SUPERSOLID PHASES FOR LATTICE BOSONS: A VARIATIONAL CALCULATION

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ABSTRACT

We consider bosons with repulsive short-range interaction on a two-dimensional lattice, e.g. Cooper pairs on a Josephson-Junction-Array (JJA). Depending on the chemical potential and the Josephson coupling energy the system is either in a superfluid or a Mott-insulating phase. Both phases are separated by a quantum phase transition. In previous meanfield calculations and Monte Carlo simulations a supersolid phase was found, which shows both crystalline order and superfluidity. In the present paper we approximate the ground state of the JJA by a variational ansatz wave function. Our results confirm the existence of a supersolid. We compare our results with those obtained from Monte Carlo simulations.

1. Introduction

Models for bosons on a two-dimensional lattice are expected to describe the low-temperature properties of superconducting films[1], ^{4}He on a substrate[2], or Cooper pairs on a JJA[3]. Because of the competition between repulsive interaction and hopping the phase diagrams are richly structured, showing Mott-insulating phases with charge order as well as superfluidity. The aim of this paper is to investigate and compare the phase diagrams for two bosonic models by means of a variational calculation.

The first model we will consider is especially applicable for JJA. The array consists of superconducting islands of capacitance C_0 connected by Josephson junctions of capacitance C_1 and Josephson coupling energy J. The capacitance matrix C_{ij} describes the Coulomb interaction of the charges. The temperature is sufficiently low, so that single quasiparticle tunneling is suppressed. A gate voltage can be applied between the islands and the substrate. The Hamiltonian of the so called Quantum-Phase model (QP) reads

$$\begin{aligned} H_{QP} &= \frac{1}{2}\sum_{i,j} n_i U_{ij} n_j - \mu \sum_i n_i - J \sum_{<i,j>} \cos(\phi_i - \phi_j) \qquad (1) \\ & [n_i, \phi_j] = i\delta_{i,j} \\ & U_{ij} = 4e^2 C_{ij}^{-1} \end{aligned}$$

The phases ϕ_i and the number of excess Cooper pairs n_i are conjugate variables. The chemical potential μ which is proportional to the gate voltage controls the average number of particles on the lattice.

Another model which describes bosons on a lattice is the Bose-Hubbard (BH) model given by the Hamiltonian [1]

$$H_{BH} = \frac{1}{2}\sum_{i,j} n_i U_{ij} n_j - \mu \sum_i n_i - t \sum_{<i,j>} (b_i^\dagger b_j + b_i b_j^\dagger) \qquad (2)$$
$$[b_i, b_j^\dagger] = \delta_{i,j} \qquad n_i = b_i^\dagger b_i$$

where $b_i^\dagger$ and b_i are boson creation and annihilation operators. In contrast to the QP model, the hopping process depends on the particle number. In the following we will study these models on a square lattice and at T=0 as we are interested in quantum phase transitions. As we will see later both models are equivalent as far as the phase boundaries are concerned in the limit of large particle numbers, if $J^* = 2J\mu/(U_0+4U_1)$ is identified with t. Furthermore we investigate the phenomenon of a supersolid phase in both models. In the supersolid phase diagonal and off-diagonal long range order coexist, as discussed below. Several authors have studied the QP model[3,4,5] and the BH model[1,6,7]. However, we do not know of any mean-field calculation investigating a supersolid phase in the BH model. Before presenting the results of such calculation in Fig. 2, we will briefly sketch some results of Ref.[1,5]

For $C_1 < C_0$, U_{ij} is short-range and we are allowed to consider repulsive on-site and nearest neighbor interaction only, i.e. $U_{ij} = U_0\delta_{i,j} + U_1\delta_{<i,j>}$. At $J = 0$ and depending on μ the system is either in a configuration where all sites are occupied with n particles, or a checkerboard configuration with n and n+1 particles per site. We consider $0 < 4U_1/U_0 < 1$. This condition guarantees stabilization of the checkerboard arrangement by nearest neighbor interaction. In both configurations the groundstate is separated from the first excited state by an energy gap. This is typical for a Mott-insulator. When J is increased the energy gap decreases and finally vanishes at a critical J. At this stage the system becomes superfluid showing ODLRO. This second order phase transition is characterized by a complex order parameter field

$$\langle\psi\rangle = \begin{cases} \langle\exp(i\phi_i)\rangle & \text{for the QP model} \\ \langle b_i\rangle & \text{for the BH model} \end{cases} \qquad (3)$$

which vanishes in the Mott-insulating phase. In the $\mu - J$ phase diagram there exist lobe-shaped, Mott-insulating regions with integer and half-integer filling, and a superfluid phase.

