Slave Boson Formulation for Interacting Boson Systems and the
Superfluid-Insulator Transition

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Abstract

A new formulation for the study of interacting bosons on a lattice is introduced. This approach is used to give analytical expressions for the Mott insulating lobes in the phase diagram and to calculate the density-density correlation function. It is also shown that, at mean-field level, this newly introduced slave boson theory coincides with mean-field theory of a suitably introduced order parameter.

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I. INTRODUCTION

There has been recently a revival of interest for interaction-induced metal-to-insulator transitions. This is due to a large extent to the discovery of high-$T_c$ materials [1] as in the cuprates it is believed that the insulating state originates from a strong Coulomb interaction in a half-filled band. Anderson’s proposal [2] that the Hubbard Model should capture the essential physics of the cuprates generated the development and the application of numerous theoretical techniques to the problem of interacting fermions on the lattice. In parallel these techniques have been applied to interacting bosons as well. In a similar way a Mott-insulating state should appear at commensurate densities due to a strong local interaction that plays the role of the Pauli principle and prevents the bosons from undergoing a Bose-Einstein condensation as known from the ideal Bose gas. This scenario has been recently discussed by Fisher et al. [3] in the framework of a suitable mean-field theory. Their result for the pure case has been confirmed by Krauth et al. [4] using Gutzwiller type of wave-function, and Sheshadri et al. [5]. Other mean-field theories have been proposed [6,7], and Quantum Monte-Carlo simulations [8,9], all confirming Fisher et al.’s result. An alternative technique is provided by introducing auxiliary bosonic fields. The slave boson representations were pioneered in the context of spin models by Holstein and Primakoff and, in particular, by Schwinger who introduced a two slave boson representation of spin 1/2 [10]. A second class of slave boson representations was introduced by Barnes and employed by others, in the context of the Anderson model of a magnetic impurity in a metal [11]. The method has been extended to lattice fermion models [12,13], and gave rise to an extensive literature. In this letter I introduce a new representation for both interacting bosons and spins on the lattice and I apply it to the Bose-Hubbard model. I point out a close connection between slave boson mean-field theory and the collective field method. The density-density correlation function in the first Mott insulating lobe is calculated.
II. FORMULATION

The new representation for both interacting bosons and spins on a lattice is based on a generalization of the slave boson representation of the fermionic Hubbard Model introduced by Kotliar and Ruckenstein [12], where each atomic state is obtained with the help of distinct slave particles subject to constraints. Here the normalized n-fold occupied state at a given site $i$ on the lattice is obtained as:

$$| n >_i \equiv b^+_{n,i} | \text{vac} > n \geq 0. \quad (1)$$

Even the empty site $| 0 >_i$ is constructed by operating with the Bose creation operator $b^+_{0,i}$ onto a new vacuum state $| \text{vac} >_i$ meaning that even the empty lattice site is not pre-existent but rather created out of a total vacuum $| 0 >_i = b^+_{0,i} | \text{vac} >_i$ in the enlarged Hilbert space. The slave bosons $b_{n,i}$ are subject to the constraint:

$$\sum_{n \geq 0} b^+_{n,i} b_{n,i} = 1 \quad (2)$$

indicating that, at each lattice site and at each time, the site has a well defined occupancy. The eigenvalues of the atomic problem with on-site interaction $U$

$$E_n = Un(n - 1) - \mu n \quad (3)$$

serve as chemical potential for the slave particles. In terms of those the physical boson creation operator reads:

$$B^+_i = \sum_{n \geq 0} \sqrt{1 + n} b^+_{n+1,i} b_{n,i} \quad (4)$$

It is a straightforward exercise to show that $B$ satisfies the canonical commutation relation provided the slave fields do it as well. This is sufficient in order to rewrite the original Hamiltonian. Taking as an example the Bose-Hubbard Model:

$$H = \sum_{i,j} t_{i,j} B^+_i B_j + \sum_i (U(B^+_i B_i - 1) - \mu)B^+_i B_i \quad (5)$$

The corresponding partition sum as expressed in the slave boson formalism reads:
\[ Z = \int \Pi_{n,i} D b_{n+1,i} D b_{n+1,i} \Pi_{i} D \lambda_{i} \exp (-S) \]  

(6)

with the action

\[ S = \int_{0}^{\beta} d\tau \sum_{n,i} b_{n,i}^{+} (\partial_{\tau} + E_{n} + i \lambda_{i}) b_{n,i} - \sum_{i} \lambda_{i} \]

\[ + \sum_{i,j,n,m} \sqrt{1+n} \sqrt{1+m} b_{n+1,i}^{+} b_{n+1,i} b_{m+1,j}^{+} b_{m,j} \]  

(7)

where the \( \lambda \)-field enforces the constraint.

