Phase diagram of ultracold atoms in optical lattices: Comparative study of slave fermion and slave boson approaches to the Bose-Hubbard model

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We perform a comparative study of the finite temperature behavior of ultracold Bose atoms in optical lattices by the slave fermion and the slave boson approaches to the Bose Hubbard model. The phase diagram of the system is presented. Although both approaches are equivalent without approximations, the mean field theory based on the slave fermion technique is quantitatively more appropriate. Conceptually, the slave fermion approach automatically excludes the double occupancy of two identical fermions on the same lattice site. By comparing to known results in limiting cases, we find the slave fermion approach better than the slave boson approach. For example, in the non-interacting limit, the critical temperature of the superfluid-normal liquid transition calculated by the slave fermion approach is closer to the well-known ideal Bose gas result. At zero-temperature limit of the critical interaction strength from the slave fermion approach is also closer to that from the direct calculation using a zero-temperature mean field theory.

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I. INTRODUCTION

Strongly correlated systems are of longstanding interest in studies of condensed matter physics. Ultra-cold atoms in optical lattices offer new opportunities to study strongly correlated phenomena in a highly controllable environment. A quantum phase transition, the superfluid/Mott-insulator transition, was demonstrated using $^87$Rb atoms in three- and one-dimensional lattices. Strongly correlated phenomena for boson systems may be studied theoretically by the Bose-Hubbard model. Experimental feasibility was established by microscopic calculations of the model parameters for cold boson atoms in optical lattices. A review of recent works on the superfluid-insulator quantum phase transition at zero temperature is given in ref. 7.

Strictly speaking, a quantum phase transition can not be observed at any finite temperature. The experimental data give only a signal that the system is towards a quantum phase transition if the temperature is extrapolated to zero. What the experiments really observed was a transition from the superfluid to the normal liquid whose compressibility is very close to zero and the system is practically a Mott insulator. Such a `classical' phase transition has been investigated recently by Dickerscheid et al. Phase diagrams for a given atom density were calculated in the temperature-interaction plane and the chemical potential-interaction plane: For a commensurate optical lattice, there are only the superfluid and the Mott insulator phases at zero temperature. At finite temperatures, starting from the superfluid phase, there is a superfluid/normal liquid phase transition while the Mott insulator phase crossovers to the normal liquid.

In order to extend the ordinary mean field approach for the Bose Hubbard model to include the finite temperature effects, the slave boson technique was used. The slave particle technique has been widely applied in dealing with the strongly correlated electron systems. In principle, the slave boson and slave fermion approaches are equivalent. However, in practical calculations, approximations still have to be used. It was well-known that in the $t$-$J$ model, the same mean field approximation using the slave boson or slave fermion leads to very different phase diagrams. It was known that the slave boson mean field approximation can qualitatively describe the phase diagram of the cuprates at finite doping. However, due to the Bose condensation of the holons, the slave boson mean field approximation does not produce correctly the ferromagnetic Mott insulator phase. One of the purposes of this work is to examine if both slave particle approaches to the Bose Hubbard model give the same physical results under the mean field approximation.

In these approaches, there is a constraint that each site can be occupied by only one slave particle. With this exact constraint, the model is very hard to solve. A standard approximation is to relax the constraint on each site to the requirement that the average slave particle per site over the lattice be equal to 1. While both approaches give the same qualitative phase diagram, we shall see that the quantitative behaviors derived from the slave fermion approach are more accurate. The advantage of the slave fermions is that the Fermi statistics automatically excludes two same type slave fermions from occupying the same site even when the constraint is relaxed. We shall see that the configurations with the multi-occupations of different types of slave fermion are far away from the mean field state we consider. Thus, these configurations will not significantly influence our results. However, the statistics of the slave particle affect the result remarkably. For repulsive interactions, there are two unsatisfactory features arising from the finite temperature mean field theory in the slave boson approach. One of them is that the critical on-site repulsive $U_c \approx 5.83$ from a direct zero temperature mean field calculation and differs from
the critical $U_c \approx 6$ in $T \to 0$ from the finite temperature mean field. This difference is much smaller with the slave fermion approach. The other was that there is a maximum $T_c$ at $U \neq 0$ in the $U$-$T$ curve which is obviously unphysical. We find that these deficiencies are corrected in the slave fermion approach. Furthermore, for $U = 0$, the critical temperature of the superfluid-normal liquid phase transition for the ideal Bose gas was well-known. We find that this critical temperature calculated by the slave fermion approach is much closer to its exact value than that by the slave boson approach.

