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Phase Transitions in Optical Lattices at Finite Temperatures

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We discuss the finite-temperature phase diagram in three-dimensional Bose–Hubbard model relevant for the Bose–Einstein condensates in optical lattices, by employing U(1) quantum rotor approach and the topologically constrained path integral, that includes a summation over U(1) topological charge. The effective action formalism allows us to formulate a problem in the phase only action and obtain analytical formulae for the critical lines beyond mean-field theory.

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1. Introduction

The quantum phase transitions of the Bose–Einstein condensates placed into the lowest vibrational level of single wells of an optical lattice in the strict sense can exist only at temperature $T = 0$ [1–3]. However, in typical experimental situations we must take into consideration thermal fluctuations in the particle number per site. The presence of the finite-temperature indicates the nonzero value of the compressibility and thus only an approximate Mott phase exists. The experimental data only signals that the system nears a quantum phase transition if the temperature is extrapolated to zero. What the experiments really observe is a transition from the superfluid to the normal liquid whose compressibility is very close to zero and the system is practically a Mott insulator.

2. Model

We start with the Bose–Hubbard (BH) Hamiltonian

$$\mathcal{H} = \frac{U}{2}\sum_i n_i^2 - \sum_{\langle i,j\rangle} t_{ij} a_i^\dagger a_j - \bar{\mu}\sum_i n_i, \tag{1}$$

where t_{ij} is the hopping matrix element with the dispersion for the simple cubic lattice $t_{\boldsymbol{k}} = 2t(\cos k_1 + \cos k_2 + \cos k_3)$, $\bar{\mu}/U = \mu/U + 1/2$ is the shifted reduced chemical potential which controls the number of bosons, and $U > 0$ is the on-site repulsion. Furthermore, $a_i^\dagger$ and a_j stand for the bosonic creation and annihilation operators that obey the canonical commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$, where $n_i = a_i^\dagger a_i$ is the boson number operator on the site i. Here, $\langle i,j\rangle$ identifies summation over the nearest-neighbor sites.

3. Method

The functional integral representation of models for correlated bosons allows us to implement efficiently the method of treatment. The partition function is written in the form

$$\mathcal{Z} = \int [\mathcal{D}\bar{a}\mathcal{D}a]\, \mathrm{e}^{-\mathcal{S}[\bar{a},a]} \tag{2}$$

and the bosonic path integral is taken over the complex fields $a_i(\tau)$ with the action $\mathcal{S}$ given by

$$\mathcal{S}[\bar{a},a] = \sum_i \int_0^\beta \mathrm{d}\tau \left[\bar{a}_i(\tau)\frac{\partial}{\partial\tau}a_i(\tau) + \mathcal{H}(\tau)\right], \tag{3}$$

where $\beta = 1/k_{\mathrm{B}}T$ and T is the temperature. Since Hamiltonian is not quadratic in the fields a_i we have to decouple first the interaction term in Eq. (1) by means of a Gaussian integration over the auxiliary scalar potential fields $V_i(\tau)$ whose periodic part $V_i^{\mathrm{P}}(\tau)$ couples to the local particle number through the Josephson-like relation $\dot{\phi}_i(\tau) = V_i^{\mathrm{P}}(\tau)$ where $\dot{\phi}_i(\tau) \equiv \partial\phi_i(\tau)/\partial\tau$. Next, we perform the local gauge transformation to the new bosonic variables

$$a_i(\tau) = b_i(\tau)\exp\left[\mathrm{i}\phi_i(\tau)\right]. \tag{4}$$

Using such a description is justified by the definition of the order parameter

$$\varPsi_{\mathrm{B}} \equiv \langle a_i(\tau)\rangle = \langle b_i(\tau)\exp(\mathrm{i}\phi_i(\tau))\rangle = b_0\psi_{\mathrm{B}}, \tag{5}$$

whose non-vanishing value signals a macroscopic quantum phase coherence (in our case we identify it as superfluid SF state, see Fig. 1). In the large U limit the amplitude $b_0 \equiv \langle b_i\rangle$ has a nonzero value, but to achieve the superfluidity, the phase variables must also become stiff and, in consequence, $\psi_{\mathrm{B}} \equiv \exp(\mathrm{i}\phi_i(\tau)) \neq 0$. Integrating the action in Eq. (3) over the bosonic fields we obtain the effective Lagrangian in terms of the phase-

