Coexistence of two kinds of superfluidity in Bose-Hubbard model with density-induced tunneling at finite temperatures

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With use of the U(1) quantum rotor method in the path integral effective action formulation, we have confirmed the mathematical similarity of the phase Hamiltonian and of the extended Bose-Hubbard model with density-induced tunneling (DIT). Moreover, we have shown that the latter model can be mapped to a pseudospin Hamiltonian that exhibits two coexisting (single-particle and pair) superfluid phases. Phase separation of the two has also been confirmed, determining that there exists a range of coefficients in which only pair condensation, and not single-particle superfluidity, is present. The DIT part supports the coherence in the system at high densities and low temperatures, but also has dissipative effects independent of the system’s thermal properties.

I. INTRODUCTION

Optical lattices provide an excellent framework for studying many-body Hamiltonians, which are difficult to replicate in solids due to their complexity and lack of control over various parameters. The Hubbard model, which contains a quantum phase transition between two ground states: the superfluid state and the Mott insulator state, is a staple of the study of strongly correlated systems in low temperatures, and its various iterations have lately been under particular scrutiny in relation to optical lattices (as well as Josephson junction arrays in the bosonic case; see [2]). Our interest lies in bosonic systems, described by the Bose-Hubbard (BH) model and its extensions. The BH model can be obtained as an approximation of a general second quantization many-body Hamiltonian, describing a gas of interacting bosons in an external potential, by cutting off all but the two most important terms, i.e. the ones that contribute most to the total energy: the on-site two-particle interaction, $U$, and $t$, the single-particle tunneling between two nearest-neighboring sites. Extended BH models are obtained by adding one or more of the cut interactions to the pure BH model. Of course, this greatly increases the complexity of the model, making exact analysis difficult – and thus a comparatively lacking section of condensed matter physics. Of all these interactions, density-induced tunneling, known also as bond-charge interaction or correlated hopping, contributes most to a system’s energy and, and thus a comparatively lacking section of condensed matter physics. Of all these interactions, density-induced tunneling, known also as bond-charge interaction or correlated hopping, contributes most to a system’s energy and, has successfully been experimentally observed on optical lattices [10][11], making it the most interesting extension to work with.

In this work, we carry out a path integral analysis of the density-induced tunneling BH model, utilizing the U(1) quantum rotor method [13][14], which replaces bosonic field operators with interacting U(1) phase fields, leading to an effective action formulation of the system’s partition function. The methods used allow us to make an explicit analytical connection between this model and an extended Quantum Phase Model (QPM) Hamiltonian, which describes pair tunnelling in bosonic many-body systems [15][16], thus showing that this behavior is anticipated by the bosonic density-induced tunneling model, provided that many-body correlations are not excluded from its analysis.

This model contains three-body correlations, as seen in the density-induced tunneling term Eq. (4), which is a product of three bosonic field operators. Previous considerations of this model [7][9][17][19] made use of mean field approximations, which do not account for such correlations, as mean fields serve as replacements for any multi-linear interactions. Thus, while the influence of density-induced tunneling on the BH phase diagram, which describe the transitions between the two ground states of the BH model – Mott insulator and superfluid – which mean fields do retain, is well documented [20], the presence of bosonic pairing has thus far remained analytically unconfirmed at finite temperatures and beyond mean field level.

Furthermore, we map the newly-acquired phase Hamiltonian onto an $S = 1$ pseudospin model [21][22] and apply a mean field approximation (which at this point does not erase the correlations we wanted to preserve; the information has been absorbed into the coefficients and the properties of the phase Hamiltonian), allowing us to obtain phase diagrams via self-consistent critical line equations. These temperature-dependent diagrams show the critical lines between the normal phase and two others: the known single-particle superfluid phase and the previously unconfirmed for density-induced tunneling BH pair condensation at finite temperatures.

