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Finite temperature superfluid transition of strongly correlated lattice bosons in various geometries

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ABSTRACT

We study finite-temperature properties of the strongly interacting bosons in three-dimensional lattices by employing the combined Bogoliubov method and the quantum rotor approach. Based on the mapping of the Bose–Hubbard Hamiltonian of strongly interacting bosons onto U(1) phase action, we study their thermodynamic phase diagrams for several lattice geometries including simple cubic, body, as well as face-centered lattices. The quantitative values for the phase boundaries obtained here may be used as a reference for emulation of the Bose–Hubbard model on a variety of optical lattice structures in order to demonstrate experimental-theoretical consistency for the numerical values regarding the location of the critical points.

1. Introduction

It is well known that the ground state of a system of repulsively interacting bosons in a periodic potential can be either in a superfluid state or in a Mott-insulting state, characterized by integer boson densities and the existence of a gap for particle–hole excitations [1]. One key piece of evidence for the Mott insulator phase transition is the loss of global phase coherence of the matter wave function. However, there are many possible sources of phase decoherence in these systems. Substantial decoherence can be induced by quantum or thermal depletion of the condensate. Experimentally, an enormous progress was made in the experimental study of cold atoms in optical lattices [2]. Cold atoms interacting with a spatially modulated optical potential resemble in many respects electrons in ion-lattice potential of a solid crystals. However, optical lattices have several advantages with respect to solid state systems. They can be made to be largely free from defects and can be controlled very easily by changing the laser field properties. Finally, ultra-cold atoms confined in optical lattice structure provide a very clean experimental realization of a strongly correlated many-body problem [3]. Moreover, in contrast to solids, where the lattice spacings are generally of order of Angstrom units, the lattice constants in optical lattices are typically three order of magnitude larger. Furthermore, variety of multi-dimensional lattices can be experimentally obtained by appropriate setup of laser beams including cubic face-centered and body-centered lattices [4,5]. For example, a three dimensional (3D) lattice can be created by the interference of at least six orthogonal sets of counter propagating laser beams. Although the initial system can be prepared at a relatively low temperature, the ensuing system after ramp-up of the lattice has a temperature which is usually higher due to adiabatic and other heating mechanisms. Recent experiments have reported temperatures on the order of $k_BT \sim 0.9t$ where t, the hopping parameter, measures the kinetic energy of bosons [6]. At such temperatures, the effects of excited states become important, motivating investigations of the *finite* temperature phase diagrams, showing the interplay between quantum and thermal fluctuations.

Therefore, the goal of this paper is to provide a study of the combined effects of a confining lattice potential and finite temperature on the state diagram of the Bose–Hubbard model in three dimensions in strongly correlated regime where the standard Bogoliubov treatment fails to describe the system and a more general framework is required. Usually, studies of bosons in optical lattices have been conducted at zero temperature and in two dimensional systems, dealing with Mott insulator-superfluid transition. In the present work, we explore the phase transition from the Mott to the superfluid state in a system of strongly interacting bosons on a cubic lattice with the chemical potential and temperature as the control parameters. Furthermore, we employ the quantum rotor method, which uses the module–phase representation of strongly correlated bosons. This introduces a conjugate to

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the density of bosons U(1) quantum phase variable, which acquires dynamic significance from the boson-boson interaction. The quantum rotor approach has been verified with other methods [7], like quantum Monte Carlo [8] or DMFT [9] giving coinciding results.

The plan of the paper is as follows: in Section 2, we introduce the microscopic Bose–Hubbard model relevant for the description of strongly interacting bosons. Furthermore, in the following Section, we briefly present technical aspects of our quantum rotor approach and in Section 4 we calculate the temperature phase diagrams. Finally, we conclude in the Section 5.

2. Model Hamiltonian

The simplest non-trivial model that describes interacting bosons in a periodic potential is the Bose Hubbard Hamiltonian. It includes the main physics that describe strongly interacting bosons, which is the competition between kinetic and interaction energy. The realization of the Bose–Hubbard Hamiltonian using optical lattices has the advantage that the interaction matrix element U and the tunneling matrix element t can be controlled by adjusting the intensity of the laser beams. Its Hamiltonian in a second quantized form reads [1]

$$\mathcal{H} = -t\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}[a^\dagger(\mathbf{r})a(\mathbf{r}')+a^\dagger(\mathbf{r}')a(\mathbf{r})] + \frac{U}{2}\sum_{\mathbf{r}}n^2(\mathbf{r}) - \overline{\mu}\sum_{\mathbf{r}}n(\mathbf{r}). \quad (1)$$

The first term is the kinetic energy of bosons moving in a given lattice within a tight-binding scheme, where t represents nearest neighbors tunneling matrix, $\mathbf{r}$ and $\mathbf{r}'$ are lattice sites and $\langle \mathbf{r},\mathbf{r}'\rangle$ denotes summation over nearest neighbors. The following introduces inter-bosonic correlations with U being the strength of the on-site repulsive interaction of bosons. Furthermore, $\overline{\mu} = \mu + (U/2)$, where μ is a chemical potential controlling the average number of bosons. The operators $a^\dagger(\mathbf{r})$ and $a(\mathbf{r}')$ create and annihilate bosons, while the boson number operator $n(\mathbf{r}) = a^\dagger(\mathbf{r})a(\mathbf{r})$ and a total number of sites is equal to N. The Hamiltonian and its descendants have been widely studied within the last years. The phase diagram and ground-state properties include the mean-field ansatz [1], strong coupling expansions [10–12], the quantum rotor approach [13], methods using the density matrix renormalization group DMRG [14–17], and quantum Monte Carlo QMC simulations [18–20].