This paper is organized as follows. In Sec. II, we give an overview of our slave particle approaches. In Sec. III, the perturbation theory is introduced. In Sec. IV, we give our main results according to the mean field theory. Section V is our conclusion.

II. SLAVE PARTICLE APPROACH

A boson operator on site $i$ may be expressed by the occupation state $|\alpha\rangle$, i.e.,

$$a_i^\dagger = \sum_{\alpha} \sqrt{\alpha + 1} (\alpha + 1)_i \langle \alpha |. \quad (1)$$

The slave particles are the auxiliary particles, which are obtained by mapping the occupation state $|\alpha\rangle_i \rightarrow a_{\alpha,i}$. According to this mapping, the original boson creating operator $a_i^\dagger$ on the lattice site $i$ may be decomposed as

$$a_i^\dagger = \sum_{\alpha=0} \sqrt{\alpha + 1} a_{\alpha+1,i}, \quad (2)$$

where $a_{\alpha,i}$ may be either the (slave) boson operator $b_{\alpha,i}$ with $[b_{\alpha,i}, b_{\beta,j}^\dagger] = \delta_{\alpha\beta\delta_{ij}}$ or the (slave) fermion operator $c_{\alpha,i}$ with $\{c_{\alpha,i}, c_{\beta,j}^\dagger\} = \delta_{\alpha\beta\delta_{ij}}$. As the auxiliary particles, they have to obey the constraint

$$\sum_{\alpha} n_{\alpha,i} = \sum_{\alpha} a_{\alpha,i}^\dagger a_{\alpha,i} = 1, \quad (3)$$

on each site, which corresponds to the completeness of the states $\sum_{\alpha} |\alpha\rangle|\alpha\rangle = 1$ and the original Bose commutation relation: $[a_i, a_j^\dagger] = \delta_{ij}$.

The Bose Hubbard Hamiltonian we will focus on reads

$$H = -t \sum_{\langle ij \rangle} \sum_{\alpha,\beta} \sqrt{\alpha + 1} \sqrt{\beta + 1} a_{\alpha+1,i}^\dagger a_{\alpha,i}^\dagger a_{\beta+1,j} a_{\beta,j} - \mu \sum_{i} \sum_{\alpha} a_{\alpha,i}^\dagger a_{\alpha,i} + \frac{U}{2} \sum_i \sum_{\alpha} (\alpha - 1) n_{\alpha,i}^2, \quad (4)$$

where the symbol $\langle ij \rangle$ denotes the sum over all nearest neighbor sites. $\mu$ is the chemical potential. The hopping amplitude $t$ and the on-site interaction $U$ are defined by

$$t = \int d\mathbf{r} W^*(\mathbf{r})\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})\right] W(\mathbf{r} + a), \quad U = g \int d\mathbf{r} |W(\mathbf{r})|^4, \quad (5)$$

FIG. 1: The dependence of the Bose Hubbard parameter $a_s U/6t$ for the three dimensional optical lattice as a function of the strength of the lattice potential $V_0$. The scattering length $a_s$ is in units of a nanometer. $V_0$ is in units of the recoil energy $E_r = \hbar^2 k^2/2m$

where $g = \frac{4\pi a_s^2 \hbar^2}{m}$ with $a_s$ the s-wave scattering length of the atoms and $m$ the mass of atom; $V(\mathbf{r})$ is the Wannier function corresponding to the lowest Bloch band and $V_0$ is the periodic optical lattice potential. In three dimensions, taking the periodic potential with a form

$$V(\mathbf{r}) = V_0 (\sin^2(kx) + \sin^2(ky) + \sin^2(kz)), \quad (6)$$

we can calculate $U$ and $t$ from the band theory [4]. In Fig. 1, we display the relation between $U/6t$ and $V_0$.

