Finite-temperature effects on the superfluid Bose–Einstein condensation of confined ultracold atoms in three-dimensional optical lattices

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Abstract
We discuss the finite-temperature phase diagram in the three-dimensional Bose–Hubbard (BH) model in the strong correlation regime, relevant for Bose–Einstein condensates in optical lattices, by employing a quantum rotor approach. In systems with strong on-site repulsive interactions, the rotor \(U(1)\) phase variable dual to the local boson density emerges as an important collective field. After establishing the connection between the rotor construction and the on-site interaction in the BH model a robust effective action formalism is developed which allows us to study the superfluid phase transition in various temperature-interaction regimes.

1. Introduction
The ability to confine ultracold quantum gases in optical lattices is already having a major impact on fields as diverse as condensed-matter physics and quantum information processing [1–3]. An optical lattice is essentially a periodic intensity pattern that is formed by the interference of two or more laser beams. The simplest optical lattice consists of the region that is formed when two laser beams with the same wavelength travelling in opposite directions meet each other and form an interference pattern. This artificial structure is able to trap an atom because the electric fields of the lasers induce an electric dipole moment in the atom. However, quantum-mechanical tunnelling allows the atoms to spread through the optical lattice to some degree. In a Bose–Einstein condensate, this tunnelling process dominates the behaviour of the atoms, which causes the system to have a perfect phase coherence between the matter waves on different lattices sites. This quantum phase transitions of the Bose–Einstein condensates loaded into the lowest vibrational level of single wells of an optical lattice in the strict sense can exist only at temperature \(T = 0\). However, in typical experimental situations we must take into consideration thermal fluctuations in the particle number per site. In the presence of the finite temperature the nonzero value of the compressibility is expected in contrast to the incompressible Mott state at \(T = 0\). The experimental data only signal 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. This issue has gained recently much attention [4–7]. Theoretical [8] and numerical [9–11] approaches have designed to these systems in three dimensions but only recently the finite-temperature effects have been studied systematically [11–13]. Yu et al. [12] presented study of the finite-temperature behaviour of ultracold Bose atoms in three-dimensional (3D) optical lattices by the slave fermion and the slave boson approaches to the Bose–Hubbard (BH) model. The finite-temperature phase diagram was also investigated by Gerbier [7] in the context of ultracold bosons confined in an optical lattice in the presence of an additional potential. Three regimes can be recognized from the phase diagram: zero-temperature quantum phase, intermediate, where Mott-insulator (MI) features persist but the superfluid (SF) region is absent and the thermal region, where the
Mott-insulator properties disappear. Despite the various theoretical approaches to the problem of the strongly interacting bosons at finite temperatures many questions still remain open and unsolved. In particular, studies of the phase transitions in the strongly correlated regime are scarce, where the repulsive energy is the main energy scale in the system and we are far from the limit of weakly interacting bosons. For these reasons, there is still a strong need for approximate but robust treatments of strongly correlated bosonic models in order to include the finite-temperature properties especially relevant for phase diagrams for the 3D system where the temperature-induced phase transition exists. The purpose of this paper is to present a robust theoretical description of correlated bosonic systems which fulfills these goals. Our main idea is to focus on the degrees of freedom associated with the relevant physical variable associated with the Mott-superfluid transition, namely a quantum phase field $U(1)$, rotor field, which is dual to the local occupation number and acquires dynamic significance from the boson–boson interaction [14].

2. The model

In the experimental parameter regime, bosonic atoms with repulsive interactions in a periodic lattice potential are perfectly described by a Bose–Hubbard model which is the simplest nontrivial model describing a bosonic many-body system on a lattice which cannot be mapped onto a single particle problem. Nevertheless it captures essential effects like a quantum phase transition from a superfluid state to a Mott-insulating state. The Hamiltonian of the model reads

