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Evolution of the critical points with the density of bosons under local three-body interactions

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ABSTRACT

We study the quantum phase transition in the one-dimensional Bose–Hubbard model with three-body local interactions for densities $\rho=2$, 3, 4 and 5 by implementing the Density Matrix Renormalization Group method. This system shows two types of phases. One phase is incompressible (corresponding to the Mott insulator state) and the other compressible (the superfluid state). The critical points found correspond to a value of the hopping parameter for which the gap energy is equal to zero. We found that the critical point increases slowly as the density of the system increases.

1. Introduction

When a system approaches absolute zero, all thermal fluctuations are frozen out while quantum fluctuations remain. These quantum fluctuations can induce a quantum phase transition in the ground state of a many-body system [1]. The study of bosonic systems has become a field of great interest in recent years due to the growing possibility of performing experiments in optical lattices [2,3]. The basic physics of strongly interacting bosons in a lattice is contained in the Bose–Hubbard model; this is a model of many bosonic particles which cannot be reduced to a model of a single particle. The bosons interact due to the Coulomb repulsion between them and the kinetic term, given as the energy for jumping to neighboring sites in the lattice [4,5]. The critical points of the quantum phase transition have been extensively studied through computational and experimental methods.

Greiner et al. [1] studied the quantum phase transition in a Bose–Einstein condensate with repulsive interactions at temperatures in the nanoKelvin range. For this, they used ultracold atoms in a three-dimensional lattice with periodic potential. They observed that the system moves from a state where the atoms are scattered throughout the lattice (the superfluid phase) to a state where they are located at each site of lattice (the Mott-insulator phase), while increasing the potential. They also observed that this transition is reversible when the potential decreases. Therefore, this transition is between an incompressible state (gap energy different from zero) and a compressible state (gap energy equal to zero) [5,6].

The critical points of the quantum phase transition for the Bose–Hubbard model with two-body local interaction have been studied via different computational methods. Kunher et al. [4] implemented the density matrix renormalization group (DMRG) method to find the ground state in a one-dimensional bosonic chain for integer and half-integer densities, obtaining the respective phase diagram; for integer (half-integer) density, the quantum phase transition is given between the Mott-insulator (charge density wave) phase and the superfluid phase. Likewise, Lauchli et al. [7] found the critical point of a one-dimensional bosonic chain, for density $\rho=1$, implementing the DMRG method and taking measurements of the von Neumann block entropy. Currently, the most accurate calculation has been carried out by Ejima et al. [8]. They used the DMRG method and extracted the Tomonaga–Luttinger parameter from the density–density correlation function, determining the critical interaction strength for the Mott insulator; in their system, they maintain $m=2000$ density-matrix eigenstates, obtaining that the critical point for $\rho=1$ ($\rho=2$) is $t_c=0.305\pm0.001$ ($t_c=0.180\pm0.001$). Recently, Danshita et al. [9] studied the critical points using the time-evolving block decimation method for arbitrary integer densities for two-body local interactions; they found that the critical point of the quantum phase transition as a function of density is well approximated by the following expression:

$$\frac{U}{D\rho t}=a+b\rho^{-c}, \tag{1}$$

where D denotes the dimensionality of the system, ρ the density, and the constants a, b, and c are numerically determined. The

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one-dimensional case is shown in Fig. 1. There it can be observed that the critical point of the phase transition decreases as the density increases. The approximation implemented by the authors differs by 5% from the result obtained by Ejima et al. [8] for $\rho=1$ and $\rho=2$.

The study of the multi-body interaction shows interesting physical properties. Büchler et al. [10] showed that polar molecules in optical lattices driven by microwave fields naturally give rise to Hubbard models with strong nearest-neighbor three-body interactions, whereas the two-body terms can be tuned with external fields. Kraemer et al. [11] reported the observation of an Efimov resonance in an ultracold gas of Caesium atoms, and experimentally observed its signature as a three-body recombination loss when the strength of the two-body interaction is varied. Johnson et al. [12] have shown that there are effective three- and higher-body interactions generated by the two-body collisions of atoms confined in the lowest vibrational states of a three-dimensional optical lattice. Will et al. [13] studied ultracold atoms in a three-dimensional optical lattice. They demonstrated the presence of effective multi-body interactions in a system of ultracold bosonic atoms in a three-dimensional optical lattice, emerging through virtual transitions of particles from the lowest energy band to higher energy bands, and Chen et al. [14] studied the Bose–Hubbard model with two- and three-body local interaction by employing the mean-field approximation. They observed the quantum phase transition between the Mott-insulator and superfluid phases for integer fillings, and found that the three-body local interaction enlarges the area of the insulating phase when the density increases.