The density-density correlation function

$$S(\vec{q}) = \left(\frac{1}{N}\right)^2 \sum_{i,j} \exp(i\vec{q}(\vec{r_i} - \vec{r_j}))\langle n_i n_j\rangle \qquad (4)$$

gives information on the arrangement of the bosons on the lattice. The insulating lobes with half filling have a nonvanishing $S(\pi,\pi)$ which signals crystalline long range

order in a checkerboard pattern. When J exceeds a critical value J_{cr1}, superfluidity sets in, but $S(\pi,\pi)$ remains nonzero[4,5], i.e. there is still a checkerboard modulation of the charge density. Finally, when J becomes larger than another critical value $J_{cr2} > J_{cr1}$, the system loses its crystalline order. The phase where the system is superfluid but still possesses the crystalline order of a solid is called supersolid.

2. Variational Ansatz Wavefunction

For $J \neq 0$ the models discussed above cannot be solved exactly. We therefore tackle the problem of a lattice of N sites with the following ansatz wavefunction for the groundstate

$$\begin{aligned} |\psi\rangle &= \prod_{i=1}^{N} \frac{1}{\sqrt{Z_i}} \sum_{n_i} \exp(-k_i(n_i - m_i)^2/2)|n_i\rangle \\ \text{where } Z_i &= \sum_{n_i} \exp(-k_i(n_i - m_i)^2) \end{aligned} \tag{5}$$

k_i and m_i are real variational parameters. The sums run from $-\infty$ to ∞ for the QP model, and from 0 to ∞ for the BH model. For $k_i \to \infty$ and m_i integer the ansatz just gives fixed particle numbers. Note that (5) is a product of single-site wavefunctions and hence a mean-field description which does not take into account correlations between sites i and j.

In order to obtain an upper bound for the groundstate energy we minimize the expectation value $E = \langle\psi|H|\psi\rangle$ with respect to k_i and m_i. The introduction of two sublattices A and B yields information about $S(\pi,\pi)$.

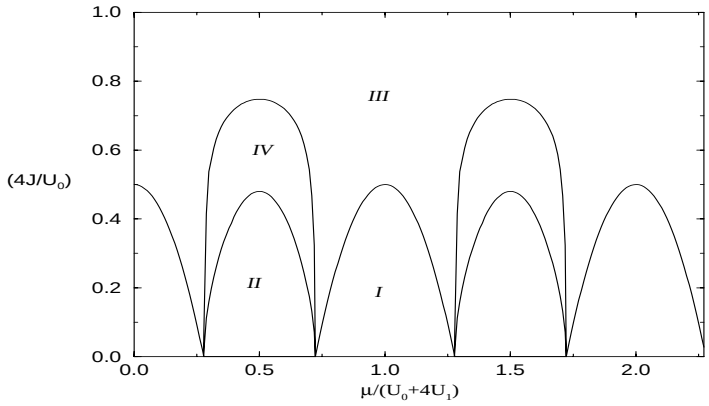

Figure 1: Phase diagram for the Quantum-Phase model with $U_1/U_0 = 0.2$ at T=0. Region *I*: insulator with 1 boson per site. $\langle\psi\rangle = 0, S(\pi,\pi) = 0$. Region *II*: insulator with checkerboard-like 0/1 occupation. $\langle\psi\rangle = 0, S(\pi,\pi) \neq 0$. Region *III*: superfluid phase. $\langle\psi\rangle \neq 0, S(\pi,\pi) = 0$. Region *IV*: supersolid. $\langle\psi\rangle \neq 0, S(\pi,\pi) \neq 0$

3. Results

Fig.1 shows the phase diagram for the QP model obtained with our variational ansatz. Both the superfluid-insulator and the crystalline order transition can be identified and agree well with previous mean-field calculations [4,5]. The phase boundaries are periodic in μ.

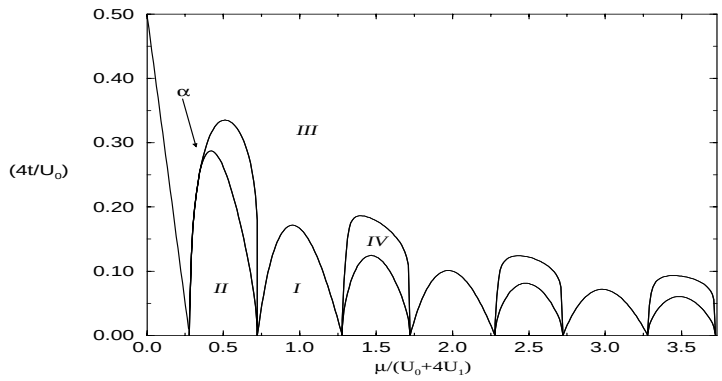

Figure 2: Phase diagram for the Bose-Hubbard model with $U_1/U_0 = 0.2$ at T=0. Regions *I-IV* are explained in Fig.1. The supersolid disappears at point α.