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

where $a_i^\dagger$ and $a_i$ 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 the summation over the nearest-neighbour sites. Furthermore, $t_{ij}$ is the hopping matrix element and describes the tunnelling of bosons between neighbouring potential wells in the simple cubic lattice and $\mu / U = \mu / U + 1/2$ is the shifted reduced chemical potential which controls the number of bosons, where $U > 0$ is the on-site repulsion. Due to the short range of the interactions compared to the lattice spacing, the interaction energy is well described by this term, which characterizes a purely on-site interaction. The interaction term tends to localize atoms to lattice sites. When the potential depth of the optical lattice is increased, the tunnelling barrier between neighbouring lattice sites is raised and the tunnelling matrix element $t$ decreases. The on-site interaction $U$ on the other hand is increased due to a tighter confinement of the wavefunction for bosons on a lattice site. Therefore the ratio $U/t$ can be continuously adjusted over a wide range by changing the strength of the lattice potential. Finally we comment on the validity of the Hamiltonian in equation (1). The Bose–Hubbard model can be obtained from the many-body Hamiltonian with the pseudo-potential interaction. However, we must assume that thermal and mean interaction energy are much smaller than the separation to the first excited band. Therefore, the exact value of the temperature (in the limit where the recoil energy is much smaller than the maximum value of the lattice depth $E_R \ll V_0$) can be calculated from the expression $k_B T \ll \hbar \omega_0$, where $\hbar \omega_0$ is the energy separated by a number of vibrational levels in an infinite periodic potential. The energy to comparison can be taken from a single site of the lattice. Moreover the hopping matrix elements are nonzero or non-negligible only to nearest neighbours, so they are always negative in the lowest band.

3. Phase action and order parameter

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

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

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

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

where $\beta = 1/k_B T$ and $T$ is the temperature. Since Hamiltonian is not quadratic in the fields $a_i$ we have to decouple first the interaction term in equation (1) by means of a Gaussian integration over the auxiliary scalar potential fields $V_i(\tau)$ whose periodic part $V_i^P(\tau)$ couples to the local particle number through the Josephson-like relation $\phi_i(\tau) = V_i^P(\tau)$, where $\phi_i(\tau) \equiv \partial \phi_i(\tau) / \partial \tau$. The phase field satisfies the periodicity condition $\phi_i(\beta) = \phi_i(0)$ as a consequence of the periodic properties of the $V_i^P(\tau)$ field. Next, we perform the local gauge transformation to the new bosonic variables

$$a_i(\tau) = b_i(\tau) \exp[\im \phi_i(\tau)]. \quad (4)$$

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

$$\Psi_B \equiv \langle a_i(\tau) \rangle = \langle b_i(\tau) \exp[\im \phi_i(\tau)] \rangle = b_0 \Psi_B \quad (5)$$

whose non-vanishing value signals a macroscopic quantum phase coherence (in our case we identify it as an SF state). The system can be then described by a macroscopic wavefunction since the many-body state is a product over identical single particle states. Therefore a macroscopic phase is well defined on each lattice site and the system is superfluid. On the other hand the atom number per site is uncertain, and therefore one would find a random atom number in a measurement. In the large $U$ limit the amplitude $b_0 \equiv b_0(\eta)$ (see figure 1) has a nonzero value, but to achieve the superfluidity, the phase variables must also become stiff and, in consequence, $\Psi_B \equiv \exp[\im \phi(\tau)] \neq 0$. Furthermore, we parametrize the boson fields $b_i(\tau) = b_0 + b_i(\tau)$ and restrict our calculations to the phase fluctuations dropping the amplitude dependence [15] which is justified in the large $U/t$ limit. The $U(1)$ group governing the phase field is compact and $\phi(\tau)$ has the topology...
of a circle, so that instanton effects can arise due to nonhomotopic mappings of the configuration space onto the gauge group $U(1)$. Accordingly, the path integral reads

$$\int [D\phi] \cdots = \sum_{\{m_i\}} \prod_i \int_0^{2\pi} d\phi_i(0) \int_{\phi(0)}^{\phi(\tau)} [D\phi_i(\tau)] \cdots$$

which is performed by taking phase configurations that satisfy boundary condition $\phi_i(\beta) - \phi_i(0) = 2\pi m_i$, where the winding numbers $n_i$ label the distinct homotopy classes of the $U(1)$ group. Thus the paths can be divided into topologically distinct classes, characterized by a winding number defined as the net number of times the worldline wraps around the system in the ‘imaginary time’ direction. Integrating the action in equation (3) over the bosonic fields we obtain the effective Lagrangian in terms of the phase-only variables

