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A THEORETICAL STUDY OF SUPER FLUID – INSULATOR PHASE TRANSITION IN A GAS OF ULTRA COLD ATOMS AND EVALUATION OF ATOM DENSITY DISTRIBUTION AS A FUNCTION OF DISTANCE FROM THE CENTRE OF TRAP (R/A) USING BOSE-HUBBARD MODEL

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Abstract: - Using the theoretical formalism of **Jakub Zakrzewski (cond-mat/0406186v3 (2005),** we have theoretically studied quantum phase transition from a super fluid to Mott insulator in a gas of ultra cold atoms and evaluated mean field particle density distribution as a function of r/a. Our theoretically evaluated results are in good agreement with the results of quantum Monte Carlo simulation results. This calculation also indicates that mean field Gutzwiller approximation allows one to simulate the dynamics of Bose-Hubbard model taking into account of realistic experimental conditions. Our theoretically evaluated results are also in good agreement with other theoretical workers.

Keywords: Bose-Hubbard model, Quantum phase transition, Super fluid-insulator phase transition, Gutzwiller trail function, Mean field approximation, Quantum Monte Carlo simulation, Wannier site function, Harmonic magnetic trap potential, Time dependent mean field dynamics, Integrated momentum distribution

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INTRODUCTION

The Bose-Hubbard model[1,2] is one of the standard models for studying the interacting particles in a cold gas placed in an optical lattice. The reported realization[3] of a quantum phase transition between super fluid (SF) and Mott insulator (MI) phase showed that one can control the parameters of the model at will. This has triggered several studies involving Bose condensate[4-9] and Bose-Fermi mixtures[10-13] placed on optical lattice. Several groups have also tried to understand the details of the experiments[3] to check the underlying physics involved in it.

A physical system that crosses the boundary between two phases changes its properties in a fundamental way. When the temperature of the system approaches zero, all thermal fluctuations die out. This prohibits phase transition in a classical system at zero temperature as their opportunity to change has vanished. However, their quantum mechanical counterparts can show fundamentally different behavior. In quantum system, fluctuations are present even at zero temperature due to Heisenberg uncertainty relation. These quantum fluctuations may be strong enough to derive a transition from one phase to another bringing about the macroscopic change. A prominent example of such a quantum phase transition is the change from the super fluid phase to Mott insulator phase in a system consisting of bosonic particles with repulsive interactions hopping through a lattice potential. This system was first studied theoretically in the context of super fluid to insulator transitions in liquid helium[14]. Jakisch etal[15] have proposed that such a transition might be observable when an ultra cold gas of atoms with repulsive interactions is trapped in a periodic potential.

Here, one considers an atomic gas of bosons at low enough temperatures that a BE condensate is formed. The condensate is a super fluid and is described by a wave function that exhibits long range coherence[16]. An intriguing situation appears when the condensate is subjected to a lattice potential in which the bosons can move from one lattice site to the next by tunnel coupling. If the lattice potential is turned on smoothly the system remains in the super fluid phase as long as the atom-atom interaction are small compared to the tunnel coupling. In this regime, a delocalized wave function minimizes the dominant kinetic energy, and also minimizes the total energy of the many body system. In the opposite limit when the repulsive atom atom interactions are large compared to the tunnel coupling, the total energy is minimized when each lattice site is filled with same number of atoms. The reduction of fluctuation in the atom number on each site leads to increased fluctuation in the phase. Thus in the state with fixed atom number per site phase coherence is lost. In addition, a gap in the excitations spectrum appears. The normal phase transition is driven by the competition between inner energy and

entropy whereas quantum phase transition is driven between the kinetic and interaction energy.

In this paper, using the theoretical formalism of J. Zakrzewski[17,18], we have theoretically studied the quantum phase transition from a super fluid to a Mott insulator in a gas of ultra cold atoms. We have also theoretically evaluated mean field particle density distribution as a function of r/a taking different set of parameters U, U_0 and κ. We have also evaluated atom density distribution (accumulations of sites) as a function of r/a by taking four sets of parameters V, N and γ_{SF} where V is lattice depth potential, N is total number of atoms and γ_{SF} is super fluid factor. Our theoretically evaluated results are in good agreement with other theoretical workers[19-21].