The phase diagram for the BH Hamiltonian is shown in Fig.2. The size of the lobes decreases with increasing μ. At point α the supersolid vanishes. This might be due to the lower bound for the particle numbers. For small μ charge fluctuations are suppressed. Hence, we conclude that they are necessary for the supersolid. Fig.3 reveals that for large μ the phase boundaries of the rescaled QP model approach those of the BH model.

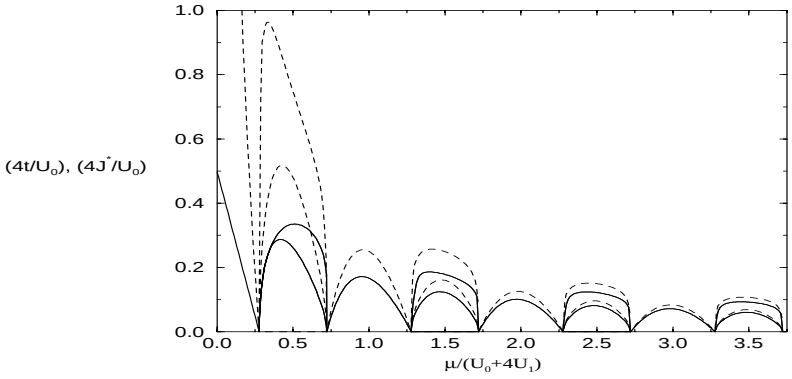

Figure 3: The phase boundaries of the Bose-Hubbard model (solid lines) and of the rescaled Quantum-Phase model (dashed lines, $J^* = 2J\mu/(U_0 + 4U_1)$).

Recently for both the BH[7] model and the QP[5] model Monte-Carlo simulations were carried out. The phase boundaries are modified under the influence of fluctuations. In Fig.4 we compare our results for the QP model with those from Ref.[5]. The Monte-Carlo data, too, show the existence of a supersolid phase. Compared with the mean-field result its size is considerably smaller. Apart from the tips of the lobes the phase boundary for ODLRO fairly well agrees with our results. At the tips of the lobes our mean-field boundary deviates from the Monte-Carlo results. This reflects the fact that in these points the critical behavior is of the 3D XY type, and not of the mean-field type.[1] For the BH model our variational approach shows a supersolid phase at half filling, in contrast to the results of Ref.[7]

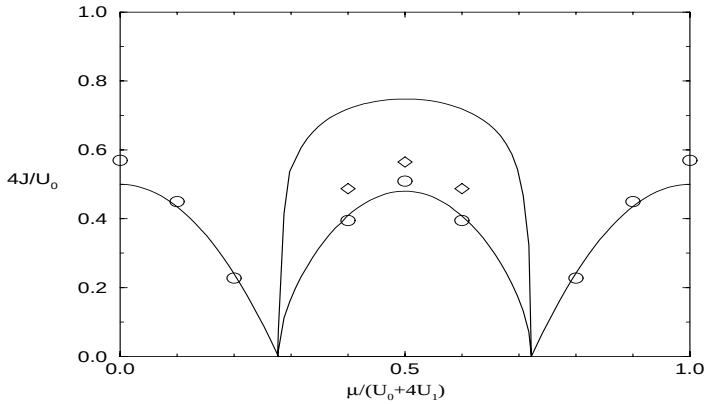

Figure 4: Our mean-field results (solid lines) for the Quantum-Phase model compared with phase boundaries ($\circ$: superfluid-insulating, $\diamond$: crystalline order) from Monte-Carlo simulations, both for $U_1/U_0 = 0.2$.

4. Summary

The T=0 properties of the BH model and the QP model which describe interacting bosons on a lattice were investigated by means of a variational ansatz wave function. We find superfluid and insulating phases as well as phases with and without crystalline order. In some regions of the phase diagram superfluidity and crystalline order coexist. Comparing our data with results from Monte-Carlo simulations, however, shows that fluctuations are essential at the tips of the lobes and at the crystalline order phase boundary and must not be neglected.

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