$$S_{ph}[\phi] = \int_0^\beta d\tau \left\{ \sum_{(i,j)} \left[ \frac{1}{2U} \dot{\phi}_i^2(\tau) + \frac{b_0^2}{2} \phi_i^2(\tau) \right] - \sum_{(i,j)} e^{\phi_j(\tau)} J_{ij} e^{-\phi_i(\tau)} \right\},$$

where the phase stiffnesses $J_{ij} = b_0^2 t_{ij}$, where the amplitude $b_0^2 = (\sum_{(i,j)} t_{ij} + \bar{\mu})/U$ originates from the saddle point condition

$$\frac{\delta S[\bar{b}, b]}{\delta b} |_{b_0^2} = 0.$$

The result of the gauge transformations is that we have managed to cast the strongly correlated problem into a system of mutually noninteracting effective bosons, submerged in the bath of strongly fluctuating $U(1)$ phase fields, whose dynamics is governed by the energy scale set by the on-site interaction $U$ that drives the Mott transition.

4. Treatment of the action of quantum rotors

Now, we devise a systematic way of treatment for the fluctuating phase fields contained in the action in equation (7) that enables us to obtain an effective nonlinear sigma-field theory that respects the symmetry properties of the model and satisfies the Mermin–Wagner theorem, thereby improving the pure mean-filed approach known from its restricted ability to deal with the spatial fluctuations. To proceed, it is convenient to replace the phase degrees of freedom by the complex field $\psi_i \equiv e^{i\phi_i(\tau)}$ which satisfies the periodic boundary condition $\psi_i(\beta) = \psi_i(0)$. This can be done by implementing the Fadeev–Popov method with the Dirac delta functional resolution of the unity: [16]

$$1 \equiv \int [D\bar{\psi} D\psi] \delta \left( \sum_i |\psi_i(\tau)|^2 - N \right) \times \prod_i \delta(\psi_i - e^{\frac{i\phi_i(\tau)}{2}}),$$

where we take $\psi_i$ as a continuous variable but constrained (on the average) to have the unimodular value. We can solve the constraint by introducing the Lagrange multiplier $\lambda$ which adds the quadratic terms (in the $\psi_i$ fields) to the action equation (7). The partition function is written in the form

$$Z = \int_{-i\infty}^{i\infty} \left[ \frac{D\lambda}{2\pi i} \right] e^{-N\beta\mathcal{F}(\lambda)},$$

where the free energy per site $\mathcal{F} = -\ln Z/\beta N$ is given by

$$\mathcal{F} = -\lambda - \frac{1}{N\beta} \ln \int [D\bar{\psi} D\psi] e^{-S_{eff}[\bar{\psi}, \psi]} S_{eff}[\bar{\psi}, \psi] = \sum_{(i,j)} \int_0^\beta d\tau d\tau' \langle [J_{ij} + \lambda \bar{\delta}_{ij}] \delta(\tau - \tau') \rangle - \gamma_{ij}(\tau, \tau') \bar{\psi}_i(\tau) \psi_j(\tau'),$$

and $\gamma_{ij}(\tau, \tau') = \langle \exp[-i(\phi_i(\tau) - \phi_j(\tau'))]\rangle$ is the two-point phase correlator associated with the order parameter field, where $\langle \cdots \rangle$ is the averaging with respect to the action in equation (7).

The action with the topological contribution, after Fourier transform, can be written as

$$S_{eff}[\bar{\psi}, \psi] = \frac{1}{N\beta} \sum_{k,\ell} \bar{\psi}_{k,\ell} \Gamma_{k}^{-1}(\omega_{k}) \psi_{k,\ell},$$

where $\Gamma_{k}^{-1}(\omega_{k}) = \lambda - J_k + \gamma^{-1}(\omega_{k})$ is the inverse of the propagator and $\omega_{k} = 2\pi \ell/\beta$ ($\ell = 0, \pm 1, \pm 2, \ldots$) stands for the Bose–Matsubara frequency, while the phase correlator, after Fourier transform, can be written as:

$$\gamma(\omega_{k}) = \frac{1}{Z_{0}} \sum_{m = -\infty}^{+\infty} \frac{e^{-\frac{i}{2}\beta U (m + \frac{\bar{\mu}}{U})^2}}{1 - 4 \frac{m + \frac{\bar{\mu}}{U}}{Z_{0}^2}},$$

where $Z_0 = \sum_{m = -\infty}^{+\infty} \exp \left[ -\frac{i}{2}\beta U (m + \frac{\bar{\mu}}{U})^2 \right]$ is the partition function for the set of non-interacting quantum rotors. Within the phase coherent state the order parameter is given by

$$1 - \psi_{k,\ell}^2 = \frac{1}{N\beta} \sum_{k,\ell} \frac{1}{\lambda_0 - J_k + \gamma^{-1}(\omega_{k})}.\]
the critical value of the Lagrange parameter \( \lambda = \lambda_0 \) that stays constant in the whole ordered phase. After summation over the Matsubara frequency the superfluid state order parameter becomes

\[
1 - \psi_B^2 = \frac{1}{4N} \sum_{\mathbf{k}} \frac{1}{\Lambda_k} \left\{ \coth \left[ \frac{1}{2} \beta U \left( \Lambda_k - \nu \left( \frac{\mu}{U} \right) \right) \right] + \coth \left[ \frac{1}{2} \beta U \left( \Lambda_k + \nu \left( \frac{\mu}{U} \right) \right) \right] \right\}.
\]

(15)

In the above equation, \( \Lambda_k^2 = (J_0 - J_0) / U + \nu^2 (\mu / U) \) and \( \nu (\mu / U) = \frac{1}{2} \arctan \left( \frac{\mu}{U} \right) - 1/2 \), where \( \nu(x) = x - \lfloor x \rfloor \) is the fractional part of the number and \( \lfloor x \rfloor \) is the floor function which gives the greatest integer less than or equal to \( x \).

5. Results

When the strength of the interaction term relative to the tunnelling term in the Bose–Hubbard Hamiltonian is changed, the system reaches a quantum critical point in the ratio of the tunnelling term in the Bose–Hubbard Hamiltonian is changed, when the strength of the interaction term relative to the repulsive energy we can achieve superfluid phase. In real physical realizations of the BH model thermal excitations are also present and also can activate a phase transition. We highlight the sole temperature effect).

A lobe-like structure (see figure 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 [15] governs the quantum phase transition. By decreasing the value of the repulsive energy we can achieve superfluid phase. In real physical realizations of the BH model thermal excitations are always present and also can activate a phase transition. We see it clearer by calculating a bosonic occupation number. Decomposing the phase field in terms of a periodic field and linear in \( \tau \) term we calculate the effects of the fixed boson number \( n_B = N^{-1} \sum \langle a_\sigma (\tau) a_\sigma (\tau) \rangle \) in the system. The total boson density \( n_B = n_B + \delta n_B \) consists of the occupation number for neutral bosons \( n_B \) and a contribution \( \delta n_B \) from a fluctuating phase field. For \( T = 0 \) we recognize steps of fixed integer filling of bosons (see figure 3). With increasing temperature, typical for the Mott state, the step-like profile becomes smoother. Therefore, bosons placed in the Mott state get energy required to move from one lattice site to another from thermal fluctuations. The temperature \( k_B T / U \sim 0.2 \), where the occupation number characteristic becomes flat, is similar to a melting temperature for the condensate slowly loaded into the optical potential in the presence of a smoothly varying trap [7]. The increasing value of the thermal energy, in analogy to the decreasing repulsive interaction [15], can lead to the situation where the sharp steps of the MI state become

![Figure 2. Phase diagram for the BH model on a cubic lattice as a function of chemical potential and temperature.](image)

![Figure 3. Bosonic occupation number \( n_B \) as a function of the chemical potential, for several values of the temperature as indicated in the plot calculated for the extreme interaction limit \((U/t = \infty)\), to highlight the sole temperature effect.](image)
indistinct (see figure 3). The Mott insulator to superfluid quantum phase transition is rigorously present only at zero temperature, whereas at finite temperature thermal fluctuations induce a phase transition between a superfluid and a normal phase. However, at sufficiently low temperatures, a remnant of the insulating phase still persists within the normal phase. In these conditions it is possible to observe a sharp crossover between a compressible normal fluid and a phase characterized by a vanishing compressibility (see figure 4). Regarding the comparison of our method with the previous approaches we found that our results are in good agreement with other calculations (including numerical quantum Monte Carlo [18], diagrammatic perturbation theory [19]) and analytical works based on the strong coupling perturbation theory [20], see table 1 and figure 5.