Here follows an outline of the contents of this publication. In Sec. II, the model Hamiltonian is defined. In Sec. III, we introduce the quantum rotor representation and derive an effective action for the model. This effective action corresponds to the phase Hamiltonian. Next, we map the obtained phase Hamiltonian onto $S = 1$ pseudospin, and calculate the critical line equations needed to analyze the thermodynamics of the system. Exemplary diagrams of order parameters and specific heat are shown and commented on in Sec. IV, followed by a summary in Sec. V.
II. MODEL HAMILTONIAN

The Hamiltonian for this model consists of two parts:
\[ \mathcal{H} = \mathcal{H}_{BH} + \mathcal{H}_{DIT}, \]
where
\[ \mathcal{H}_{BH} = \frac{U}{2} \sum_{i} n_i (n_i - 1) - \sum_{\langle i, j \rangle} t_{ij} a_i^\dagger a_j - \mu \sum_{i} n_i \]

is the pure Bose-Hubbard model Hamiltonian, with \( a_i^\dagger \), \( a_i \) being the bosonic creation and annihilation operators respectively, obeying the canonical commutation relation \([a_i, a_j^\dagger] = \delta_{ij}\), and \( n_i = a_i^\dagger a_i \) being the boson number operator on site \( i \). Further, \( U > 0 \) is the on-site repulsion, \( \mu \) the chemical potential, \( \langle i, j \rangle \) identifies a summation over nearest neighbor sites, and \( t_{ij} \) is the hopping integral, the dispersion of which on a bipartite lattice in \( d \) dimensions is
\[ t(k) = 2t \sum_{l=1}^{d} \cos k_l. \]

This work focuses on the properties of the BH model with density-induced tunneling on a simple cubic lattice. We also assume that hopping is isotropic, \( t_{ij} = t \). The density-induced tunneling (DIT) term is
\[ \mathcal{H}_{DIT} = -T \sum_{\langle i, j \rangle} \left[ a_i^\dagger (n_i + n_j) a_j + a_j^\dagger (n_i + n_j) a_i \right], \]
with density-induced tunneling amplitude \( T \). The full Hamiltonian can be rewritten in a pure BH-like form:
\[ \mathcal{H} = \frac{U}{2} \sum_{i} n_i^2 - J \sum_{\langle i, j \rangle} a_i^\dagger a_j - \mu \tilde{\mu} n_i, \]
with the coefficients
\[ J = t - 2T, \]
\[ \tilde{\mu}_{ij} = \bar{\mu} + 4T a_i^\dagger a_j, \]
\[ \bar{\mu} = \frac{U}{2} + \mu - 2T. \]

It is worth mentioning that the shifted chemical potential \( \tilde{\mu}_{ij} \) is now an operator, due to the presence of the density-induced tunneling amplitude \( T \).

III. METHOD

A. Quantum rotor approximation

Using the quantum rotor method [13], we will rewrite the model as phase-only, and then carry out transformation to a pseudospin model, much as in [21].

1. Hubbard-Stratonovich and gauge transformations

The path integral formulation of the partition function is
\[ Z = \int [\mathcal{D}a][\mathcal{D}a^\dagger] e^{-S[a,a^\dagger]}, \]
where \( S \) is the effective action,
\[ S = \sum_{i} \int_{0}^{\beta} d\tau \bar{a}_i(\tau) \frac{\partial}{\partial \tau} a_i(\tau) + \int_{0}^{\beta} d\tau H(\tau). \]

The bosonic field operators \( a_i^\dagger, a_i \) are now represented by complex fields \( a_i(\tau) \) and \( \bar{a}_i(\tau) = H[\bar{a}(\tau), a(\tau)] \) is our Hamiltonian (Eq. [4]). Our first step is decoupling the bilinear term in \( H \) by a Hubbard-Stratonovich transformation, introducing the auxiliary fields \( V_i(\tau) \):
\[ e^{-\frac{1}{2} \mu \sum_{\langle i, j \rangle} \int_{0}^{\beta} d\tau n_i^2(\tau)} = \int \frac{dV}{2\pi} e^{-\frac{1}{2} \int_{0}^{\beta} d\tau \left( V_i(\tau)^2 - iV_i(\tau)n_i(\tau) \right)}, \]
which allows us to split the effective action (Eq. [9]) into two terms, one of which is independent of the fields \( a_i(\tau) \):
\[ Z = \int [\mathcal{D}a][\mathcal{D}a^\dagger] e^{-S_1[a,a^\dagger]} \int \frac{dV}{2\pi} e^{-S_2[n,V]}, \]
\[ S_1 = \int_{0}^{\beta} d\tau \left[ \sum_{i} \bar{a}_i(\tau) \frac{\partial}{\partial \tau} a_i(\tau) - J \sum_{\langle i, j \rangle} \bar{a}_i(\tau) a_j(\tau) \right], \]
\[ S_2 = \sum_{i} \int_{0}^{\beta} d\tau \left[ \frac{1}{2U} V_i^2(\tau) - (iV_i(\tau) + \bar{\mu}) n_i(\tau) \right]. \]

