Quantum Critical Point in Strongly Correlated $^{87}\text{Rb}$ Atoms in Optical Lattice

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Abstract

In this paper, the Bosonic projected variational method is proposed to study the strongly correlated $^{87}\text{Rb}$ atoms in optical lattice. A global phase diagram is obtained by this method. There exist two characteristic lattice depths $V$ for $^{87}\text{Rb}$ atoms in optical lattice: one is $V = 9.5E_r$ to label the maximum height of the 'zero-momentum' peak of condensation, the other is the quantum critical point for the superfluid-insulator (SI) transition at $V = 12.3E_r$. As a result of strongly correlated effect for lattice Bosons, the suppressed superfluid state is predicted near the SI transition with the suppressed superfluid density and the very slowly velocity of the sound-like excitons.

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During the last years a spectacular development in the storage and manipulation of cold atoms in optical lattices has taken place. An superfluid-insulator (SI) transition was observed for $^{87}$Rb atoms trapped in a three-dimensional optical lattice potential by changing the potential depth [1]. The SI transition is the appearance of a excitation gap. In the superfluid regime, there is no excitation gap and instead one observes a series of 'Bragg-peaks' around the characteristic 'zero-momentum' peak of a condensate in the absence of an optical lattice. The existence of this gap has been verified experimentally by applying a phase gradient in the Mott-insulator. This experimental progress has revived the interest in the Bose-Hubbard (BH) model as a generic Hamiltonian for strongly correlated bosons [2], by which the quantum phase transition can be described [3–18].

In this paper we intend to examine the physics in $^{87}$Rb atoms by studying a Bose-Hubbard model using a variational method for bosonic systems [19]. In the new approach, the on-site repulsion is treated exactly, while the kinetic energy is studied variationally, so that it is suitable to examine some issues in strongly correlated Bosonic systems. The variational method applied to the Bose-Hubbard model in three-dimension demonstrates a quantum phase transition from a superfluid with suppressed superfluid density for smaller intra-site Coulomb repulsion $U$ to a Mott insulator for larger $U$ at unit filling $\frac{N}{L} = 1$. There exists a quantum critical point (QCP) for the homogenous phase. We calculate the superfluid density near the QCP and show the existence of the suppressed superfluid state which is a kind of ”gossamer” phenomenon. The idea of ”gossamer” (superconducting) state is that the “insulator” might actually be a thin, ghostly superconductor which is proposed by Laughlin [20,21]. In a suppressed superfluid state, the superfluid density is very thin and the velocity of the sound-like excitons is very slow, in contrast to the conventional superfluid state.

The system is based on confining cold $^{87}$Rb atoms in the periodic potential of an optical lattice [1]. In the simplest case, three orthogonal, independent standing laser fields with wave vector $k$ produce a separable three dimensional lattice potential $V(x, y, z) = V \left( \sin^2 kx + \sin^2 ky + \sin^2 kz \right)$ with a tunable amplitude $V \gg E_r = \hbar^2 k^2 / 2m$. Starting from the standard pseudopotential description the interatomic potential is replaced by an
effective contact interaction of the form $U(\vec{x}) = \frac{4\pi^2a_s}{m} \cdot \delta(\vec{x})$ containing the exact s-wave scattering length $a_s$. With $\hat{a}_i^\dagger$ as the creation operator of a boson at site $i$ and $\hat{n}_i$ as the density operator, the Hamiltonian reads

$$\hat{H} = -J \sum_{<ij>} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1)$$

(1)

The bandwidth parameter $J$ is essentially the gain in kinetic energy due to nearest neighbor tunneling $J = \frac{4}{\sqrt{\pi}E_r} \left(\frac{V}{E_r}\right)^{3/4} \exp -2 \left(\frac{V}{E_r}\right)^{1/2}$. The relevant interaction parameter $U$ is thus given by an integral over the on-site wave function via $U = \sqrt{\frac{2}{\pi}}ka_sE_r \left(\frac{V}{E_r}\right)^{3/4}$.

We consider $|\Psi\rangle = \hat{P}_p |\Phi_0\rangle$ as a variational wavefunction to examine the ground state of the above effective BH model for $^{87}$Rb atoms in optical lattices. $|\Phi_0\rangle$ is the wavefunction of the Bose-condensed ground state for non-interacting Bosons

$$|\Phi_0\rangle = \exp(\sqrt{N} e^{i\phi_0} \hat{a}_{k=0}^\dagger)|0\rangle$$

(2)

where $N$ is the number of Bosons. The order parameter $\langle \Phi_0 | \hat{a}_{k=0} \hat{a}^\dagger_{k=0} |\Phi_0\rangle = e^{i\phi_0} \sqrt{N}$ shows an off diagonal long range order. $\hat{P}_p$ is the Bosonic partial projection (BPP) operator defined as

$$\hat{P}_p = \prod_{m=2}^N \prod_i \left[1 - \prod_{j=0, j\neq m}^N (\hat{N}_i - j) \cdot (1 - \varepsilon_m)\right].$$