MATERIALS AND METHODS

The Bose-Hubbard Hamiltonian describing the system takes the form[22]

$$H = -J\sum_{<i,j>} a^{+}_{i}a_{j} + \frac{U}{2}\sum_{i} n_i(n_i - 1) + \sum_{i} W_i n_i \qquad (1)$$

Where $n_i=a_i^{+}a_i$ is occupation number operator at site i (with a_i being the corresponding annihilation operator) W_i denotes the energy offset of the ith lattice sites due to external harmonics component of the atom. U is the interaction energy and J is the tunneling coefficient. $\Sigma_{<i,j>}$ denote a sum over nearest neighbor. The strength of the tunneling term is characterized by the hopping matrix element between adjacent sites i,j

$$J = -\int d^3x w(x - x_i)\left(\frac{-\hbar^2\nabla^2}{2m} + V_{lat}(x)\right)w(x - x_i) \qquad (2)$$

Where $w(x-x_i)$ is the single particle Wannier function localized to the ith lattice site, $V_{lat}(x)$ is optical lattice potential and m is the mass of a single atom. The repulsion between two atoms on a single lattice site is given by on-site interaction matrix element U

$$U = \left(\frac{4\pi\hbar^2 a}{m}\right)\int |w(x)|^4 d^3x \qquad (3)$$

Where a is the scattering length of an atom. One first considers the standard homogeneous situation in which all W_i's are equal. The last term of equation (1) becomes proportional to the number of bosons and may be dropped. The only remaining parameter of the model is the ratio

U/J. When tunneling dominates the system in its ground state is super fluid while in the opposite case it becomes the Mott insulator. The border line between the two phases depends on the chemical potential. The effective chemical potential at each site is given by

$$\mu_i = \mu - W_i \qquad (4)$$

Now to find the mean field ground state, one minimizes

$$< E >= \langle G | H - \mu N | G \rangle \qquad (5)$$

Where N= $\Sigma_i n_i$ and $|G\rangle$ is Gutzwiller trial function

$$|G\rangle = \prod_{i=1}^{N1} (\sum_{n=0}^{n_m} f^{(i)}{}_n |n > i\rangle \qquad (6)$$

Where the number of parameters $f_n^{(i)}$ depends on the number of site as well as the maximal occupation of a given site n_m. At each site I, one takes a solution for $f_n^{(i)}$ corresponding to the homogeneous B-H model with the effective chemical potential μ.

Now the difference of the on-site energy W_i and the chemical potential μ is expressed as

$$W_i - \mu = -U_0 + \frac{U}{2} + \kappa x^2{}_i \qquad (7)$$

Where x_i is the position vector of site i. U and U_0 are different taken to match the results with mean field solution with quantum Monte Carlo results[23]. The momentum distribution is given by[24]

$$n_k = |\phi(k)|^2 \sum_{i,j} e^{ik.(r_i - r_j)} < a^+{}_i a_i > \qquad (8)$$

Where **k** is the wave vector, ϕ(k) is Fourier transform of Wannier site function. In order to characterize whether the state is closer to super fluid or Mott insulator, one defines the super fluid factor γ_{SF}

$$\gamma_{SF} = \frac{1}{N} \Sigma < a_i >< a^+{}_i > \qquad (9)$$

γ_{SF} =0.0 for pure MI state.

Now, one applies time dependent variational principle[25]. One takes minimum of expression

$$\langle G(t)|i\hbar\frac{\partial}{\partial t}-H(t)+\mu N|G(t)\rangle \quad \text{=minimum} \quad (10)$$

Here H(t) is time dependent Hamiltonian . μ is also time dependent. $|G(t)\rangle$ is variational wave function. The minimum of equation (10) gives the set of first order differential equation for $f_n^{(i)}(t)$

$$i\hbar\frac{d}{dt}f^{(i)}{}_n=[\frac{U}{2}n(n-1)+n(W_i-\mu)]f^{(i)}{}_n-J[\phi^*{}_i\sqrt{n+1}f^{(i)}{}_{n+1}+\phi_i\sqrt{n}f^{(i)}{}_{n-1}] \quad (11)$$

Where $$\phi_i=\Sigma_{<j>}\langle G(t)|a_j|G(t)\rangle \quad (12)$$

In equation (12) the sum as indicated by subscript in bracket is over the nearest neighbor only. Now when U and J change the chemical potential corresponding to the mean field solution with a given number of particles N also changes. The dynamics of μ depends upon the evolution of two states $|G_1\rangle$ and $|G_2\rangle$ with different average number of particles.

$$N_2=\langle G_2|\hat{N}|G\rangle=N_1+\delta N=\langle G_1|\hat{N}|G_1\rangle+\delta N \quad (13)$$

The chemical potential at given time will be

$$\mu(t)=\frac{[\langle G_2(t)|H(t)|G_2(t)\rangle-\langle G_1(t)|H(t)|G_1(t)\rangle}{\delta N} \quad (14)$$

This approach is used to find out the numerical results shown in table

The freely expanding atomic cloud after some delay was recorded by a destructive absorption imaging which is reflected in the momentum distribution[26]. Since the absorption images are taken along two orthogonal axes the quantity measured in fact is the integrated momentum distribution which is given by

$$N(k_x,k_y)\alpha\int dk_z n_k \quad (15)$$

For clouds released from low optical lattice when tunneling dominates and the super fluid behavior is expected the signal reflects Bragg peaks due to interference of the atoms coming from different lattice sites. At increased lattice depth above $13E_\gamma$ (where E_γ is the recoil energy of the Rb atom) the interference maxima immersed in the incoherent background. This behavior is associated with the quantum phase transition from SF to MI phase.