In the slave particle language, the one-component Bose Hubbard Hamiltonian in a $d$-dimensional cubic lattice with $L$ sites reads

$$H = -t \sum_{\langle ij \rangle} \sum_{\alpha,\beta} \sqrt{\alpha + 1} \sqrt{\beta + 1} a_{\alpha+1,i}^\dagger a_{\alpha,i}^\dagger a_{\beta+1,j} a_{\beta,j} - \mu \sum_{i} \sum_{\alpha} a_{\alpha,i}^\dagger a_{\alpha,i} + \frac{U}{2} \sum_i \sum_{\alpha} (\alpha - 1) n_{\alpha,i}^2, \quad (7)$$

With the constraint $\delta$, the standard path integral integral leads to the partition function of the system

$$Z = T \text{re}^{-\beta H} = \int D\alpha D\bar{\alpha} D\lambda e^{-S_E}, \quad (8)$$

$$S_E[\bar{\alpha}, \alpha, \lambda] = \int_0^{1/T} dr \left\{ \sum_i \sum_{\alpha} \bar{a}_{\alpha,i}\partial_\tau - \alpha \mu + \frac{U}{2} \delta(\alpha - 1) - i\lambda_i |a_{\alpha,i} + i \sum \lambda_i \right\}$$

where we have taken $\hbar = k_B = 1$. $\bar{a}_{\alpha,i}$ is equal to the complex conjugate $b_{\alpha,i}^\dagger$ of the bosonic field $b_{\alpha,i}$ for the
slave boson while being the Grassmann conjugate $\bar{c}_{\alpha i}$ of the fermion field $c_{\alpha i}$ for the slave fermion. The integrals over the Lagrange multiplier field $\lambda_i(\tau)$ from the constraint come:

$$\prod_i \delta(\sum_\alpha n_i^\alpha - 1) = \int D\lambda \exp \left[ \int_0^\beta \sum_i \lambda_i \times (\sum_\alpha n_i^\alpha - 1) d\tau \right].$$

(9)

In the sense of the $\delta$-function, the $\lambda_i$ fields have to be real to ensure the constraint is correctly taken into account.

To decouple the four slave particle term in the Hamiltonian, we introduce a Hubbard-Stratonovich field $\Phi_i$ which is a bosonic field and may be identified as the order parameter of the superfluid. The integral

$$\int D\Phi D\Phi^* \exp \left[ - \int d\tau \sum_{\langle ij \rangle} \left( \Phi_i^\alpha - \sum_\alpha \sqrt{\alpha + 1} a_{\alpha+1,i} \right) \right. \left. \cdot \left( \Phi_j^\alpha - \sum_\alpha \sqrt{\alpha + 1} a_{\alpha+1,j} \right) \right],$$

(10)

is obviously a constant. The partition function can be written as

$$Z = \int D\Phi D\Phi^* D\bar{a}_\alpha D a_\alpha D\lambda e^{-S_{eff}[\Phi, a, \lambda]},$$

$$S_{eff}[\Phi, a, \lambda] = \int d\tau \left[ \sum_\alpha \bar{a}_{\alpha,i} \partial_\tau a_{\alpha,i} - \alpha \mu - \frac{U}{2} \alpha(\alpha - 1) - i\lambda_1 a_{\alpha,i} + i \sum_i \lambda_i + i \sum_{\langle ij \rangle} (\Phi_i^\alpha \Phi_j - \Phi_i^\alpha \sum_\alpha \sqrt{\alpha + 1} a_{\alpha+1,i} \right. \left. \cdot \left( \Phi_j^\alpha - \sum_\alpha \sqrt{\alpha + 1} a_{\alpha+1,j} \right) \right].$$

(11)

This effective action is the starting point of the slave particle approach. The slave boson and the slave fermion representations are only reexpression of the original Bose Hubbard model. Both of them are equivalent to the original model before any approximation. So far, all formal transformations we made are rigorous.