Next, we shift the electrochemical potential \( V_i(\tau) = V_i^T(\tau) - \frac{\bar{\mu}}{2} \), getting
\[ S_2 = \sum_{i} \int_{0}^{\beta} d\tau \left[ \frac{1}{2U} \left( V_i^T(\tau) \right)^2 - \frac{1}{2U} \bar{\mu}^2 + \right. \]
\[ - \left. \frac{V_i^T(\tau) \bar{\mu}}{iU} - iV_i^T(\tau) n_i(\tau) \right]. \]

\( V_i^T \) is further split into static and periodic parts,
\[ V_i^T(\tau) = V_i^S(\tau) + V_i^P(\tau), \]
which are defined as follows:
\[ V_i^S(\tau) = \frac{1}{\beta} V_i^T(\omega_m = 0), \]
\[ V_i^P(\tau) = \frac{1}{\beta} \sum_{m=1}^{+\infty} (V_i^T(\omega_m) e^{i\omega_m \tau} + c.c.), \]
where $\omega_m = 2\pi m/\beta$ for integer values of $m$ are the bosonic Matsubara frequencies. We then bind the periodic part of the field $V_i^P(\tau)$ from Eq. (18) to a $U(1)$ phase field $\phi(\tau)$ via Josephson coupling:

$$V_i^P(\tau) = \dot{\phi}_i(\tau),$$

noting that $\phi(\tau)$ is also periodic:

$$\phi_i(\beta) = \phi_i(0).$$

The partition function in Eq. (12) is now split into three terms:

$$Z = \int [D\phi] e^{-S_1[\phi,\phi]} \int dV \int \beta e^{-S_3[n,V]} \int D\phi e^{-S_1[n,\phi]},$$

where $S_1$ remains unchanged as in Eq. (13) and

$$S_2 = \beta \sum_i \left[ \frac{1}{2U} (V_i^S)^2 + \int_0^\beta d\tau \left( \frac{-\tilde{\mu}^2}{2U} - \frac{i\mu}{2U} \left( \sum_j g_{ij} \dot{b}_j(\tau) + \sum_{j', j''} g_{jj'} \dot{b}_j(\tau) \dot{b}_{j'}(\tau) \right) \right) \right],$$

$$S_3 = \sum_i \int_0^\beta d\tau \left[ \frac{1}{2U} (\dot{\phi}_i(\tau))^2 - \frac{\tilde{\mu}}{iU} \dot{\phi}_i(\tau) \right].$$

The next step is a local gauge transformation:

$$a_i(\tau) = e^{i\phi_i(\tau)} b_i(\tau),$$

$$\tilde{a}_i(\tau) = e^{-i\phi_i(\tau)} \tilde{b}_i(\tau),$$

which must also be applied to the chemical potential, as defined in Eq. (7). This transformation, combined with the parametrization $b_i(\tau) = \tilde{b}_i(\tilde{\tau})$ we carry out later on, reduces $S_2$ entirely to a constant, so it can be ignored in the path integral formulation. This leaves us with

$$Z = \int [Db] \int D\phi e^{-S_1[\tilde{b},\tilde{b}]} e^{-S_3[n,\phi]},$$

the effective action terms now being

$$S_1 = \int_0^\beta d\tau \sum_{\langle i,j \rangle} \left[ \tilde{b}_i(\tau) \left( \frac{1}{2U} \sum_{j'} g_{ij} \dot{b}_j(\tau) \dot{\phi}_{j'}(\tau) + \sum_{j''} g_{jj'} \dot{b}_j(\tau) \dot{b}_{j'}(\tau) \right) \right],$$

$$S_3 = \sum_i \int_0^\beta d\tau \left[ \frac{1}{2U} (\dot{\phi}_i(\tau))^2 - \frac{\tilde{\mu}}{iU} \dot{\phi}_i(\tau) \right],$$

