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Temperature effects on superfluid phase transition in Bose-Hubbard model with three-body interaction

Introduction

In optical lattices the behaviour of contained atoms is governed mainly by two-body interactions. However, there are experimental indications that also three-body interactions should be taken into account [1, 2]. In this work we present the finite temperature phase diagram of strongly interacting lattice bosons in the framework of the Bose-Hubbard model and study its dependence on the three-body interactions strength. In the calculations we used the mean-field approximation and the resolvent method, which is based on the contour integral representation of the partition function [3].

The model

To describe an ultracold gas of bosons in an optical lattice, the Bose-Hubbard model, which successfully captures Mott-insulator-superfluid phase transition [4], is utilized. The Hamiltonian in second-quantized form is given by:

$$\hat{H}_{\mathrm{BH}} = -J\sum_{\{ij\}}(\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) - \sum_i \mu \hat{n}_i + \sum_i \hat{V}_i,$$

where:

- $\hat{a}_i$ and $\hat{a}_i^\dagger$ are bosonic creation and annihilation operators at the i-th site of the lattice,
- $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the particle number operator,
- J_{ij} is the hopping matrix element,
- μ is the chemical potential.

The summation index i runs from 1 to N - the number of the lattice sites. The V_i term contains two- and three-body interactions and is given by:

$$\hat{V}_i = \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) + \frac{W}{6}\hat{n}_i(\hat{n}_i - 1)(\hat{n}_i - 2),$$

where U and W measure two- and three-body repulsive interaction strength.

The method

To describe the superfluid phase of the system under study we introduce the order parameter $\Phi_i = \langle \hat{a}_i \rangle$. The mean-field approximation leads to the following Hamiltonian:

$$\hat{H} = \sum_i \left[-Jz\Phi(\hat{a}_i + \hat{a}_i^\dagger - \Phi) - \mu \hat{n}_i + \hat{V}_i \right],$$

which is the sum of local terms. Since the corresponding statistical sum Z factorizes, we can omit the index i. One can split the Hamiltonian into two parts:

$$\hat{H}_0 = \hat{V} - \mu \hat{n},$$

which in the strong coupling regime is considered as the unperturbed Hamiltonian and

$$\hat{H}' = -Jz\Phi\left(\hat{a} + \hat{a}^\dagger - \Phi\right),$$

which plays role of the perturbation. Next, we express the statistical sum Z by the resolvent of the full mean-field Hamiltonian $(z - \hat{H})^{-1}$:

$$Z = \int_\Gamma \frac{dz}{2\pi i} e^{-\beta z} \mathrm{Tr}\,(z - H)^{-1},$$

which can be expanded in the series:

$$Z = \tilde{Z}_0 - \beta \int_0^1 \frac{dg}{g} \int_\Gamma \frac{dz}{2\pi i} e^{-\beta z} \mathrm{Tr} \sum_{n=1}^{\infty} [(z - \hat{H}_0)^{-1} g \hat{H}']^n.$$