### III. Perturbation Theory

The physical meaning of the $\Phi$ field may be seen by using its equation of motion:

$$\langle \Phi_i \rangle = \sum_\alpha \sqrt{\alpha + 1} a_{\alpha+1,i} = \langle a_i \rangle.$$

(13)

This means that $\Phi_i$ indeed serves as an order parameter field. Near the Mott transition, this order parameter is small and one can use perturbation theory to solve the system described by the action $S_{eff}$. The difficulty is that there is no way to exactly solve the problem if the $\lambda$ field varies from site to site. A widely-used approximation is to relax the constraint by replacing the local constraint Lagrange multiplier $\lambda_i(\tau)$ by an imaginary time- and site-independent field $\lambda$. That is, relaxing the condition of exactly one slave particle per site to one with an average of one particle per site. It implies that multi-occupation of the slave particles on the same site is allowed. For slave bosons, this relaxation allows the same type of the boson to multi-occupy a single site. However, for the same type of slave fermions, multi-occupation of the same site is automatically forbidden by the Pauli principle. The value of $\lambda$ will be variationally determined.

To do the perturbation calculation, it is convenient to make a Fourier transformation for the fields $A_i = a_i, \Phi_i$ and $\lambda_i$:

$$A_i = \frac{1}{\sqrt{L^3}} \sum_{k,n} A_{\alpha,kn} e^{ik \cdot i - i\omega_n \tau},$$

(14)

where the Matsubara frequencies $\omega_n = 2\pi n T$ for bosonic fields and $\omega_n = (2n + 1)\pi T$ for fermionic fields. The approximation of the site-independent of $\lambda_i$ implies that all $\lambda_{k,n} = \lambda_{0,0} = \lambda \sqrt{L^3}$.

After all these preparations and then some algebra, we arrive the effective action to second order of the order parameter field,

$$S_{E,eff}[\Phi^*, \Phi] = \beta \Omega_0 - \sum_{k,n} \Phi_{k,n}^* G^{-1}(k, i\omega_n) \Phi_{k,n},$$

(15)

where $\Phi_{k,n}$ is the Fourier component of $\Phi_i$ and the zero order thermodynamic potential is given by

$$\Omega_0 = iL \lambda + \frac{L}{\beta} \sum_\alpha \ln(1 + e^{-\beta \epsilon_0(\alpha)}),$$

(16)

where $\beta = 1/T$ and $\epsilon_0(\alpha) = -i\lambda - \alpha \mu + \alpha(\alpha - 1)U/2$ and $- (\alpha)$ sign corresponds to the slave boson (slave fermion) approximation. The Green’s function is defined by

$$- G^{-1}(k, i\omega_n) = \epsilon_k + \epsilon_k^\alpha \sum_\alpha (\alpha + 1) \frac{n^{\alpha} - n^{\alpha+1}}{i\omega_n + \mu - \alpha U},$$

(17)

where the dispersion $\epsilon_k = 2t \sum_i \cos(k, a_i)$ with $z$ the nearest neighbor partition and $a$ the lattice spacing vector of a $d$-dimensional cubic lattice. The bosonic Matsubara frequency $\omega_n = \frac{2\pi n}{a}$. The slave particle occupation number is given by

$$n^\alpha = \frac{1}{\exp[\beta [-i\lambda - \alpha \mu + \alpha(\alpha - 1)U/2]] + 1},$$

(18)

corresponding to the slave boson and slave fermion, respectively.
IV. MEAN FIELD THEORY

We focus on repulsive interactions with $U > 0$ in this paper. According to Landau theory, the condition $G^{-1}(0,0) = 0$ may be used to determine the critical point of the phase transition between the superfluid and the normal liquid $^3$.

The key difference between the slave boson and slave fermion is their quantum statistics, which leads to the sign difference $\mp$ in equation (18). The difference appears because we have approximated all $\lambda_i(\tau)$ by a real constant $\lambda$. We discuss the zero temperature and the finite temperature cases separately.

