Local quantum coherence and the superfluid phase

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Abstract

Superfluidity ,in the strong interaction limit, is associated to non vanishing off diagonal elements of the average density matrix associated to a local state i.e. to the occurrence of a macroscopic quantum coherence phenomenon. In the Hard Core Bosons model the local state is a quantum superposition of a Spin up state (site s occupied by a particle) or a Spin down state (empty site). In the Hubbard model the local state is a superposition of the two degenerate components of the ground state of the local part of the Hamiltonian at half filling . This approach allows a systematic expansion around the mean field at fixed order parameter in terms of the coordination number of the lattice and of deviation from half-filling. In the Hubbard case this expansion simplifies in the limit of a large ratio of the interaction strength to the hopping amplitude where Hard core bosons model results are recovered as expected.

Key words: Superfluid; Bose-Hubbard model; Phase transition;

1. Introduction

An interacting Bose particles system on a lattice shows at vanishing temperature a superfluid behavior for non integer occupation number and a transition from superfluid to Mott insulator at integer occupation number. This transition has been recently observed[1] in a Bose system which condensates on a optical lattice. The traditional weak coupling theory is unable to explain this behavior as discussed by Van Oosten et *al*[2]. An alternative mean field theory has been introduced by Sheshadri et *al*[3] and developed by Van Oosten[2].

The aim of this paper is to show that the Bose-Hubbard model, in the large interaction strength limit, corresponds to a suitable XY model in the presence of a transverse field which vanishes for semi-integer occupation numbers.

Let's first discuss the nature of the ground state in the atomic limit This limit is obtained from Bose-Hubbard Hamiltonian

$$H = -\sum_{i,j} t_{ij} b_i^+ b_j + \sum_i (\varepsilon_i - \mu_i) n_i + \frac{U}{2} \sum_i n_i (n_i - 1) \quad (1)$$

neglecting the hopping amplitude t_{ij}. An integer occupation number $< n_i >= n_0$ is obtained by choosing a chemical potential such that ground state corresponds to $n = n_0$. For non integer occupation number we split the local hamiltonian in a part which has a degenerate ground state with two components corresponding to the eigenstate $n = n_0$ and $n = n_0 + 1$, i.e. for $\mu_0 = \varepsilon + U n_0$ ant the other where the deviation $\Delta\mu = \mu_0 - \mu$ is taken into account. We assume as a trial eigenstate $|GS >= \cos(\theta)|n_0 > + \sin(\theta)|n_0 + 1 >$ and choose the anomaly θ minimizing the perturbation which arise from $\Delta\mu$ and the hopping term. It is worth to note the we assume the same ground state in each site or, in other words we start with a broken gauge symmetry ground state. An elementary calculation gives the variational θ dependent energy density

$$E(\theta) = -\frac{t}{4}(n_0 + 1)\sin^2(2\theta) + \Delta\mu(n_0 + \sin^2(\theta) \quad (2)$$

where $t = \sum_j t_{ij}$. The minimum is obtained for $\Delta\mu = \frac{t}{2}(n_0 + 1)\cos(2\theta)$. The average occupation number is given by:

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$$< n_i >= n_0 + \frac{1}{2} - \frac{\Delta\mu}{t(n^0+1)} \quad (3)$$

Hence the superfluid ground state is expected to occur if $\left|\frac{\Delta\mu}{t}\right| < \frac{1}{2}$. It is also worth to recall that the superfluid behavior is associated to the possibility of a current in the ground state as a response to a vector potential which makes the hopping amplitude complex ($J \propto (n_0+1)(1-(2\frac{\Delta\mu}{t(n_0+1)})^2)$). We see that in the present approximation the superfluid density vanishes as the occupation number becomes an integer. Further contribution of the order $\frac{t^2}{U}$ will modify this result and open the possibility of a superfluid Mott-insulator transition at finite U

2. Magnetic model and Mean field theory

It is convenient to use the eigenstates of the degenerate part of the hamiltonian to compute statistical averages. In the large U limit the contribution which has a non vanishing weight derives from the ground states subspace. It means that we can neglect all operators which either act outside of the subspace or make transitions inside or outside. The Bose-Hubbard Hamiltonian can be simplified with the following approximation

$$\begin{aligned} b_i &\sim \sqrt{n_0+1}|n_0 >< n_0+1| \\ b_i^+ &\sim \sqrt{n_0+1}|n_0+1 >< n_0| \\ n_i &\sim (n_0+1)|n_0+1 >< n_0+1| + n_0|n_0 >< n_0| \end{aligned} \quad (4)$$

Moreover we can introduce the Pauli operators associated to the two level subspace and finally obtain the XY model in the presence of a transverse field apart from a term which is a constant in the ground state subspace

$$H = \frac{\Delta\mu}{2}\sigma_z - (n_0+1)\sum_{ij} t_{ij}\sigma_i^+\sigma_j^- \quad (5)$$

The mean field approximation gives the following result

$$m = \tanh(\beta t(n_0+1)m) \quad (6)$$

$$\cos(2\theta) = \frac{\Delta\mu}{2t(n_0+1)m} \quad (7)$$

The order parameter is given by $< \sigma_x >$ and is equal to $m\sin(2\theta)$ and the average occupation number does not depend on the temperature. In the vanishing temperature limit this result coincides with the previous one. The finite U correction to mean field can be easily derived by the resolvent method as a systematic expansion of resolvent matrix element given by continuous fractions

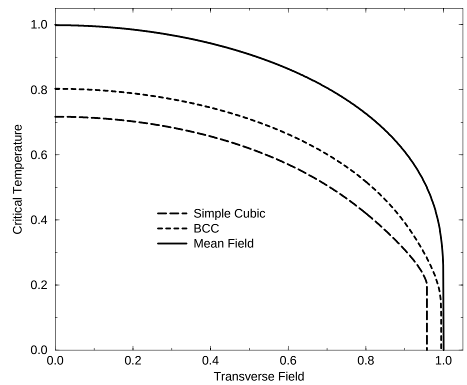

Fig. 1. Critical temperature at first order in $\frac{1}{z}$ for different lattices.

$$R_{n,m} =< n|\frac{1}{i\omega - H_0 - H_p}|m > \quad (8)$$

where n ,m refer to eigenstate of the local Hamiltonian H_0 and H_p is the deviation from the semi-integer occupation and the hopping term in the mean field approximation

3. Beyond the mean field

On the basis of quantum information concepts it is possible to define the broken symmetry phase in terms of the functional

$$\Omega = \ln Tr\left\{ e^{-\beta H} \exp\left[\sum_i \lambda_i(\beta)\,(\sigma_i\cdot n_i - m_i)\right]\right\} \quad (9)$$

which depends on the amplitude of the order parameter m_i and the symmetry breaking direction n_i[4]. The symmetry breaking direction n_i is shown to coincide with the direction associated to the mean field approximation in the zero order approximation in $\frac{1}{z}$. A suitable T - product expansion allows to define first correction to mean field.

The main advantage is that this expansion turns out to be uniform in m. As a result of a straightforward calculation we obtain the critical temperature as a function of $\Delta\mu$ for various lattices

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