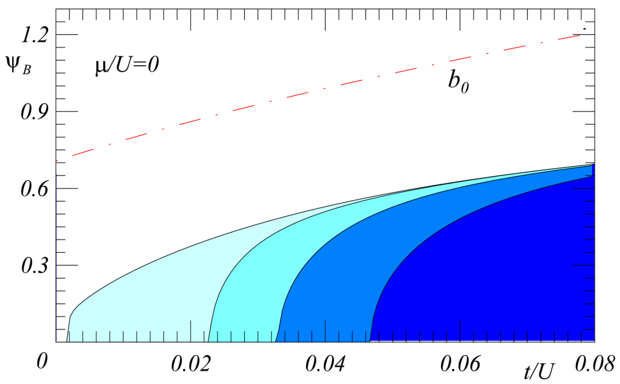

Fig. 1. Superfluid order parameter ψ_{B} for several values of relative temperature $k_{\mathrm{B}}T/U = 0.00, 0.05, 0.10, 0.20$ from the left to the right and fixed chemical potential. Dashed-dotted line is the amplitude b_0 of the order parameter.

only variables

$$\mathcal{S}_{\mathrm{ph}}\phi = \int_0^\beta \mathrm{d}\tau \Bigg\{ \sum_i \left[\frac{1}{2U} \dot{\phi}_i^2(\tau) + \frac{1}{\mathrm{i}} \frac{\bar{\mu}}{U} \dot{\phi}_i(\tau) \right] - \sum_{\langle i,j \rangle} \mathrm{e}^{\phi_i(\tau)} J_{ij} \mathrm{e}^{-\phi_j(\tau)} \Bigg\}, \tag{6}$$

with the phase stiffnesses $J_{ij} = b_0^2 t_{ij}$, and the amplitude $b_0^2 = \left(\sum_{\langle i,j \rangle} t_{ij} + \bar{\mu} \right) / U$.

4. Results

To proceed, we replace the phase degrees of freedom by the complex field ψ_i which satisfies the quantum periodic boundary condition $\psi_i(\beta) = \psi_i(0)$. This can be conveniently done using the Fadeev–Popov method with the Dirac delta functional representation [4]. Within the phase coherent state the superfluid state order parameter becomes

$$1 - \psi_{\mathrm{B}}^2 = \frac{1}{4N} \sum_{\boldsymbol{k}} \frac{1}{\Lambda_{\boldsymbol{k}}} \left\{ \coth \left[\frac{1}{2} \beta U \left(\Lambda_{\boldsymbol{k}} - v \left(\frac{\mu}{U} \right) \right) \right] + \coth \left[\frac{1}{2} \beta U \left(\Lambda_{\boldsymbol{k}} + v \left(\frac{\mu}{U} \right) \right) \right] \right\}. \tag{7}$$

In the above equation $\Lambda_{\boldsymbol{k}}^2 = \left(J_0 - J_{\boldsymbol{k}} \right) / U + v^2(\mu/U)$ and $v(\mu/U) = \mathrm{frac}(\mu/U) - 1/2$, where $\mathrm{frac}(x) = x - [x]$ is the fractional part of the number and $[x]$ is the floor function which gives the greatest integer less than or equal to x. The finite-temperature phase diagram of the model can be calculated from Eq. (7) by introducing the density of states for simple cubic lattice in order to perform the sum over the lattice wave vectors

$$\rho(\xi) = \frac{1}{\pi^3 t} \int_{a_1}^{a_2} \frac{\mathrm{d}\epsilon}{\sqrt{1-\epsilon^2}} \Theta \left(1 - \frac{|\xi|}{3t} \right) \times \boldsymbol{K} \left(\sqrt{1 - \left(\frac{\xi}{2t} + \frac{\epsilon}{2} \right)^2} \right) \tag{8}$$

with $a_1 = \min(-1, -2 - \xi/t)$ and $a_2 = \max(1, 2 - \xi/t)$; $\boldsymbol{K}(x)$ is the elliptic function of the first kind [5].

