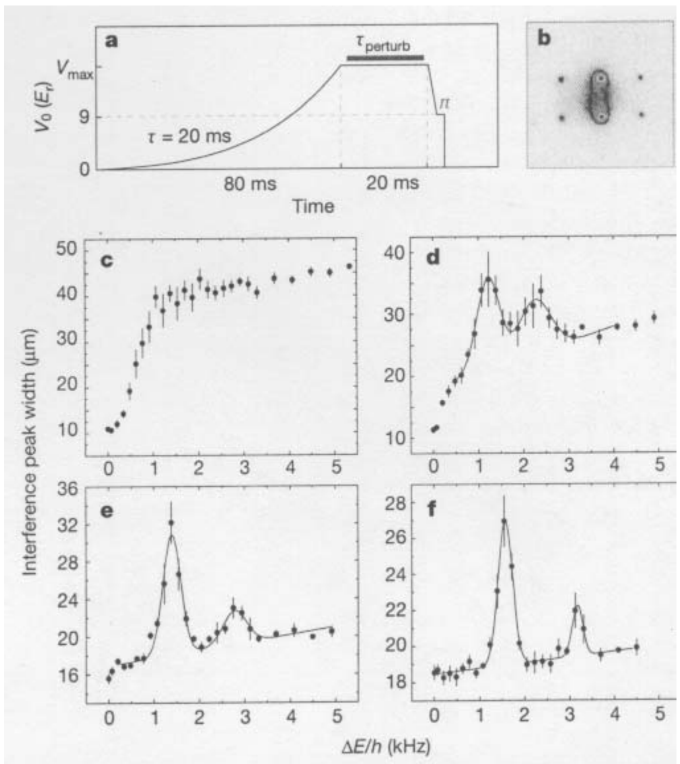

Figure 4: **a. Exptl. sequence: The optical lattice potential is increased in 80ms to a potential depth of V_0. Then the atoms are held for a time of 20ms ($\tau_{perturb}$) during which a potential gradient is applied. The optical potential is lowered again within 3ms to $V_0 = 9E_r$. Now the system is in superfluid state. Again, a potential gradient is applied for $300\mu s$ to change the phases of adjacent atoms by π. Finally the trap potential is suddenly lowered to zero. b. Excitations created by the applied potential gradient. c-f Width of the interference peak versus energy difference ΔE between adjacent sites for different values of V_{max} and $\tau_{perturb}$. c. $V_{max} = 10E_r$,$\tau_{perturb} = 2ms$ d. $V_{max} = 13E_r$,$\tau_{perturb} = 6ms$ e. $V_{max} = 16E_r$,$\tau_{perturb} = 10ms$ f. $V_{max} = 20E_r$,$\tau_{perturb} = 20ms$ The $\tau_{perturb}$ is increased to take into account the higher tunneling times for higher value of V_{max}**

excitation probability. These are excitations in the Mott insulator phase and the location of the first peak on the energy axis gives a measure of the exciation gap Δ or the minimum energy difference between adjacent sites for which the system can be perturbed.

It is observed that the system goes through a transition between $V_0 = 10E_r$ and $V_0 = 13E_r$. U is taken to be $13E_r$ and this value is used in a band structure calculation to numerically compute the critical value of U/J. It is found that $U/J = 36$ which is close to the mean field prediction of $U/J = 5.83 \times z$, where the number of nearest neighbours z here is six.

4 Breaking the Translational Symmetry

Theoretical curiosity in this problem arises from noting that the harmonic trapping potential breaks the translational symmetery of the lattice. Whether the physics is fundamentally different in this as compared to the unconfined case is a matter of inspection. Recent quantum Monte Carlo studies of the Bose Hubbard Hamiltonian modified by the harmonic potential indicate that the breaking of translational invariance has non-trivial effect on the phase diagram. The Bose Hubbard Hamiltonian is modified to[2]:

$$\mathcal{H} = -t \sum_{<i,j>} (a_i^\dagger a_j) + U \sum_i n_i(n_i - 1) + V_c \sum_i (i - L/2)^2 n_i \qquad (10)$$

where V_c is the curvature of the trapping potential and L is the number of sites. The local density is defined as $n_i = \langle a_i^\dagger a_i \rangle$ and the local compressibility as $\kappa_i = \partial n_i / \partial \mu_i$. A world-line quantum Monte Carlo algorithm is used in canonical ensemble to study the Hamiltonian (10)

4.1 Quantum Monte Carlo results

Fig. 5 shows the evolution of the local density with increasing total occupancy of the lattice. Fig. 6 shows the compressibility profile κ_i associated with the local density n_i [2]. It can be clearly seen that the local density becomes almost zero in selected regions as the number of atoms is increased. The consequence of these profiles is that the global compressibility is never zero as opposed to the unconfined case. The number of bosons versus the chemical potential graph is devoid of the plateaus which are characteristic of the Mott insulator phase for unconfined bosons. The state diagram for this model is complicated and will not be discussed here. The basic features are: There are Mott regions even at incommensurate fillings. But these regions are localized and they grow and shrink with the ratio of t/U. The state diagram as is worked in this analysis, has Mott insulator regions that are in co-existence with superfluid state and hence the formation of these regions is not a true quantum critical phenomenon as it is in the unconfined case.