### Table 1. Comparison of the maximum of the critical value for $t/U$ parameter (as a function of the normalized chemical potential $\mu/U$) at the tip of the first ($n_B = 1$) Mott lobe for square lattice with several numerical (QMC: quantum Monte Carlo [18], DPT: diagrammatic perturbation theory [19]) and analytical work (SCPT: strong coupling perturbation theory [20]). QRA: our calculations using the quantum rotor approach.

| $t/U$ | QMC | DPT | PA | QRA |
|-------|-----|-----|----|-----|
| 0.03408(2) | 0.03407 | 0.34737 | 0.03215 |
| $\mu/U$ | 0.389 | 0.393 | 0.37905 | 0.41 |

Figure 5. The comparison of the zero-temperature phase diagram calculated from the diagrammatic perturbation theory [19] (DPT) and our results obtained in the frame of the quantum rotor approach (QRA) with $n_B = 1, 2, 3$ and 10. We found that the critical value $(t/U)_{\text{crit}}$ (see also table 1) for the tip of the $n$-th Mott-insulator lobe is always slightly lower than obtained from DPT and Monte Carlo simulations [18].
References

[1] Jaksch D, Bruder C, Cirac J I, Gardiner C W and Zoller P 1998 Phys. Rev. Lett. 81 3108
[2] Greiner M, Mandel O, Esslinger T, Hansch T W and Bloch I 2002 Nature 415 39
[3] Fisher M P A, Weichman P B, Grinstein G and Fisher D S 1989 Phys. Rev. B 40 546
[4] Buonsante P and Vezzani A 2004 Phys. Rev. A 70 033608
[5] Plimak L I, Fleischauer M and Olsen M K 2004 Phys. Rev. A 70 013611
[6] Pupillo G, Williams C J and Prokof’ev N 2006 Phys. Rev. A 73 013408
[7] Gerbier F 2007 Phys. Rev. Lett. 99 120405
[8] Kampf A P and Zimanyi G T 1993 Phys. Rev. B 47 279
[9] Prokof’ev N V, Svistunov B V and Tupitsyn I S 1998 Phys. Lett. A 238 253
Prokof’ev N V, Svistunov B V and Tupitsyn I S 1998 J. Exp. Theor. Phys. 87 310
[10] Alet F, Wessel S and Troyer M 2005 Phys. Rev. E 71 036706
[11] Capogrosso-Sansone B, Prokof’ev N V and Svistunov B V 2007 Phys. Rev. B 75 134302
[12] Yue Yu and Chui S T 2005 Phys. Rev. A 71 033608
[13] Pollet L, Kollath C, van Houcke K and Troyer M 2008 arXiv:0801.1887
[14] Kopeč T K 2004 Phys. Rev. B 70 05451
See also Zhao E and Paramekanti A 2007 Phys. Rev. B 76 195101
[15] Polak T P and Kopeč T K 2007 Phys. Rev. B 76 094503
[16] Kopeč T K and José J V 1999 Phys. Rev. B 60 7473
[17] Abramovitz M and Stegun I 1970 Handbook of Mathematical Functions (New York: Dover)
[18] Capogrosso-Sansone B, Güney Söyleş S, Prokof’ev N and Svistunov B 2008 Phys. Rev. A 77 015602
[19] Teichmann N, Hinrichs D, Holthaus M and Eckardt A 2009 Phys. Rev. B 79 100503
[20] Freericks J K, Krishnamurthy H R, Kato Y, Kawashima N and Trivedi N 2009 arXiv:0902.3435