RESULTS AND DISCUSSION

In this paper using the theoretical formalism of Jakub Zakrzewski[17,18], we have studied mean field dynamics of super fluid –insulator phase transition in a gas of ultra cold atoms. We have evaluated mean field particle distribution (on site filling factor) n as s function of r/a and mean field atom density distribution (accumulation of sites) also as a function of r/a with different set of parameters. **In table T1,** we have shown the evaluated results of mean field particle distribution 'n' as a function of r/a with different sets of parameters; (a) U=24, U_0=-11.08, κ=0.19531 (b) U=32, U_0=-28.08, κ=0.19531 (c) U=80, U_0 =-65, κ=0.97656. U is the interaction energy, U_0 is the energy required to make a particle-hole excitation, κ is the parameter to match the result of mean field with Quantum Monte Carlo results. Our evaluated results indicate that mean particle distribution n decreases with r/a. the decrease is more sharply pronounced in case of (a) in comparison to (b) and (c) . **In table T2,** we again repeated the calculation by taking three different values of U, U_0 and κ shown in (d), (e) and (f). In this case the value of n is large in (f) and small in (d). Here, also n decreases with r/a. **In table T3,** we have shown the evaluated results of mean field atom density distribution (occupation of sites) as a function of r/a. Here, we have taken three sets of parameters V, N and γ_{SF} known as lattice depth potential, Total number of particles, E_γ recoil energy, Super fluid factor. In calculation, we have taken four sets of parameters (a) V=$9E_\gamma$, N=99771, γ_{SF}=0.95 (b) V=$13E_\gamma$, N=99502, γ_{SF}=0.40 (c) V=$16E_\gamma$, N=95408, γ_{SF}=0.11 (d) V=$22E_\gamma$, N=94572, γ_{SF}=0.01. Here, the chemical potential μ has been adjusted to have the average number of atoms 10^5. This leads to more than two atoms per site in the center of the trap. To characterize whether the state is closer to being super fluid or Mott insulator, we take super fluid factor γ_{SF}. The case V=$9E_\gamma$ seems almost fully super fluid when V=$13E_\gamma$ shows first traces of insulating phase. The transition is completed for significant fraction of sites at V=$16E_\gamma$ while for deepest lattice V=$22E_\gamma$,SF fraction is restricted to vary narrow regions separately different integer occupations. In **table T4,** we have given the interference peak widths (μm) as a function of energy difference between neighboring sites ΔE/Ћ due to potential gradient applied. Here, we have also taken four different sets of potential gradient (a) $10E_\gamma$ (b) 13 E_γ (c)16 E_γ and (d) 20 E_γ. The results shown in tableT4 are fits to the data based on two Gaussian peaks on the tops of the linear backgrounds. The obtained results can

be interpreted as follows: If excitations have been created during the application of the potential gradient at the potential depth $V_0=V_{max}$ then one is not able to return to perfectly coherent super fluid state by taking the potential to a depth Vo=9 E_γ. Here, excitations in the Mott insulator phase will lead to excitations in the lower energy band in the super fluid case. These excitations are simply phase fluctuations between lattice sites. It also causes a broadening of the interference maxima in the interference pattern. Our theoretical results indicate that in case (a) $V=10E_\gamma$ the state is completely super fluid state. In this case no peak values are seen. In case (b) V= 13 E_γ two peak values are observed as a function of $\Delta E/\hbar$. Similarly in case of (c) and (d) two peak values are observed. These all results show the dynamical process of restoring coherence coming from Mott insulator Phase. There is some recent calculations[27-35] which also reveals the same behavior.

CONCLUSION

From the above theoretical analysis and investigations, we have come across the following conclusions

(1) In the theoretical study of quantum phase transition from a super fluid to a Mott insulator in a gas of ultra cold atoms, we observed that as the potential depth of the lattice is increased, a transition is observed from a super fluid to Mott insulator phase. In the super fluid phase each atom is spread out-over the entire lattice with long range phase coherence. But in the insulating phase atoms are localized at individual lattice sites with no phase coherence across the lattice. This phase is characterized by a gap in the excitation spectrum.