The limit of infinite local interaction simply results in restricting the number of slave fields to be 2. In this case it is worth noting that the \( b \)-fields can be taken as fermionic and the action (7) describes a quantum \( X-Y \) model in an external magnetic field \( \mu/\mu_{B} \). But in the following I shall keep the \( b \)-fields as bosonic. The action (7) is invariant under a \( U(1) \) gauge transformation which allows to eliminate the phase of one slave field at the price of introducing a time-dependent \( \lambda \)-field.

**III. RESULTS**

a) HARD-CORE LIMIT.

As a first example of handling the action (7) I consider the hard-core limit in the saddle-point approximation. This yields, for \( |\mu| \leq |t_{0}| \), where \( t_{0} \equiv t(k = 0) \):

\[ b_{0}^{2} = \frac{t_{0} + \mu}{2t_{0}} , \quad b_{1}^{2} = \frac{t_{0} - \mu}{2t_{0}} \]  

and both phase boundaries of the insulating state are properly recovered. Namely they read \( \mu = -2dt \) and \( \mu = 2dt \) for the empty (\( b_{1} = 0 \)) and the full (\( b_{0} = 0 \)) systems. Whereas the density \( \rho \) is given by \( |b_{1}|^{2} \), the superfluid density as taken from \( \rho_{s} \sim |<B>|^{2} = |b_{0}b_{1}|^{2} \) is very different from \( \rho \) and they only coincide in the low density limit. To obtain the gaussian fluctuations I first take advantage of the \( U(1) \) gauge symmetry of \( S \) eq. (7) in order to take the \( b_{0} \)-field as real. I can then integrate out both \( b_{0} \) and \( \lambda \) fields. After having introduced the mean-field parameters the action reads:
\[ S_{GF} = \frac{1}{2} \sum_k (b'_{1,-k}, b''_{1,-k}) \begin{pmatrix} \alpha_k & \omega_n \\ -\omega_n & \beta_k \end{pmatrix} \begin{pmatrix} b'_{1,k} \\ b''_{1,k} \end{pmatrix} \] (9)

where \( \alpha_k = \beta_0 (t_k - t_0) - 4b_0^2 t_k \) and \( \beta_k = \beta_0 (t_k - t_0) \). This yields the spectrum

\[ \omega^2 = (t_k - t_0)^2 - 4b_0^2 b_1^2 t_k (t_k - t_0) =_{k \to 0} 2t_0^2 b_0^2 b_1^2 k^2 \] (10)

which is linear in \( k \) for small \( k \) as expected in a superfluid state as a consequence of the spontaneously broken \( U(1) \) symmetry.

There is another way to tackle the slave boson action eq. (7). One can decouple the hopping term by introducing a single Hubbard-Stratonovich field \( \Phi \). The action then becomes bilinear in all slave boson fields which can then be integrated out exactly. One then finds

\[
Z = \int D\Phi D\lambda \exp \left( -\int_0^\beta d\tau (-\sum_{i,j} \Phi^*_i \tau_{i,j} \Phi_j + \sum_i i\lambda_i) \right) \prod_{n,i} \frac{1}{1 - \exp (-\beta(i\lambda_i + \xi_n))} \] (11)

where, in the occupation number space, \( \xi_n \) are the eigenvalues of \( M_{m,n} \equiv E_n \delta_{m,n} + \sqrt{1 + m^2 \Phi \delta_{m+1,n}} + \sqrt{n^2 \Phi^* \delta_{m,n+1}} \), where the \( E_n \) are the eigenvalues of the atomic problem (eq. (3)) and \( \Phi \) is treated in mean-field approximation. Due to the particular form of eq. (11) the constraint can be handled exactly. In terms of the order parameter \( \Phi \), the action reads:

\[
S = -\frac{\beta}{t_0} |\Phi|^2 - \ln \left( \sum_n \exp (\beta \xi_n) \right). \] (12)