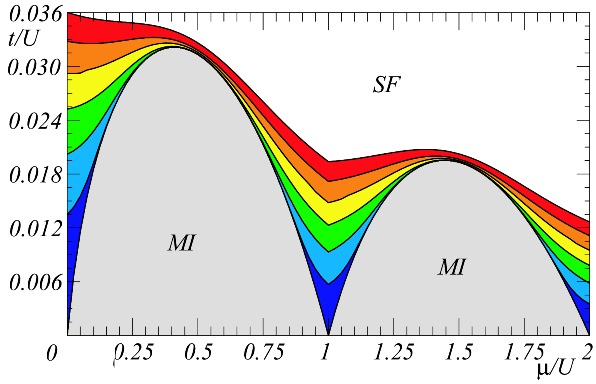

Fig. 2. Phase diagram for BH model for a simple cubic lattice as a function of chemical potential and several values of relative temperature $k_{\mathrm{B}}T/U = 0.00, 0.01, 0.02, 0.03, 0.04, 0.05, 0.06$ (different gray regions from bottom). The Mott insulator phase is found within each lobe of integer boson density. Above the critical lines the superfluid region takes place.

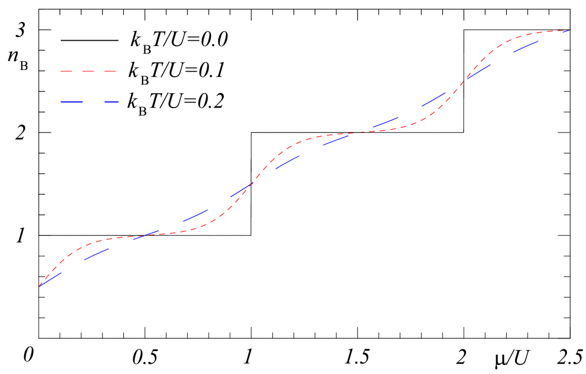

Fig. 3. Bosonic occupation number n_{B} as a function of the chemical potential, for several values of relative temperature and for $t/U = 0$ (the atomic limit).

A lobe-like structure (see Fig. 2), similar to the zero--temperature case, becomes flat with increasing temperature. The lobes with a larger boson occupation number are more stable against temperature. The stability comes from higher values of the repulsive energy U. Therefore, at temperature $T = 0$ the interaction in the system [6] governs the quantum phase transition. Decreasing value of the repulsive energy we can achieve superfluid phase. With increasing temperature, typical of the Mott state, steps-like profile becomes smoother (see Figs. 3 and 4). Therefore, bosons placed in the Mott state get energy required to move from one lattice site to another from thermal fluctuations. The temperature $k_{\mathrm{B}}T/U \approx 0.2$, where the occupation number characteristic becomes flat, is similarly recognized as a melting temperature for the condensate slowly loaded into the optical potential in the presence of a smoothly varying trap [7].

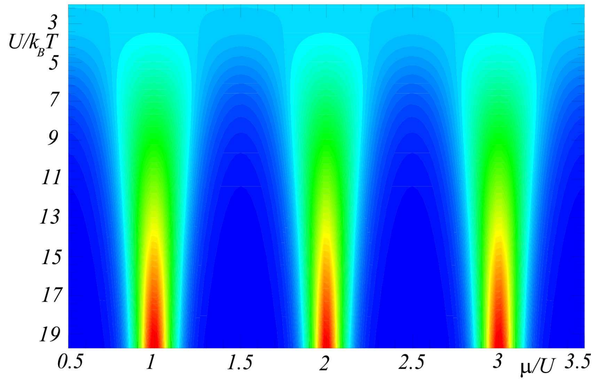

Fig. 4. Density plot of the compressibility $\kappa = \partial n_{\mathrm{B}}/\partial\mu$ as a function of the temperature for $t/U = 0$. Shading around the integer values μ/U corresponds to high values of κ whereas the gray shading marks the region of diminishing compressibility.

5. Summary

In this paper we have presented a study of the finite-temperature transition in the three-dimensional Bose–Hubbard model. We employed the U(1) quantum rotor approach and a path integral formulation with inclusion of summation over topological charge, explicitly tailored for the BH Hamiltonian. This method can give the thermodynamics of the Bose–Hubbard model in the limit of strong interactions. Our aim was then to analyze the phase transitions that may occur in such system at finite temperature, as well as to determine the general features of the phase diagrams. We demonstrated the evolution of zero temperature Mott lobes and Mott plateaus when the temperature is increasing.

Acknowledgments

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