(2) Our theoretical calculation show that the mean field Gutzwiller approximation allows ones to simulate the dynamics of inhomogeneous Bose-Hubbard model and calculates the mean-field particle density distribution as a function of r/a. The obtained results are in good agreement with the quantum Monte Carlo simulation results.

Table T1: An evaluated result of mean-field particle distribution 'n' as a function of r/a with different sets of parameters (a) U=24, U_0=-11.08, κ=0.19531 (b) U=32, U_0=-28.08, κ=0.19531 (c) U=80, U_0 =-65, κ=0.97656. U is the interaction energy, U_0 is the energy required to make a particle-hole excitation, κ is the parameter to match the result of mean field with Quantum Monte Carlo results.

r/a	<-------n----------→		
	(a)	(b)	(c)
1.0	0.562	1.000	1.000
1.5	0.508	0.982	0.984
2.0	0.476	0.917	0.942
2.5	0.403	0.843	0.936
3.0	0.365	0.796	0.904
4.0	0.308	0.702	0.896
5.0	0.284	0.654	0.845
6.0	0.237	0.606	0.726
7.0	0.186	0.532	0.637
8.0	0.105	0.474	0.548
9.0	0.084	0.286	0.406
10.0	0.006	0.205	0.316
12.0	0.000	0.005	0.006

Table T2: An evaluated result of mean-field particle distribution 'n' as a function of r/a, the others parameters are (d) U=80, U_0=-90.0, κ=1.03062 (e) U=80.0, U_0=-120.08, κ=2.00375 (f) U=80, U_0 =-150.0, κ=1.75781.

r/a	<-------- n----------→		
	(d)	(e)	(f)
0.5	1.000	1.526	2.058
1.0	0.985	1.438	1.897
1.5	0.976	1.407	1.820
2.0	0.966	1.328	1.769
2.5	0.931	1.304	1.705
3.0	0.892	1.286	1.658
3.5	0.824	1.232	1.606
4.0	0.786	1.205	1.584
5.0	0.723	1.195	1.532
6.0	0.683	1.167	1.505
7.0	0.636	0.678	0.652

8.0	0.432	0.439	0.504
9.0	0.324	0.340	0.368
10.0	0.242	0.228	0.254
12.0	0.017	0.007	0.090

Table T3: An evaluated result of mean-field atom density distribution (accumulation of sites) as a function of r/a. others parameters are (a) V=9E_γ, N=99771, γ_{SF}=0.95 (b) V=13E_γ, N=99502, γ_{SF}=0.40 (c) V=16E_γ, N=95408, γ_{SF}=0.11 (d) V=22E_γ, N=94572, γ_{SF}=0.01.Here three sets of parameters V, N and γ_{SF} are known as lattice depth potential, Total number of particles, E_γ recoil energy, Super fluid factor

r/a	<----Atom density distribution---→			
	(a)	(b)	(c)	(d)
2	2.232	2.142	2.058	2.163
4	2.156	2.056	1.942	2.104
5	2.084	1.972	1.906	1.986
10	1.892	1.904	1.854	1.954
15	1.806	1.844	1.786	1.902
18	1.546	1.607	1.422	1.567
20	0.862	1.538	1.368	1.524
22	0.588	0.675	0.954	1.496
24	0.505	0.627	0.836	1.476
25	0.462	0.508	0.655	1.443
27	0.404	0.422	0.624	1.402
30	0.327	0.365	0.596	0.176
35	0.158	0.278	0.243	0.104
40	0.053	0.074	0.084	0.074

Table T4 : An evaluated result of interference peak width(μm) as a function of energy difference between neighboring lattice sites ΔE/ħ due to potential gradient applied (V_{max}=10E_γ (b) 13E_γ (c) 16E_γ (d) 20 E_γ

ΔE/ħ (KHz)	<-----Interference peak width (μm)---------→			
	(a)	(b)	(c)	(d)
0	10.25	10.86	16.25	18.57
1.0	15.68	12.58	18.84	20.26
1.5	20.46	22.47	32.35	28.42
2.0	28.75	38.15	28.20	17.29

2.5	33.26	30.26	22.16	23.25
3.0	37.49	32.39	24.58	24.16
3.5	41.86	37.15	23.86	27.89
4.0	43.24	30.42	21.29	22.42
4.5	44.59	29.59	22.58	23.67
6.0	45.16	32.57	23.09	20.34
6.5	47.27	33.11	28.13	18.29
7.0	49.58	39.56	29.24	17.56
8.0	55.06	38.29	26.12	24.42

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