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Pairing Mechanism at Finite Temperatures in Bosonic Systems

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The pure Bose–Hubbard model, a staple of optical lattice-related research that describes bosonic condensation, is examined at finite temperatures. Advanced analytical methods are used, most importantly path integrals and quantum rotors. A first-order trace approximation is commonly applied while integrating over bosonic fields to obtain a phase-only model. Here, a second-order trace approximation is considered instead. This extension leads to an effective phase model with two types of superfluid, i.e., standard Bose–Einstein condensation and additional temperature-driven bosonic pair condensation. This effective model is further treated with a self-consistent harmonic approximation in order to compare the two superfluids. This analysis shows that the pairing mechanism strengthens the condensate phase at finite temperatures.

topics: Bose–Hubbard model, path integral, phase Hamiltonian, phase transition

1. Introduction

The quantum phase transition between the two ground states of the Bose–Hubbard (BH) model, i.e., the superfluid (SF) state and the Mott insulator (MI) state, is a staple of the study of strongly-correlated systems in low temperatures [1–5], particularly on optical lattices. The transition to the normal state is also observed at finite temperatures [4–7].

Atom pairs have been observed in the depletion of an equilibrium interacting Bose gas by Tenart et al. [8], who used helium 4 and combined long time-of-flight (TOF) with three-dimensional detection method.

Many-body correlations (MBCs) are always present in optical lattice systems, even when only the standard Hamiltonian is used to analyze experimental data [9–11]. In the BH model with density-induced tunnelling, MBCs lead to bosonic pair condensation [12]. However, MBCs are not the only possible source of bosonic pairing.

We carry out a path integral analysis of the Bose–Hubbard model, using the U(1) quantum rotor method [3]. The usual strategy in quantum rotor approaches is to reach a phase-only effective model and perform Gaussian integration. The next step is the series expansion of the Green's function of the effective model. This expansion is usually approximated to first-order terms only. We show that temperature-driven pair condensation is anticipated by this model, provided terms of higher order are also preserved.

The self-consistent harmonic approximation [13] is applied to the effective phase model. The order parameters are calculated to map the transitions between the normal phase and two others: single-particle Bose–Einstein condensate (BEC) and pair condensate. Introducing the density of states allows us to analyse and compare the properties of this model in different geometries, although here we focus on a simple cubic lattice. The methods used provide a natural way to analyze effective many-body correlations.

2. Methods

The Hamiltonian of the Bose–Hubbard model is

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

with on-site repulsion $U > 0$, chemical potential μ, hopping integral $t_{ij} = t$, and annihilation a_j (creation $a_i^\dagger$) operator of a particle at j-th site. The path integral partition function and the effective action are, respectively,

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

and

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

The Hubbard–Stratonovich and gauge transformations allow us to integrate over bosonic fields, bringing us to a phase-only model with the following partition function

$$\mathcal{Z} = \int \mathcal{D}\varphi \, \exp\left[-\sum_i \left\{ \int_0^\beta \mathrm{d}\tau \left(\frac{1}{2U} \left(\dot{\varphi}_i(\tau)\right)^2 + \frac{\bar{\mu}}{\mathrm{i}U} \dot{\varphi}_i(\tau) \right) + \mathrm{Tr}\left[\ln\left(G^{-1}\right) \right] \right\} \right], \tag{4}$$

where

$$G^{-1} = G_0^{-1} - T = G_0^{-1}\left(1 - TG_0\right), \tag{5}$$

$$G_0^{-1} = \left(\frac{\partial}{\partial\tau} + \bar{\mu} \right) \delta_{ij}, \tag{6}$$

$$T = t_{ij}\, \mathrm{e}^{-\mathrm{i}\left(\varphi_i(\tau) - \varphi_j(\tau)\right)}. \tag{7}$$

The trace can be approximated to the second order as

$$\mathrm{Tr}\left[\ln\left(G^{-1}\right) \right] = -\mathrm{Tr}\left[\ln\left(G_0\right) \right] - \mathrm{Tr}\left[\left(TG_0\right) \right] - \frac{1}{2U} \mathrm{Tr}\left[\left(TG_0\right)^2 \right]. \tag{8}$$