(3)

If the on-site repulsive interaction between bosons is large enough, there exist little possibly of high occupation states, we can introduce the Bosonic partial projection (BPP) operator to describe the strongly correlated effects. If $\varepsilon_m = 0$, the Bosonic partial projection operator $\hat{P}_p$ turns into the Bosonic completely projection operator $\hat{P}_c$, the ground state $|\Psi\rangle$ is reduced into a Mott insulator state with gapped excitons. If $\varepsilon_m = 1$, there is no interaction between Bosons, the Bosonic partial projection operator $\hat{P}_p$ turns into constant number $\hat{P}_p = 1$, and the ground state turns into a Bose-condensation state with massless excitons $E \sim \alpha q^2$.

The variational energy for the ground state becomes

$$E_g = \langle \Psi | \hat{H} | \Psi \rangle / \langle \Psi | \Psi \rangle$$

$$= \langle \hat{H}_t \rangle + UD_2 + 3UD_3 + ... + \frac{N(N-1)}{2} UD_N.$$ 

(4)
The occupation numbers are $D_2, D_3, \ldots D_N$. The variational kinetic energy $\langle H_t \rangle$ is

$$\langle H_t \rangle = \langle \Psi \mid -J \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_j + \text{h.c.}) \mid \Psi \rangle / \langle \Psi \mid \Psi \rangle = g_J E_0$$

where $E_0$ the kinetic energy for non-interaction Bose systems

$$E_0 = \langle \Phi_0 \mid -J \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_j + \text{h.c.}) \mid \Phi_0 \rangle / \langle \Phi_0 \mid \Phi_0 \rangle. \quad (6)$$

$g_J$ is renormalization factor for kinetic energy to be determined.

In the thermodynamics limit $N \to \infty$, we choose the maximum term of the variational wavefunction $|\Psi\rangle$ and obtain the condition

$$\varepsilon^2_m = \frac{d_m(x + d_2 + 2d_3 + \ldots + (N - 1)d_N)^{m-1}}{(1 - x - 2d_2 - 3d_3 \ldots - Nd_N)^m}, \quad (7)$$

where $x = (N - D_2 - D_3 - \ldots D_N)/L$ describes the empty concentration. $L$ is the number of the site. From the condition we have the renormalization factor for the kinetic energy

$$g_J = \sum_{m=1}^{N} C_m A^m B^{m-2}, \quad (8)$$

$$C_m = \varepsilon_{m-1}\varepsilon_m + \varepsilon_2\varepsilon_{m-2}\varepsilon_{m-1} + \varepsilon_2\varepsilon_3\varepsilon_{m-3}\varepsilon_{m-2} + \ldots$$

$$+ \varepsilon_i\varepsilon_{m-i-1}\varepsilon_{m-i+1} + \ldots + \varepsilon_{m-1}\varepsilon_{m}.$$  

with $A^m = 1 - x - 2d_2 - 3d_3 \ldots - Nd_N$ and $B = x + d_2 + 2d_3 + \ldots + (N - 1)d_N$.

In the strong interaction limit, one has $\varepsilon^2_m \simeq \frac{d_m(x + d_2)^m}{(1 - x - 2d_2)^m}$. The renormalization factor for the kinetic energy is obtained as

$$g_J \simeq (d_2 + x)(1 - x - 2d_2)$$

$$+ \ldots 2\sqrt{d_{m-2}d_{m-1}[(d_2 + x)(1 - x - 2d_2)]^{1/2}} + \ldots.$$  

where $d_m = \frac{D_m}{L}$ are determined by the equations

$$\frac{\partial E_g(d_m)}{\partial d_m} = 0.$$
In this paper we solve the equations by the approximation up to $d_2$ without considering $d_m$, $m > 2$ [22]. The renormalization factor is obtained as $g_J \approx (1 - x - 2d_2)(2d_2 + x + 2\sqrt{d_2(d_2 + x)})$. $d_2$ is determined by the minimum energy condition $\frac{\partial E_0}{\partial d_2} = 0$ as $d_2 \simeq \frac{1}{4}[1 - (\frac{U}{24J})]$. In the following paper we consider a BH model with unit filling $N/L = 1$ or $x = 0$.