A. Zero Temperature

In the zero temperature limit, Dickerscheid et al $^8$ investigated commensurate fillings and assume the number of particles of each well to be fixed at some value $\alpha'$: $n_i^\alpha = \delta_{\alpha,\alpha'}$ in mean field theory. This mean field assumption works for both kinds of slave particles. In terms of $G^{-1}(0,0) = 0$ and the Green’s function $^9$, it is easy to calculate the phase boundaries in the $\mu-U$ plane $^8$: The Mott insulator phase is in the regimes where $\bar{\mu}$ lies between $\mu_\pm'$:

$$\bar{\mu}_\pm' = \frac{1}{2} U (2 \alpha' - 1) \pm \frac{1}{2} \sqrt{U^2 - 2U (2 \alpha' + 1) + 1}$$

Here $\bar{\mu} = \mu/zt$ and $U = U/zt$. It is easy to check that for $U > 0$, $\mu$ is positive. Eq. (19) reproduce results of previous mean field studies $^8$. For the first Mott lobe, $\alpha' = 1$, the critical temperature is given by the zero of the square root in (19), which gives $\bar{U}_c \approx 5.83$. The quantum Monte Carlo calculation showed the critical $U_c$ is somewhat smaller: $\bar{U}_c \approx 4$ $^8$.

B. Finite Temperature

We next turn our attention to the finite temperature behavior. For an site-independent parameter $\lambda$, the relaxed constraint associated with $^8$ may be derived by taking a saddle point approximation for $\lambda$, i.e., minimizing the thermodynamic potential: $\partial \Omega / \partial \lambda = 0$. The particle conservation condition reads $-\partial \Omega / \partial \mu = N$. The corresponding saddle point equations are given by

$$N_s \sum_\alpha (1 - n^\alpha) - \frac{i}{\beta} \sum_{\mathbf{k},\mathbf{n}} G(\mathbf{k}, i \omega_n) \frac{\partial G^{-1}(\mathbf{k}, i \omega_n)}{\partial \lambda} = 0,$$

$$N_s \sum_\alpha \omega_n n^\alpha + \frac{1}{\beta} \sum_{\mathbf{k},\mathbf{n}} G(\mathbf{k}, i \omega_n) \frac{\partial G^{-1}(\mathbf{k}, i \omega_n)}{\partial \mu} = N.$$ (20)

In these equations, all the possible multi-occupant states are included.

FIG. 2: The critical temperature of the normal-superfluid phase transition as a function of the interaction $U$. The solid curve is for the $\alpha = 0, 1, 2$ slave fermions. The dash curve is for the $\alpha = 0, 1, 2$ slave bosons. The down-triangles for the $\alpha = 0, 1, 2, 3$ slave fermions. The up-triangles for the $\alpha = 0, 1, 2, 3$ slave bosons. The data for the slave bosons are taken from $^8$. The arrows indicate the position of the maxima of the critical temperature. The longer bar on the $T_c$-axis is the critical temperature ($T_c^{ideal} = 1.18$) for the ideal Bose gas in three-dimensional lattice.

FIG. 3: The $\alpha = 1$ slave fermion number versus $U/zt$ at the critical point of the phase transition. The solid curve is for three slave fermions and the dash line is for four slave fermions. The empty circles represent the unphysical results with $n^\alpha > 1$ at the "critical temperature".

The mean field approximation implies the last terms in the above two equations may be neglected, which gives

$$\sum_\alpha n^\alpha = 1,$$

$$\sum_\alpha \omega_n n^\alpha = N/L.$$ (21)

From the first equation, we see that all multi-occupancy of the different types slave particles are excluded in the mean field approximation $^8$. The difference between
the slave boson and slave fermion approaches is shown only on their different statistics. The critical point of the superfluid/normal liquid phase transition, in terms of \( G^{-1}(0,0) = 0 \), is determined by

\[
\sum_{\alpha} (\alpha + 1)n^{\alpha+1} - n^{\alpha} = 1. \tag{22}
\]

We now restrict to the commensurate state and take the total density to \( n = N/L = 1 \). To be able to solve eqs. \( \alpha \) and \( \beta \), one must make a cut-off in \( \alpha \). For a cut off of \( \alpha_M = 2 \) so that only \( \alpha = 0,1,2 \) are allowed, these equations can be analytically solved. The resulting equations have been solved by Dickerscheid et al. in the slave boson case \( \delta \). They are also easily solvable for the slave fermion case. For a given \( U, \mu = U/2 \) and \( n^1 = (U+3)/9 \) for both kinds of slave particles the critical point is determined by

\[
T_c = \frac{U}{2} \left[ \ln \left( \frac{U - 24(U+3)}{U - 6(U+12)} \right) \right]^{-1}, \quad \text{(boson)} \tag{23}
\]