where

$$g_{ij} = \delta_{ij} \frac{\partial}{\partial \tau} - J e^{-i\phi_{ij}(\tau)} - \frac{4\beta\tilde{\mu}}{U} T e^{-i\phi_{ij}(\tau)},$$

$$g_{ij}^2 = \frac{8\beta}{U} T^2 e^{-2i\phi_{ij}(\tau)}.$$

Here we have denoted $\phi_{ij}(\tau) = \phi_i(\tau) - \phi_j(\tau)$. The similarity to an extended Quantum Phase Model (QPM) Hamiltonian can already be seen at this point in the presence of both $e^{-i\phi_{ij}(\tau)}$ and $e^{-i2\phi_{ij}(\tau)}$ dependent terms, which correspond to cosine and double cosine parts of the action. The cosine expression can be found in the QPM and describes the superfluid phase. The double cosine term, then, must correspond to condensation of bosonic pairs. Therefore we can clearly see from Eq. (30) the impact of the additional term Eq. (4) on the original bosonic system. Due to $J$ having been defined as $J = t - 2T$, our cosine term contains two parts dependent on $T$:

$$+ 2T e^{-i\phi_{ij}(\tau)} - \frac{4\beta\tilde{\mu}}{U} T e^{-i\phi_{ij}(\tau)}.$$

The first part reduces the bosonic condensation with an amplitude $2T$, irrespectively of the temperature and densities. The second term competes with the first, strengthening the superfluid phase in regions of higher densities and low temperatures. This can come as a surprise in comparison with the effective model some naively assume, which consists of two independent parts:

$$H = J_1 \sum_{\langle i,j \rangle} \cos(\phi_{ij}) + J_2 \sum_{\langle i,j \rangle} \cos(2\phi_{ij}).$$

To maintain physical clearness and integrity, the coefficients in this model cannot be assumed and must be rigorously derived. As it turns out, $J_1$ and $J_2$ are not constant and might also be temperature dependent, as we show later.

Furthermore we notice also the pair condensation term, which can lead to pair condensation. Its dependence is proportional to $\sim T^2$, rather than a linear dependence, as that of $\sim t$ in the cosine term.

To sum this part up, we emphasize that apart from pair condensation, we distinguish two contrasting effects on the superfluid phase that stem from the density induced term. In the whole range of temperatures the DIT tends to have a dissipative influence on the original bosonic system, but the situation can be different for higher densities and low temperatures, where it works in favor of the superfluid phase. Up to now, all calculations have been exact and the phenomena we analyze stem from the density induced term. The assumptions made in order to obtain the phase diagram we discuss in the next paragraph.

2. Matrix form of effective action

Before we go further with calculations, we must concentrate on the regions we are interested in and physical phenomena we would like to describe. We do not focus on the lob-like phase diagram, which has already been established in the mean field approximation and which would have to be calculated in a different way. Instead,
we would like to explore the specific heat (CH) of the system and ask the question whether a second $\lambda$-like peak appears therein that would provide clear proof of a second phase transition: in our case, the condensation of bosonic pairs. Because the CH measures energy fluctuations, it provides useful information about the system we analyze. From now on, we make the necessary assumptions and explain what information might be lost due to those assumptions.

The next step in order to achieve a phase-only model is getting rid of $b_i$ by carrying out the following integral:

$$\int [DB_i DB_j] e^{-S_1[b,b]} .$$

(33)

For this to be possible, $S_1$ in Eq. (27) must be quadratic in bosonic field variables. The quadruple term is split using a Wick average:

$$\sum_{(i,j)} b_i^\dagger b_j^\dagger b_j^\prime b_j^\prime \approx \sum_{(i,j)} \left[ \langle b_i b_j \rangle b_i^\dagger b_j^\prime + \langle b_j^\prime b_j \rangle b_j^\dagger b_j + \langle 4 \langle b_j b_j^\prime \rangle + \delta_{ij} \rangle b_i^\dagger b_j \right] ,$$