Note that in the BPP approach and at unit filling case $N/L = 1$ or $x = 0$, $d_2$ is a measure of the mobile carrier density. At $d_2 = 0$, we have $\langle H_t \rangle = 0$. This state describes a Mott insulator. On the other hand, the case with $d_2 > 0$ describes superfluid state. We expect a transition from the Mott insulator at larger $U$ to the superfluid at smaller $U$ as $U$ decreases passing through a critical point $U_c$. The transition point $U_c$ is given by

$$U_c = (\frac{-\partial g_J}{\partial d_2})|_{d_2=0} \frac{E_0}{N} = 24J$$

or $(\frac{V}{E_t})_c = \frac{1}{4}\ln^2(\frac{\sqrt{2k_0}}{48}) \simeq 12.3$. For $U > U_c = 24J$, there is no solution for physical values of $d_2$, indicating that $d_2 = 0$.

If $U \leq U_c$ ($\frac{V}{E_t} < 12.3$), $d_2 > 0$ ($\varepsilon_2 > 0$), the ground state is a superfluid state.

Within the BPP approximation, the suppressed superfluid density $\langle \Phi | \hat{n}_{\vec{k}=0} | \Phi \rangle$ is

$$\frac{\langle \Phi | \hat{n}_{\vec{k}=0} | \Phi \rangle}{\langle \Phi_0 | \hat{n}_{\vec{k}=0} | \Phi_0 \rangle} = g_J = \frac{1}{2}[1 - (\frac{U}{U_c})^2].$$

In this state, the mobile carrier density $d_2$ is fixed and the excitons are the phase fluctuations - phasons. To consider the dynamics of phasons, the quantum states are defined as

$$| \tilde{\Psi} \rangle = \hat{P}_p \exp(\sum_j e^{i\varphi_j} a_j^+) | 0 \rangle.$$  

The effective Hamiltonian becomes

$$H_{eff} = \langle \tilde{\Psi} | -J \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_j + h.c.) + \frac{U}{2} \sum_i n_i(n_i - 1) | \tilde{\Psi} \rangle / \langle \tilde{\Psi} | \tilde{\Psi} \rangle$$

$$\sim -\rho_p \sum_{\langle ij \rangle} \cos(\varphi_i - \varphi_j) + U \sum_i (\frac{d}{d\varphi_i})^2,$$

where $\rho_p = \frac{d}{4}[1 - (\frac{U}{U_c})^2]$ is the phase stiffness. As a result the effective model of the SF state turns into a quantum four dimensional XY model with long range order. The transition temperature $T_c$ is scaled as $T_c \sim \rho_p^{2/3}$ [2].


In the SF regime, there is no excitation gap and instead the homogeneous system exhibits a sound like mode - phason with frequency $\omega(q) = cq$. The associated sound velocity is $c = \sqrt{\frac{1}{4}JU[1 - (\frac{U}{U_c})^2]}$. It is the correlated effect drives the BEC-like $q^2$ spectrum to superfluid-like $q$ type.

The SF phase of $^87$Rb atoms in an optical lattice can thus quite generally be characterized by the fact that at reciprocal lattice vectors $\vec{q} = 0$, the momentum distribution $n_0$ has a peak with the height as [1,24]

$$n_0 = L \cdot \langle \Phi | \hat{n}_{\vec{k}=0} | \Phi \rangle |w(0)|^2$$

$$\sim L \frac{1}{2} \left[ 1 - \sqrt{2}ka_s \exp(-\sqrt{4V/E_r}) \right] \left( \frac{V}{E_r} \right)^{3/2}.$$  

The fact that the peaks in the momentum distribution at $\vec{q} = 0$ initially grow with increasing depth of the lattice potential is a result of the strong decrease in spatial extent of the Wannier function $w(\vec{x})$, which entails a corresponding increase in its Fourier transform $w(\vec{q}) \propto (\frac{V}{E_r})^{3/4}$. Beyond a critical lattice depth around $V = 9.5E_r$, this trend is reversed, however, and the superfluid density eventually disappear completely at $U = U_c$ ($V = 12.3E_r$).

If $U > U_c$ or $(\frac{V}{E_r})_c > 12.3$, $d_2 = 0$ and $\varepsilon_2 = 0$ ( $d_m = 0$ and $\varepsilon_m = 0$, $m > 2$), the ground state is a Mott insulator, of which the wave function is