\[
\bar{T}_c = \frac{U}{2} \left[ \ln \left( \frac{U + 12(U+3)}{U - 6(U+2)} \right) \right]^{-1}, \quad \text{(fermion)} \tag{24}
\]

where \( \bar{T}_c = T_c/zt \). There is no analytical solution when \( \alpha_M \geq 3 \), but the equations may be numerically solved. The results of four types of the slave bosons have been presented in Ref. \( \delta \). We have solved the slave fermion equations for \( \alpha_M = 3 \). In Fig. 2, we plot the critical temperature as a function of \( U \). Below \( T_c \), it is superfluid phase and above \( T_c \), it is normal liquid phase. \( T_c = 0 \) is a triplet critical point of the superfluid, normal liquid and Mott insulator phases.

We now make a comparison with the results in Fig. 2 from the two approaches. The critical temperature for a given \( U \) from the slave boson approach is higher than that from the slave fermion one. Two further analyzes can show that the slave fermion result may be more appropriate. The bar located at \( \bar{T} = 1.18 \) on the \( \bar{T} \)-axis is the exact critical temperature for the ideal Bose gas on the three-dimensional lattice in the long wave length limit \( \epsilon \). It is obvious that the critical temperature at \( U = 0 \) from the slave fermion approach is better than that from the slave boson approach. As mentioned in \( \delta \), there are two unsatisfactory features for slave bosons: one is that the zero-temperature critical interaction \( U \) is moved to \( U_c = 6 \) from solving eqs. \( \alpha \) and \( \beta \) and is different from zero-temperature result \( U_c \approx 5.83 \) from given by eq. \( \epsilon \). Another is the existence of a local maximum in the position of the phase boundary indicated by the arrows in Fig. 2. We see that both features are improved by the slave fermion approach. Although the three slave fermion result still gives \( U_c = 6 \) at \( T = 0 \), the four fermion result has moved \( U_c \) to about 5.85, which is very close that the well-known zero-temperature mean field result \( U_c \approx 5.83 \).

Note that there are solutions of \( U > 6 \) in eq. \( \gamma \) where the ‘critical temperatures’ are nonzero, which are shown by filled circles in Fig. 2. However, these solutions correspond to \( n^1 > 1 \) and \( n^0 < 0 \). Thus, these points are not physical. The similar situation appears for four slave fermions but these points move to \( U > 5.85 \) (shown by the empty circles in Fig. 2). To verify these ‘critical temperatures’ are not physical, we depict \( n^1 \) at the critical point as a function of \( U \) in Fig. 3. We see that \( n^1 > 1 \) after \( U > 5.85 \) All of these evidences show the critical point indeed moves to around \( U_c \approx 5.85 \) at \( T = 0 \), which is in good agreement with the zero temperature mean field result, \( U_c = 5.83 \).

The second feature in the slave boson result is the local maximum in the \( U-T_c \) curves (see the arrows in Fig. 2). As we see, this maximum comes from the finite \( \alpha_M \) approximation getting worse as \( U \rightarrow 0 \). This feature is greatly improved in the slave fermion \( U-T_c \) curves. The positions of the maximum of the critical temperature for slave fermions are in about \( U \approx 1.2 \) for three fermions and near \( U = 0.2 \) for four fermions, which are much closer to zero than 2.15 and 1.8 in the slave boson curves. Furthermore, \( \Delta T/T_c^\text{max} < T_c(U = 0) \approx 0.25 \) and \( \Delta T/T_c^\text{max} \approx 15\% \) for slave bosons while \( \Delta T/T_c^\text{max} \approx 2\% \) for slave fermions. The local maximum appears because the cut-off \( \alpha \leq 3 \) is not appropriate as \( U \rightarrow 0 \).

Both these two quantitative improvements from the slave fermion approach over the slave boson approximation come from the exclusion of the same types of the slave fermions, due to the Pauli principle. From eqs. \( \alpha \) and \( \beta \), we can calculate the derivative \( dT_c/dU \). It is seen that the boson statistics of the slave boson sharpens the slope the \( T_c-U \) curve in small \( U \).