(34)

which in our case gives

$$S_1 = \int_0^\beta d\tau \left[ \sum_{(i,j)} \tilde{b}_i (\tau) g_{ij}^1 b_j (\tau) + \sum_{(i,j)} g_{ij}^2 \left( \langle b_j b_j^\prime \rangle \tilde{b}_i^\dagger \tilde{b}_i + \langle \tilde{b}_i^\dagger \tilde{b}_i \rangle b_j b_j^\prime \right) \right] ,$$

(35)

where

$$g_{ij}^1 = \delta_{ij} \frac{\partial}{\partial \tau} - J e^{-i\phi_{ij}(\tau)} - \frac{4\mu}{U} T e^{-i\phi_{ij}(\tau)} + - \frac{8}{U} T^2 e^{-i2\phi_{ij}(\tau)} \cdot (4 \langle b_j b_j^\prime \rangle + \delta_{ij}) ,$$

(36)

and $g_{ij}^2$ remains unchanged as in Eq. (30). This part is rather formal; nonlocal interactions are excluded in the process. We rewrite $S_1$ in matrix form, expanding the usual one- or two-dimensional description of the Bose Hubbard model by introducing a four-dimensional Nambu-like space:

$$S_1 = \bar{B} \Gamma B ,$$

(37)

where the vectors consist of bosonic fields,

$$\bar{B} = ( \tilde{b}_i \ b_j \ \tilde{b}_j \ b_j ) ,$$

(38)

$$B = \begin{pmatrix} b_i \\ \tilde{b}_i \\ b_j \\ \tilde{b}_j \end{pmatrix} ,$$

(39)

and the matrix itself takes the form

$$\Gamma = \begin{pmatrix} 0 & \frac{1}{2} \delta_{ij} \Delta_i & \frac{1}{2}S_{ij} & 0 \\ \frac{1}{2} \delta_{ij} \Delta_i & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \delta_{ij} \Delta_i \\ \frac{1}{2}S_{ij} & 0 & \frac{1}{2} \delta_{ij} \Delta_i & 0 \end{pmatrix} ,$$

(40)

with

$$S_{ij} = \delta_{ij} \frac{\partial}{\partial \tau} - J e^{-i\phi_{ij}(\tau)} - \frac{4\mu}{U} T e^{-i\phi_{ij}(\tau)} + - \frac{8}{U} T^2 e^{-i2\phi_{ij}(\tau)} \cdot (4 \langle b_j b_j^\prime \rangle + \delta_{ij}) ,$$

(41)

$$\Delta_i = \frac{8}{U} T^2 e^{-i2\phi_{ij}(\tau)} \langle b_i b_i \rangle ,$$

(42)

$$\Delta_i = \frac{8}{U} T^2 e^{-i2\phi_{ij}(\tau)} \langle \tilde{b}_i \tilde{b}_i \rangle .$$

(43)

After analytically diagonalizing $\Gamma$, the non-phase field dependent part of the partition function, Eq. (33), is now a Gaussian integral,

$$\int [DB_i DB_i DB_j DB_j] e^{-\int_0^\beta d\tau' B \Gamma' B} = \det \Gamma' = e^{Tr \ln \Gamma'^{-1}} ,$$

(44)

where $\Gamma'$ is the diagonalised matrix,

$$\Gamma' = \begin{pmatrix} -\lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_1 & 0 & 0 \\ 0 & 0 & -\lambda_2 & 0 \\ 0 & 0 & 0 & \lambda_2 \end{pmatrix} ,$$

(45)

with eigenvalues

$$\lambda_1 = \frac{1}{2} \sqrt{\Delta_i \Delta_i - S_{ij} \sqrt{\Delta_i \Delta_i}} ,$$

(46)

$$\lambda_2 = \frac{1}{2} \sqrt{\Delta_i \Delta_i + S_{ij} \sqrt{\Delta_i \Delta_i}} .$$

(47)

The entire partition function from Eq. (26) can be written in the form

$$Z = \int D\phi e^{-\sum f_{ij}^3 d\tau \left[ \sqrt{\phi_{ij}(\tau)^2 - \dot{\phi}_{ij}(\tau)} \right] } e^{Tr \ln \Gamma' } .$$

(48)

We approximate, as usual, the trace of $\Gamma'$, to have quadratic terms in the action only

$$Tr \ln \Gamma' \approx \ln (\Delta_i \Delta_i - S_{ij}^2) \approx \ln (G_{0}^{-1})^2 + G_{0}^2 \left[ \Delta_i \Delta_i - (S_{ij})^2 \right] + 2S_{ij} G_0 ,$$