$$| \Phi > = \hat{P}_c | \Phi_0 > = L^{-1/2} \prod_l (|1_l >).$$

The energy gap describes the energy difference between the ground state with $D_2 = 0$ and the excited state with $D_2 = 1$ as $\Delta E \approx -24J \cos(aq/2) + U$. The excited energy $\Delta E$ is from $(U - 24J)$ to $(U + 24J)$ with the center at $U$. $\Delta$ is the Mott gap for Boson exciton defined as $\Delta = (U - 24J)$. Deep in the MI phase, this gap has size $U$, which is just the increase in energy if an atom tunnels to an already occupied adjacent site. The existence of this gap has been verified experimentally by applying a phase gradient in the MI and measuring the resulting excitations produced in the SF at smaller $V/E_r$ [1]. Near the Mott transition, the gap closes $\Delta = (U - 24J) = 0$. The signal of the Mott gap $\Delta$ disappeared around $V = 12.3E_r$ ($U = 24J$), which was taken also as another definition of the critical point of the SI transition.
Above results predict two characteristic lattice depths: $V = 9.5E_r$ and $V = 12.3E_r$. Near the lattice depth around $V = 9.5E_r$, the 'zero-momentum' peak has maximum height at which the condensation is most robust. Beyond this point, the phase coherence becomes weak. The other characteristic lattice depth is $V = 12.3E_r$ which is just the QCP for the SI transition. At this point the 'zero-momentum' peak disappears together with the opening of a gap for particle-hole excitons. From the experiments by M. Greiner, at almost the same point $V \approx 13E_r$ the 'zero-momentum' peak of a condensate has maximum height and the Mott gap $\Delta$ opens. Thus there exist only one characteristic lattice depth. The difference between our results and the experiments is due to the inhomogeneous [1,4,25]. In this paper our theory is based on the homogenous phase without considering the inhomogeneous phase. The inhomogeneous phase in the BH model from BPP method will be explored elsewhere.

In strongly correlated limit near the SI critical point $0 < \frac{U - U_c}{U_c} \ll 1$, a new class of superfluid state appears - the suppressed superfluid state. The wavefunction for so called the suppressed superfluid state is read as

$$|\Phi > = \hat{P}_p|\Phi_0 > = L^{-1/2} \prod_l (|0_l > + |1_l > + \sum_{n_l=1}^{N} \varepsilon_{n_l} |n_l >),$$

$$\varepsilon_{n_l} \approx \frac{d_m(x + d_2)^{m-1}}{(1 - x - 2d_2)^m} \ll 1.$$

It is obviously that the superfluid density for the suppressed superfluid is suppressed seriously by correlations

$$n(\vec{q} = 0) = \langle \Phi | \hat{n}_{\vec{q}=0} |\Phi \rangle = \frac{1}{2} (1 - (\frac{U}{U_c})^2) \to 0,$$

a quantitative measure of the suppressed superfluid. Another feature for the suppressed superfluid is the existence of a very slowly velocity of the phasons. The associated sound velocity turns into zero $c = \sqrt{\frac{1}{4} J U [1 - (\frac{U}{U_c})^2]} \to 0$. The third character for the suppressed superfluid is the pinned chemical potential at the center of the gap.

Let us now consider the evolution of chemical potential. The chemical potential $\mu$ is $\mu = \mu_0 + \frac{\partial g}{\partial x}$. The term originates from the $x$ dependences of $g_J$ in the variational procedure [21], which will be important in calculation of the chemical potential of the state.
\[
\frac{\partial g}{\partial x} = 1 - 2(2d_2 + x) - 2\sqrt{d_2(d_2 + x)} \\
+ (1 - 2d_2 - x)\sqrt{(d_2 + x)/d_2}.
\] (18)

In the limit \(x \to 0, U \to U_c\), \(\frac{\partial g}{\partial x} \sim 2 - 8d_2\), one has

\[
\mu \to \mu_0 + \frac{U}{2}.
\] (19)

Our results show that the suppressed superfluid state is a similar phenomenon to the gossamer superconductivity. From the results of the partial projection to the Gutzwiller variational method, the ground state for strongly correlated electrons may be superconducting at half filling due to some kinds of attraction mechanism [21]. In this paper it is shown that because of the partial projection, there exists the suppressed superfluid state at unit filling \(N/L = 1\) in the region of \(0 < \frac{U - U_c}{U_c} \ll 1\). The Bose condensation can be suppressed seriously by strongly correlated effect.

In summary, we have used the Bosonic projected variational method to study the Bose-Hubbard model which is the effective model for strongly correlated \(^{87}\text{Rb}\) atoms in the optical lattice. And we obtain a global phase diagram of the homogenous phase and give two results: two characteristic lattice depths in phase diagram and the existence of the "gossamer"-like state near the SI transition.

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**Figure Captions**

Fig.1

This figure shows the double occupation rate $d_2$ and the triple occupation rate $d_3$ of $\gamma = \frac{U}{E_0}$.

Fig.2

Phase diagram for the Bose-Hubbard model under unit filling. In this figure the scales at left axis and right axis are $T_c(U \rightarrow 0)$ and $U_c$, respectively. $\frac{\nu_0}{E_c}$ is the parameter for Bosons in optical lattice.
This figure "becfig1.jpg" is available in "jpg" format from:

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