We next investigate if the finite \( \alpha_M \) approximation is good or not. For this purpose, we plot \( n^1 \) \((\alpha_M = 3)\) versus \( U \) at the critical temperature (Fig. 4). It is seen that the occupancy of the 0th, 1st and 2nd types of the slave fermion is of the order \( 10^{-1} \) from \( U = 1 \) to 4. However, \( n^3 \) decreases quickly as \( U \) increases. For \( U = 1, n^3 \approx 0.05 \) but \( \approx 0.009, 5 \times 10^{-4} \) and \( 2 \times 10^{-5} \) for \( U = 2,3 \) and 4, respectively. This means that for a large enough \( U \), the \( \alpha_M = 3 \) cut-off is a good approximation. In the regime of small \( U \), a larger \( \alpha_M(>3) \) is required if we would like to have a quantitatively reliable result. For \( \alpha_M = 3 \), we see that, from Fig. 2, \( T_c(U = 0, \alpha_M = 3) \approx 0.98 \). It may be expected that as \( \alpha_M \) increases, \( T_c(U = 0) \) should be close to, e.g. 1.18 in three dimensions, the ideal Bose gas critical temperature. The approximation getting worse for small \( U \) means the contribution from large \( \alpha(>3) \) can not be neglected. The maximum of the critical temperature in Fig. 2 comes from neglecting these degrees of freedom corresponding to large \( \alpha \). Taking a larger \( \alpha_M \), it may be anticipated that the maximum of \( T_c \) may disappear as \( T_c(U = 0) \) tends to 1.18. To reveal the quantitative behavior of the system for small \( U \) more precisely, we have to work at a larger \( \alpha_M \). The numerical work is still in progress which will be present elsewhere.
C. Incommensurate State

It was also known that in the incommensurate state, there is no Mott insulator phase for any value of $U$. To confirm this point, we calculate two incommensurate fillings with $n = 0.9$ and $0.75$. As Fig. 5 shown, only a normal-superfluid transition in the phase diagram is found and there is no Mott insulator phase.

V. CONCLUSION

In summary, we have made a comparative study of the finite temperature phase diagrams with the slave boson and the slave fermion mean field theory for the Bose Hubbard model. We found that both slave particle mean field theories are qualitatively the same but the slave fermion approach is quantitatively more accurate. Many other results obtained in Ref. 8 by the slave boson approach are valuable and may be improved by the slave fermion approach by replacing the bosonic occupation number with the fermionic occupation number. This approach can be generalized to the two-component Bose Hubbard model with $b^\dagger_{i,\uparrow} = \sum_{\alpha,\alpha'} \sqrt{\alpha_{\uparrow} + 1} c^\dagger_{\alpha + 1,\alpha' \downarrow}$ and $b^\dagger_{i,\downarrow} = \sum_{\alpha,\alpha'} \sqrt{\alpha_{\downarrow} + 1} c^\dagger_{\alpha + 1,\alpha' \downarrow}$, while for Bose-Fermi mixture Hubbard model, a slave boson composite fermion mixture approach with $b^\dagger_i = \sum_n \sqrt{\alpha + 1} (c^\dagger_{i,\alpha + 1} c_{i\alpha} + b^\dagger_{i,\alpha + 1} b_{i\alpha})$ and $f_i = \sum_{\alpha} c^\dagger_{i,\alpha} b_{i\alpha}$ or $= \sum_n b^\dagger_{i,\alpha} c_{i\alpha}$, will be required. Here $c^\dagger_{i,\alpha}$ may be thought as a composite fermion 12. These will be worked out elsewhere.

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To eliminate the multi-occupied configuration beyond the mean field state, one has to deal with the fluctuation corresponding to $\delta \lambda_i = \lambda_i - \lambda$. However, it is very difficult to solve this problem.

In the long wavelength limit, the critical temperature for the three-dimensional ideal Bose gas is given by $T_{\text{ideal}}^c = \frac{2\pi}{9} \left( \frac{\rho a^3}{g(0)} \right)^{2/3}$ with $g(x) = \sum_{m=1}^{\infty} \frac{e^{mx}}{m}$. For the present case, $\rho a^3 = n = 1$ and then $T_{\text{ideal}}^c = 2.61^{-2/3} \times \frac{1}{10} \approx 1.18$. 