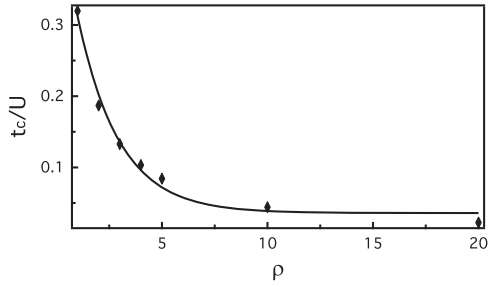

Fig. 1. Behavior of the critical point for a Bose–Hubbard model with two-body local interaction. The data were taken from [9].

Inspired by the above, we study the quantum phase transition in the one-dimensional Bose–Hubbard model with three-body local interactions, for densities $\rho=2$, 3, 4 and 5 by implementing the density matrix renormalization group method.

In the next section, we show the Bose–Hubbard model with pure three-body interaction. Subsequently, we show the gap energy for four values of the hopping term, and finally we discuss the behavior of the critical point of the quantum phase transition as a function of density.

2. Critical points of the Bose–Hubbard model

The Bose–Hubbard Hamiltonian of bosons interacting via local three-body terms is given by

$$H=-t\sum_i(b_i^\dagger b_{i+1}+b_i b_{i+1}^\dagger)+\frac{W}{6}\sum_i n_i(n_i-1)(n_i-2), \tag{2}$$

where $b_i^\dagger$ and b_i are the creation and annihilation operators, respectively, at site i, $n_i=b_i^\dagger b_i$ is the local number of particles, and i varies along the sites of a one-dimensional lattice of size L. The first term of Eq. (2) models the kinetic energy of the atoms, and the parameter t indicates the tunneling force or hopping between adjacent sites. The second term represents the short-range interaction between three bosons, and the parameter W characterizes its strength. The energy scale is set by choosing $W=1$.

The critical point of the quantum phase transition, when the density remains constant, can be calculated as the value t for which the energy gap is zero; the energy of excitation for adding or removing a particle is given by

$$\mu^p(L)=E_0(L,N+1)-E_0(L,N), \tag{3}$$

$$\mu^h(L)=E_0(L,N)-E_0(L,N-1), \tag{4}$$

where μ^p (μ^h) is the energy necessary to add (remove) a particle and $E_0(L,N)$ is the energy of the ground state for a chain of size L with N particles. This transition is of the Kosterlitz–Thouless type, and the gap is given by

$$E_g=\mu^p-\mu^h\sim\exp\left(\frac{cte}{\sqrt{t_c-t}}\right), \tag{5}$$

but the energy gap closes very slowly, and small errors in the energy lead to an error in the location of critical point t_c [4];

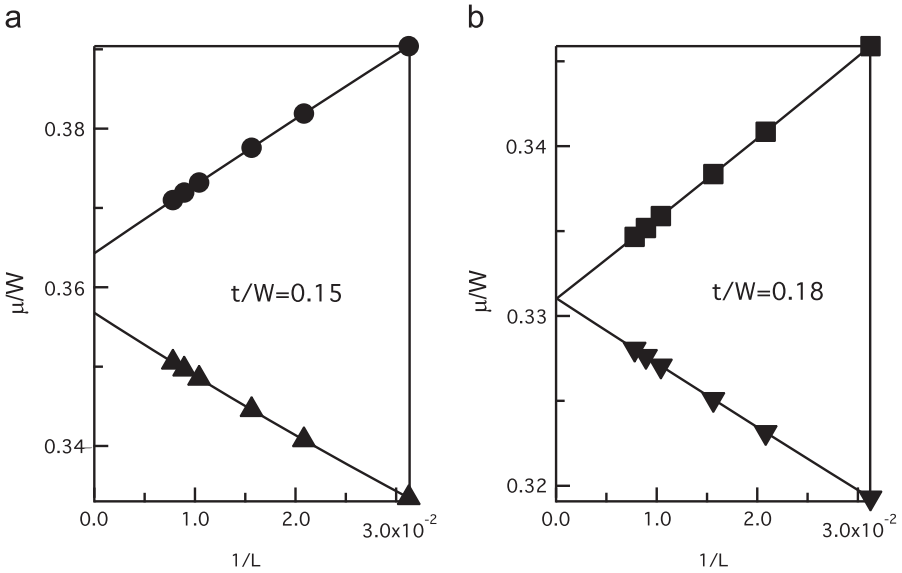

Fig. 2. Dependence of system size on the chemical potential for $\rho=2$. In the left (right) panel we have a Mott-insulator (superfluid) state. The solid lines are the quadratic fit.