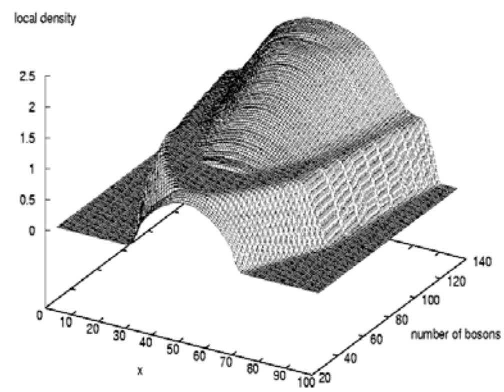

Figure 5: The evolution of the local density n_i as a function of increasing number of bosons. $V_c = 0.008$, $L = 100$ and $U = 4$ At low fillings the system is in the superfluid phase. Mott insulator behavior appears as the density is increased. But then at larger fillings a superfluid begins to form at the center of the trap.

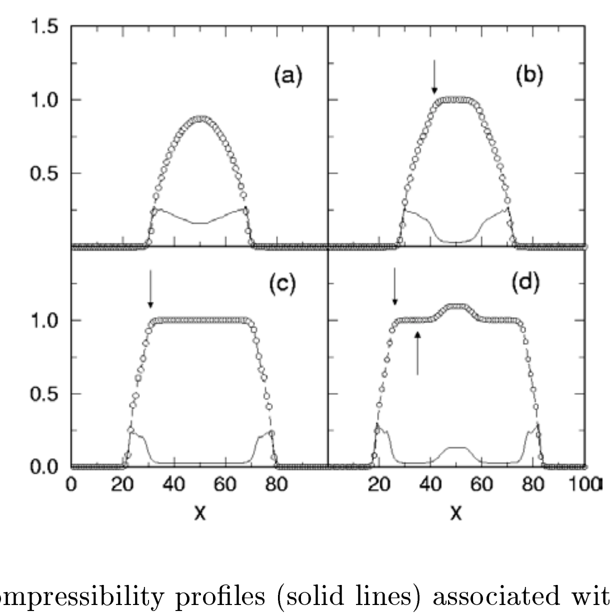

Figure 6: Cuts show compressibility profiles (solid lines) associated with local density profiles. **a.** $N = 25$, **b.** $N = 33$, **c.** $N = 5o$ **d.** $N = 60$

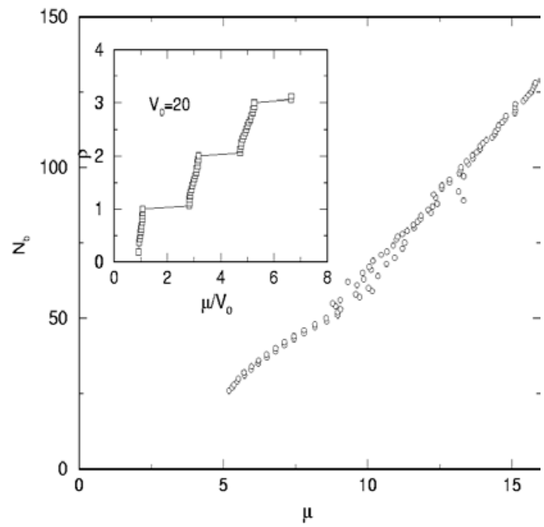

Figure 7: Number of bosons as a function of chemical potential. The global compressiblity does not go to zero. The inset shows the behaviour for confined case and we note the familiar plateaus

5 Conclusion

We have studied the quantum phase transition in lattice bosons. The experiment outlined here successfuly describes the physics of strongly interacting bosons on a lattice. Like the unconfined case, the bosons inside an optical trap undergo a superfluid to Mott insulator transtion when tunneling between the neighboring lattice sites is decreased. The Mott insulator state is an emergent state of matter and excitations in this state are entirely dictated by interactions. However, due to the presence of the harmonic trapping potential, the density of atoms inside the trap is not constant. This inhomogeneity leads to localized Mott insulator domains coexisting with the superfluid state. An immediate outcome of this is we have a superfluid - Mott insulator transition even at incommensurate densities unlike the unconfined case. The global compressibility also shows non-vanishing values even though the Mott insulator state is present.

Future work might focus on studying the dynamics of the superfluid - Mott insulator transition. Also besides changing the tunneling matrix element, it should be possible to study the transtion by changing the atom-atom interaction using Feshbach resonances. Lastly, the effect of disorder in the unconfined case is to introduce an intermediate Bose glass phase where the compressiblity is non-zero but finite. One can introduce a quasi-crystalline order in the optical lattice and look for the existence of the Bose glass phase in confined systems.

The Mott insulator state can be a good candidate for the realization of a Heisenberg-limited atom interferometer [8], which should be capable of improved level of precision. The Mott insulator phase also opens a new experimental realization of recently proposed quantum gates with neutral atoms [9]

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