In the hard core limit, the 2 eigenvalues \( \xi_\sigma \) are given by \( 2\xi_\sigma = -\mu \pm \sqrt{\mu^2 + 4 |\Phi|^2} \). This result is well known in the context of the ferromagnetic \( X - Y \) model and usually serves as a pedagogical starting point for the discussion of the paramagnetic-ferromagnetic transition in this model [10]. Solving the saddle-point condition which follows from the action (12) yields the \((\mu, T)\) phase diagram where the phase boundary between the superfluid and the normal states is given by \( \mu = 2T_c t h^{-1}(\mu/2dt) \). This might serve as a description of the \( \lambda \)-transition in \( ^4He \). Assuming that the \( ^4He \) atoms are sitting on a lattice that is half-filled and that they only experience a hard-core interaction yields the ratio \( T_c/T_{BE} = 0.7 \), which is identical to the ratio \( T_{c}^{exp}/T_{BE} \) as obtained with the help of the experimental data.
b) FINITE U PROBLEM.

In the saddle-point approximation the slave-boson action becomes:

\[ S = \sum_n |b_n|^2 (E_n + \lambda_0) - \lambda_0 \]

\[ + \sum_{n,m} \sqrt{1+n} \sqrt{1+m} \ b^*_{n+1} b_n t_0 b_{m+1} b^*_{m} \]  

(13)

I minimized numerically both eq. (12) and eq. (13). Even though both approaches yield very different looking equations, it turns out that they deliver identical results at zero temperature. The difficult problem of minimizing the slave-boson action is handled in the following way. First of all one phase can be removed owing to the gauge symmetry of the action. Second the phase of the physical Bose field can not be determined by the saddle-points equations, as usual in a superfluid state, but all the others are readily seen to be equal to the latter, so as to minimize the kinetic energy. There is thus a single Goldstone mode. The constraint expresses the fact that the \( N \) bosons to be considered are restricted to the surface of a \( N \) dimensional hyper-sphere which I parameterize in polar coordinates. I am thus left with determining the angles. It turns out that the number of angles that differ from zero gradually reduces when the interaction is raised up. This is exemplified in fig. 1 where I show the amplitude of the first 4 bosonic fields as a function of the interaction strength at density \( \rho = 1 \). Even for moderate coupling, say \( U = t \), only the first 5 fields differ from 0. This implies that amplitude fluctuations are very substantially weakened as compared to the ideal Bose gas. This physical effect persists down to any finite interaction strength.

The Mott insulating state is reached when a single \( b \)-field differs from 0. In this case the superfluid density, which vanishes, is very different from the density which takes (here) the value 1. We meet a very different situation as in the weakly interacting Bose gas theory, where both quantities are identical due to Galilean invariance at zero temperature [17]. How they start to deviate from each other is shown in the inset of fig. 1, where I plot \( |< B >|^2/\rho \) as a function of the interaction strength at density \( \rho = 1 \).

The phase diagram (fig. 2) shows Mott insulating states corresponding to commensurate densities, which are identical to those obtained by [3]. They are in good agreement with
QMC results by Trivedi and Ullah [9], even though the insulating lobes are somewhat too small. This is a drawback of the method which is well-known from similar calculations for interacting fermions [12]. This originates in the fact that the action (7), even though exact, does not yield the correct non-interacting limit at mean-field level. Phase fluctuations in this approach are somewhat atypical. At finite temperature they are expected to cause the superfluid-normal transition. Even though there are a lot of phases that fluctuate, only a single one is relevant, all other being massive. This is in contrast to the fermionic Hubbard model where all phases but one can be gauged away and the fluctuations of the remaining one leads to a massive mode that is then not expected to destroy the condensate [15]. Here the fluctuations bring a rich excitation spectrum. Considering as an example the gaussian fluctuations in the $n = 1$ insulating lobe leads to a decoupling of the propagator matrix. After having integrated out the (real) $b_1$ field and the constraint field and introduced

$$\alpha_k \equiv E_0 - E_1 + |b_1|^2 t_k \quad \text{and} \quad \beta_k \equiv E_2 - E_1 + 2|b_1|^2 t_k$$

one obtains:

$$S_{GF} = \sum_{n \geq 3, k} b^*_{n,k} (-i\omega_n + E_n - E_1) b_{n,k}$$

$$+ \sum_k (b^*_{0,k}, b_{2,-k}) \begin{pmatrix} -i\omega_n + \alpha_k & \sqrt{2}|b_1|^2 t_k \\ \sqrt{2}|b_1|^2 t_k & i\omega_n + \beta_k \end{pmatrix} \begin{pmatrix} b_{0,k} \\ b^*_{2,-k} \end{pmatrix}$$