3. U(1) quantum rotor formulation

The quartic form of the Hamiltonian makes it very difficult to deal with it in all the different regimes. The aim of this chapter is to rewrite it so that a systematic approach can be developed to accommodate strongly interacting regime, In the following, we use a theory that goes beyond the simple Bogoliubov approximation which has been recently developed that incorporates the phase degrees of freedom via the quantum rotor approach to describe regimes beyond the very weakly interacting one [21]. This scenario provided a picture of quasi-particles and energy excitations in the strong interaction limit, where the transition between the superfluid and the Mott state is be driven by phase fluctuations. Taking advantage of the macroscopically populated condensate state, we have separated the problem into the amplitude of the Bose field and the fluctuating phase that was absent in the original Bogoliubov problem [22].

The statistical sum of the system defined in Eq. (1) can be written in a path integral form with use of complex fields, $a(\mathbf{r}\tau)$ depending on the "imaginary time" $0 \le \tau \le \beta \equiv 1/k_BT$, (with T being the temperature) that satisfy the periodic condition $a(\mathbf{r}\tau) = a(\mathbf{r}\tau+\beta)$:

$$Z = \int [\mathcal{D}\overline{a}\mathcal{D}a]e^{-\mathcal{S}[\overline{a},a]}, \quad (2)$$

where the action $\mathcal{S}$ is equal to

$$\mathcal{S}[\overline{a},a] = \int_0^\beta d\tau\, \mathcal{H}(\tau) + \mathcal{S}_\mathcal{B}[\overline{a},a], \quad (3)$$

where the Berry term is

$$\mathcal{S}_\mathcal{B}[\overline{a},a] = \sum_{\mathbf{r}}\int_0^\beta d\tau\, \overline{a}(\mathbf{r}\tau)\frac{\partial}{\partial\tau}a(\mathbf{r}\tau).$$

Now, we are briefly introducing the quantum rotor approach [23]. The fourth-order term in the Hamiltonian in Eq. (1) can be decoupled using the Hubbard–Stratonovich transformation with an auxiliary field $V(\mathbf{r}\tau)$:

$$e^{-(U/2)\sum_\mathbf{r}\int_0^\beta d\tau n^2(\mathbf{r}\tau)} \propto \int \frac{\mathcal{D}V}{\sqrt{2\pi}} e^{\sum_\mathbf{r}\int_0^\beta d\tau[-(V^2(\mathbf{r}\tau)/2U)+iV(\mathbf{r}\tau)n(\mathbf{r}\tau)]}. \quad (4)$$

The fluctuating "imaginary chemical potential" $iV(\mathbf{r}\tau)$ can be written as a sum of static $V_0(\mathbf{r})$ and periodic function:

$$V(\mathbf{r}\tau) = V_0(\mathbf{r}) + \delta V(\mathbf{r}\tau), \quad (5)$$

where using Fourier series:

$$\delta V(\mathbf{r}\tau) = \frac{1}{\beta}\sum_{\ell=1}^{\infty}\delta V(\mathbf{r}\omega_\ell)(e^{i\omega_\ell\tau}+e^{-i\omega_\ell\tau}), \quad (6)$$

with the Bose–Matsubara frequencies are $\omega_\ell = 2\pi\ell/\beta$ and $\ell = 0, \pm 1, \pm 2, \ldots$.

3.1. Phase action

Introducing the U(1) phase field $\phi(\mathbf{r}\tau)$ via the Josephson-type relation:

$$\dot{\phi}(\mathbf{r}\tau) = \delta V(\mathbf{r}\tau) \quad (7)$$

with $\dot{\phi}(\mathbf{r}\tau) = \partial\phi(\mathbf{r}\tau)/\partial\tau$ we can now perform a local gauge transformation to new bosonic variables:

$$a(\mathbf{r}\tau) = b(\mathbf{r}\tau)e^{i\phi(\mathbf{r}\tau)}, \quad (8)$$

where

$$\zeta(\mathbf{r}\tau) = e^{i\phi(\mathbf{r}\tau)} \quad (9)$$

with $\phi(\mathbf{r}\tau)$ being U(1) phase variable. Concerning the amplitude in Eq. (8), the operator splits into a sum:

$$b(\mathbf{r}\tau) = b_0 + \delta b(\mathbf{r}\tau). \quad (10)$$

Since, the strongly correlated limit is dominated by phase fluctuations, we neglect a contribution coming from $\delta b(\mathbf{r}\tau)$ in subsequent calculations. After the variable transformations the statistical sum becomes

$$Z = \int [\mathcal{D}\overline{b}\mathcal{D}b][\mathcal{D}\phi]e^{-\mathcal{S}[\overline{b},b,\phi]} \quad (11)$$

with the action

$$\mathcal{S}[\overline{b},b,\phi] = \mathcal{S}_0[\phi] + \mathcal{S}_\mathcal{B}[\overline{b},b] - t\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\int_0^\beta d\tau[e^{i\phi(\mathbf{r}'\tau)-i\phi(\mathbf{r}\tau)}\overline{b}(\mathbf{r}\tau)b(\mathbf{r}'\tau)+h.c.] + \sum_{\mathbf{r}}\int_0^\beta d\tau[U|b_0|^2-\overline{\mu}]\overline{b}(\mathbf{r}\tau)b(\mathbf{r}\tau) \quad (12)$$