Further, G_0 is expanded as the sum of two components, i.e., the bosonic G_0 and the imaginary time-dependent $G(\tau)$, which after Fourier transform are

$$G_0 = b_0^2 = \frac{2\left(zt + \bar{\mu}\right)}{U}, \tag{9}$$

$$\Gamma = \frac{1}{\beta} \sum_n \frac{-\mathrm{i}\omega_n + \bar{\mu}}{\omega_n^2 + \bar{\mu}^2}. \tag{10}$$

These transformations lead to an effective phase model with

$$\mathcal{S}\left[\varphi\right] = \int_0^\beta \frac{\mathrm{d}\tau}{U} \sum_i \left(\frac{\partial\varphi_i}{\partial\tau} \right)^2 + \int_0^\beta \mathrm{d}\tau \left[-J \sum_{\langle i,j \rangle} \cos(\varphi_{ij}) - J' \sum_{\langle i,j \rangle} \cos(2\varphi_{ij}) \right] \tag{11}$$

and exact expressions for the two coefficients

$$\frac{J}{t} = \frac{2\left(zt + \frac{1}{2}U + \mu\right)}{U}, \tag{12}$$

$$\frac{J'}{t} = \frac{t}{U} \left[\frac{2\left(zt + \frac{1}{2}U + \mu\right)}{U} \right]^2 + \frac{\frac{t}{U} z}{2\sinh^2\left(\frac{1}{2}\beta\left(\frac{1}{2}U + \mu\right)\right)}. \tag{13}$$

The interaction terms represent two different ordered phases, with two order parameters, namely $\Psi_\varphi \equiv \langle \cos(\varphi_i) \rangle$ (single) and $\Psi_{2\varphi} \equiv \langle \cos(2\varphi_i) \rangle$ (pair). The imaginary time-dependent part of J' disappears in the zero temperature limit.

The self-consistent harmonic approximation is applied, with the trial function

$$\mathcal{S}_0\left[\varphi\right] = \int_0^\beta \mathrm{d}\tau \left[\frac{1}{U} \sum_i \left(\frac{\partial\varphi_i}{\partial\tau} \right)^2 + \frac{K}{2} \sum_{\langle i,j \rangle} \varphi_{ij}^2 \right]. \tag{14}$$

According to the variational principle for free energy, one reads

$$\mathcal{F} \leq \tilde{\mathcal{F}} = \mathcal{F}_0 + \frac{1}{\beta} \langle \mathcal{S} - \mathcal{S}_0 \rangle. \tag{15}$$

Minimising $\tilde{\mathcal{F}}$ by requiring that $\delta\tilde{\mathcal{F}} = 0$ yields the eponymous self-consistent equation for K

$$J\, \mathrm{e}^{-\frac{1}{2}D_{ij}} - K = 0, \tag{16}$$

where $D_{ij} = \langle \varphi_{ij}^2 \rangle$. Summing over nearest neighbours and introducing the density of states allows us to obtain an analytical expression for D_{ij}

$$D_{ij} = \frac{1}{z} \int \mathrm{d}\xi \sqrt{\frac{(z-\xi)\,U}{2K}} \coth\left(\frac{\beta}{2} \sqrt{\frac{(z-\xi)\,KU}{2}} \right). \tag{17}$$

The single and pair order parameters

$$\Psi_1 = \left\langle \cos(\varphi_i) \right\rangle = \mathrm{e}^{-\frac{1}{2}\left\langle \varphi_i^2 \right\rangle}, \tag{18}$$

$$\Psi_2 = \left\langle \cos(2\varphi_i) \right\rangle = \mathrm{e}^{-2\left\langle \varphi_i^2 \right\rangle}, \tag{19}$$

can also be calculated. The use of the density of states allows us to analyse their properties and critical behaviour both analytically and numerically, in various geometries. The following results have been generated for a three-dimensional simple cubic lattice.