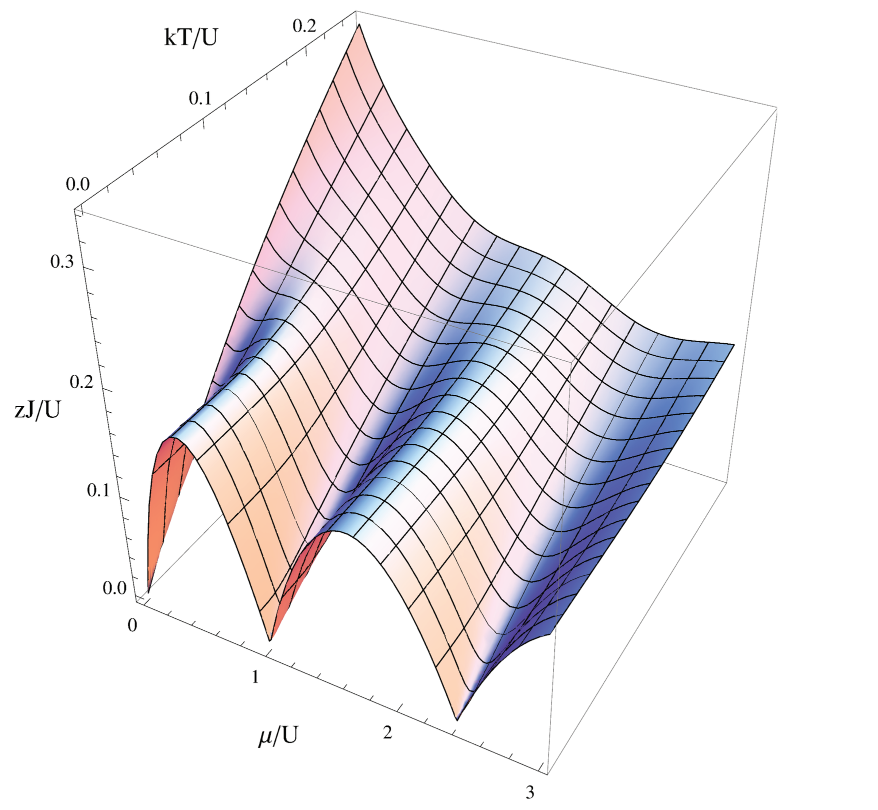

Figure 1: The plot of the critical surface separating the disordered (below the surface) and superfluid state (above the surface) for the Bose–Hubbard model with three-body interaction in the three-dimensional plot defined by the $T - J - \mu$ variables. The three-body interaction parameter was set to $W/U = 0.4$.

The contour of the integration Γ surrounds all singularities of the resolvent. In our case this expansion is of the form:

$$Z = e^{-\beta J z \Phi^2}\left(Z_0 + Z_2\Phi^2 + Z_4\Phi^4 + \ldots\right),$$

where

$$Z_0 = \mathrm{Tr}\, e^{-\beta \hat{H}_0} = \sum_{n=0}^{\infty} e^{-\beta E_n}$$

is the partition function of the unperturbed Hamiltonian with energy levels given by

$$E_n = \frac{U}{2}n(n-1) + \frac{W}{6}n(n-1)(n-2) - \mu n$$

and

$$Z_2 = -\beta J^2 z^2 \sum_{n=0}^{\infty} e^{-\beta E_n}\left(\frac{n}{E_n - E_{n-1}} + \frac{n+1}{E_n - E_{n+1}}\right).$$

Due to its complexity, we do not write the fourth order term explicitly. In the resolvent method the calculation of Z_k terms in the partition function expansion is divided into two stages:

- Calculation of the trace
- Calculation of the contour integral

Both steps do not require advanced computations, which make the resolvent method very efficient. The detailed calculations can be found in [5].

Phase Diagram

In order find the finite temperature phase diagram of the corresponding system, one needs to calculate the free energy $f = -1/\beta \ln Z$. The expansion of the free energy up to the fourth order of the order parameter has the form:

$$f = f_0 + \left(Jz - \frac{1}{\beta}\frac{Z_2}{Z_0}\right)\Phi^2 - \frac{1}{\beta}\left(-\frac{Z_2^2}{2Z_0^2} + \frac{Z_4}{Z_0}\right)\Phi^4,$$

where $f_0 = -1/\beta\ \ln Z_0$. In Landau theory, at a point of the phase transition the coefficient in front of Φ^2 vanishes, which yields to the following equation for the critical line:

$$zJ = \frac{\sum_{n=0}^{\infty} e^{-\beta E_n}}{\sum_{n=0}^{\infty} e^{-\beta E_n}\left(\frac{n+1}{E_{n+1} - E_n} - \frac{n}{E_n - E_{n-1}}\right)}.$$