(14)

It follows that the spectrum is split into a set of localized high energy excitations (for $n \geq 3$) and a continuum which arises from the small $n$ part of the action. Looking for a vanishing gap provides expressions for the superfluid-insulator lines for the $N$-th lobe ($N \geq 1$):

$$\frac{\mu}{U} = 2N - 1 - \frac{dt}{U} \pm \sqrt{\left(\frac{dt}{U}\right)^2 - (2N + 1)\frac{2dt}{U} + 1}$$

(15)

This is the analytical expression for the Mott-insulating lobes which can be obtained either with this method or with the collective field approach. In turn physical response functions such as the density-density correlation function can be computed. The Mott gap following from the low energy part vanishes at the tip of the lobe where the spectrum is changing from being gapful and massful to gapless and massless. At this particular point I calculated numerically for $N = 1$ the density-density correlation function $N(q, \omega)$ on the 2-d square
lattice which is displayed in fig. 3. The latter is vanishing identically for \( k = 0 \) reflecting the incompressibility of the system. As a result charge fluctuations are mostly high energetic and inhomogeneous up to a fraction of low but finite energy excitations resulting into a gapless incompressible state. The spectrum is very broad and is extending well over the band width of the corresponding non-interacting Fermi system. It mostly consists of a two-peak structure following from the two modes of the fluctuation matrix. At low momentum and energy the imaginary part of \( N(q, \omega) \) is obtained as:

\[
\text{Im}N(q, \omega) = \frac{\Theta(\omega - cq)}{16} \frac{q^2}{\sqrt{\omega^2 - (cq)^2}}
\]

with the sound velocity \( c = 4t/\sqrt{6\sqrt{2} - 8} \). This response function thus exhibits an integrable singularity at the threshold. As a result the DC conductivity is finite and takes the universal value \( e^2/16\hbar \) where \( e \) denotes the charge of the bosons. However a finite value for the DC conductivity heavily relies on the particular form of \( \text{Im}N(q, \omega) \) as found in eq (16). Keeping in mind that all self-energy corrections to the slave boson propagators are neglected makes it unlikely that such a peaked behavior is a genuine feature of the model. Moreover an additional symmetry of the Hamiltonian appearing at a discrete set of points of the phase diagram corresponding to the tip of the lobes could not be identified. Thus self-energy corrections must exist. Here the holon and doublon propagators only coincide for small energy and momentum. The differences are responsible for the 2-peak structure in \( \text{Im}N(q, \omega) \) rather than a 1-peak structure. Calculations of \( N(q, \omega) \) away from the tip of the lobe yields similar looking results apart from a gap as obtained from eq (15). The detailed expression for \( N(q, \omega) \) as well as additional calculations in the superfluid domain that are in progress, will be published elsewhere [18].

**Conclusion**

In this paper the superfluid-insulator transition that occurs in interacting bosons systems is considered. To this aim an auxiliary boson representation is introduced and I showed that the slave boson mean-field theory is identical to a mean-field theory on an order parameter. Despite of its apparent complexity it allowed to obtain an analytical expression for the Mott insulating lobes as well as for the density-density correlation function. This newly introduced
framework is used to show that many energy scales appear in the excitation spectrum. In the strong coupling regime it consists of a continuum of low energy excitations and a set of localized high energy excitations. The latter are weakening the amplitude fluctuations in a substantial way, even for moderate coupling.

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FIGURE CAPTIONS. FIG. 1 Amplitude of the slave boson fields $b_n$ as functions of the interaction strength at the commensurate density $\rho = 1$. The curves A,B,C,D correspond respectively to $n = 0, 1, 2, 3$. Inset: $|<B>|^2$ as a function of the interaction strength at the commensurate density $\rho = 1$.

FIG. 2 Chemical potential versus hopping phase diagram at zero temperature. The insulating lobes correspond to the densities 1 and 2.

FIG. 3 Density-density correlation function at the tip of the first Mott lobe on the square lattice as functions of frequency. The curves A, B, C, D are calculated for wave-vectors on the diagonal of the first Brillouin zone for respectively $q_x = (1, 2, 3, 5)\pi/5$. 