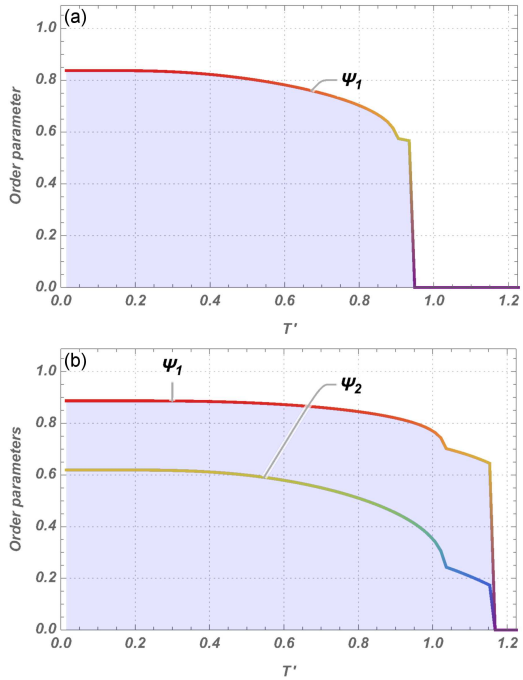

Fig. 1. The single Ψ_1 and pair Ψ_2 order parameters on a simple cubic lattice for $t/U = 0.085$. (a) Model without pair term. (b) Model with pair term.

3. Results

Figure 1 shows a comparison of the temperature dependence of order parameters in two models: (i) single order parameter in the standard phase model, without a pair term,

$$\mathcal{S}[\varphi] = \int_0^\beta \mathrm{d}\tau \left[\frac{1}{U} \sum_i \left(\frac{\partial \varphi_i}{\partial \tau} \right)^2 - J \sum_{\langle i,j \rangle} \cos(\varphi_{ij}) \right], \tag{20}$$

and (ii) single and pair condensate order parameters in the full version (11). The single hopping is $t/U = 0.085$ and the chemical potential is $\mu/U = 1.5$. The temperature is $T' = T/U = 1/(\beta U)$.

In the extended phase model, the pair condensate is generated by imaginary time dynamics. Similar to pairing generated by density-induced tunnelling (DIT) [12], the presence of the $\cos(2\varphi_{ij})$ pair term in (11) strengthens the condensate phase, meaning the superfluid survives in higher temperatures. However, in this case, there is no phase separation; the critical temperature is the same for single and pair condensates.

Figure 2 shows the entropy

$$S = -\frac{\partial \tilde{\mathcal{F}}}{\partial T}, \tag{21}$$

with and without the $\cos(2\varphi_{ij})$ term. The comparison is presented for two values of the single hopping, $t/U = 0.015$ and $t/U = 0.085$.

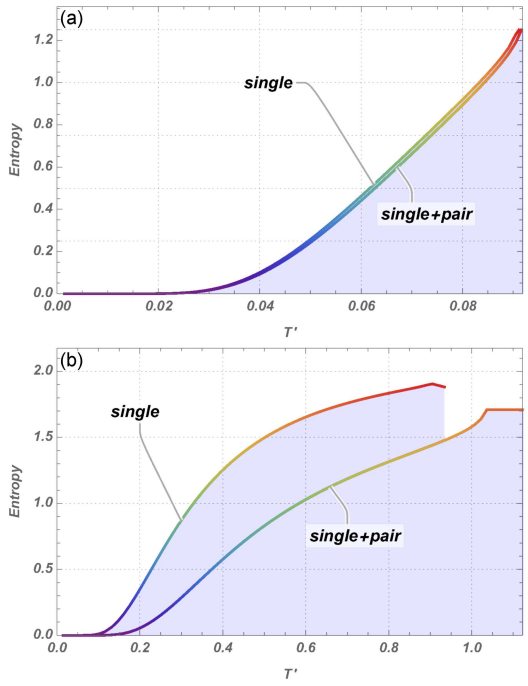

Fig. 2. Dependence of entropy on temperature on a simple cubic lattice in the single model (20) and in the single + pair model (11) for (a) $t/U = 0.015$; (b) $t/U = 0.085$.

4. Conclusions

The results shown in this work are obtained by a quantum rotor path integral analysis of the Bose–Hubbard model. The standard procedure is to obtain phase-only effective models, perform Gaussian integration, and series expansion of the result of this integration. We expand on this procedure by including higher-order terms in the effective action after the series expansion. We show that temperature-driven pair condensation is anticipated by one of the second-order terms in this model. This finite temperature pair condensation is driven by imaginary time dynamics.

In addition to generating pair condensation, bosonic pairing also strengthens the superfluid phase, which means it survives at higher temperatures.

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