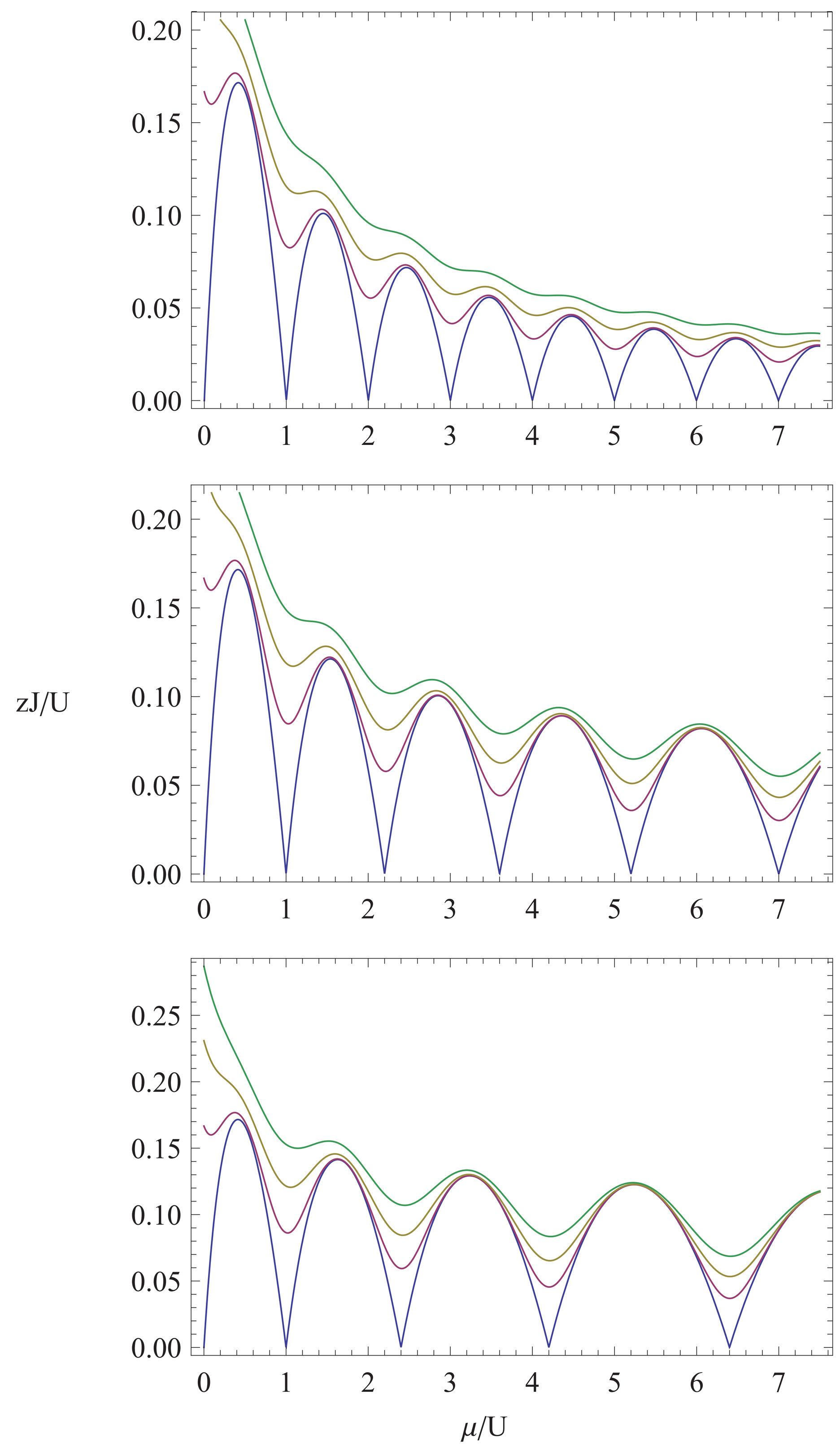

Figure 2: Phase diagram of the Bose–Hubbard system showing evolution of the Mott lobes for several values of the three body interaction $W/U = 0,\ 0.2,\ 0.4$ (panel a, b and c, respectively) in the plane defined by the chemical potential μ and the tunnelling parameter J (the on-site interaction U serves as an energy scale) for several values of the temperature ($kT/U = 0, 0.1, 0.15, 0.20$, curves from the bottom to the top).

The above equation divided by the two-body interaction strength U defines a hyper-surface in the space of the following parameters:

- The reduced temperature kT/U and chemical potential μ/U
- The dimensionless hopping term J/U and three-body interaction strength W/U

Figure 1 contains the plot of the critical surface for a fixed value of the parameter W. As one can see, the finite temperature dilutes the Mott lobes and diminishes the superfluid phase. Figure 2 presents the evolution of the insulating Mott lobes for increasing temperature and various choices of the three-body interaction strength W/U. As it increases, the subsequent Mott lobes widen.

Conclusions

We have investigated the effect of the three body interactions on the Bose-Hubbard model using both the mean field approach to the on-site hopping term and the resolvent method – which turned out to be very efficient method for calculation of the partition function. Subsequently we have found the phase diagram and depicted its dependence on various parameters of interest.

References

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