(49)

where now

$$S_{ij}' = - Je^{-i\phi_{ij}(\tau)} + \frac{4\mu}{U} T e^{-i\phi_{ij}(\tau)} + + \frac{8}{U} T^2 e^{-i2\phi_{ij}(\tau)} \cdot (4 \langle \tilde{b}_j b_j^\prime \rangle + \delta_{ij}) .$$

(50)

We parametrize the boson fields, $b_i (\tau) = b_{ij} + b_{ij}' (\tau)$, assuming any fluctuations are contained in the phase and
fixing the amplitude at a constant value. This approach can be very successful when the dynamics of a system depend both on the amplitude and phase. The coherence of the latter provides the phase transition between ordered (superfluid) and disordered (normal insulator) phase. Thus, \( G_0 = \frac{b_0^2}{2} \) can be calculated by minimizing the Hamiltonian, \( \partial H (b_0) / \partial b_0 = 0 \), giving

\[
b_0^2 = \frac{z (t - 4T) + \left( \frac{U}{2} + \mu \right)}{U - 8zT},
\]

which finally brings us to the final form of the Hamiltonian,

\[
\langle \bar{b}_i \bar{b}_j \rangle = b_0^2 \langle \bar{b}_0^2 \rangle = b_0^4 \Psi_{2\phi},
\]

where \( \psi_{2\phi} = \langle e^{i2\phi_i} \rangle = \langle e^{-i2\phi_i} \rangle \) is the pair condensation order parameter, in which we neglect the chirality of the phase. The average \( \langle \bar{b}_i b_j \rangle \) is equal to

\[
\langle \bar{b}_i b_j \rangle = b_0^2 \langle e^{i[\phi_i(\tau) - \phi_j(\tau)']} \rangle = b_0^2 G_{ij} (\tau, \tau'),
\]

where

\[
G_{ij} (\tau, \tau') = \delta_{ij} e^{\frac{i\gamma_{ij}}{2} (\tau - \tau')} \cdot \gamma_{ij} (\tau, \tau')
\]

is the Green’s function [13], with

\[
\gamma_{ij} (\tau, \tau') = \frac{\sum_i \exp \left[ -\frac{U}{2} \left( n_i + \frac{\mu}{2} \right) \right]}{\sum_i \exp \left[ -\frac{U}{2} \left( n_i + \frac{\mu}{2} \right) \right]} \left( n_i + \frac{\mu}{2} \right),
\]

\[
\approx \frac{\coth \left( \frac{\mu}{2} \right) + \coth \left( \frac{U}{2} + \frac{\mu}{2} \right)}{2}.
\]

After these operations, the final form of the partition function, barring constant terms and (as a second-order approximation) quadrupolar phase exponent terms, is

\[
\mathcal{Z} = \int D\phi \left[ e^{-\sum_i \int_0^\beta d\tau \left( \frac{1}{2} \partial^2 \phi_i(\tau) - \frac{\partial}{\partial \phi_i(\tau)} \right)} \times e^{\sum_{\langle i,j \rangle} \int_0^\beta d\tau \left( \epsilon_1 e^{-i2\phi_{ij}(\tau)} + \epsilon_2 e^{i\phi_{ij}(\tau)} \right)} \right],
\]

where

\[
\epsilon_1 = \left[ \frac{z (t - 4T) + \bar{\mu}}{U - 8zT} \right]^2 \frac{64\bar{\mu} T^3 - 16 (t - 2T) T^2}{U^2}
\]

\[
\times \left\{ 2 \left[ \coth \beta \mu + \coth \beta (\mu + U) \right] + 1 \right\} + \frac{z (t - 4T) + \bar{\mu}}{U - 8zT} \left[ \frac{8\bar{\mu}}{U} T - 2 (t - 2T) \right],
\]

\[
\epsilon_2 = \left[ \frac{z (t - 4T) + \bar{\mu}}{U - 8zT} \right]^2 \times \left[ (t - 2T)^2 + \left( \frac{4\bar{\mu}}{U} T \right)^2 - 2 (t - 2T) \frac{8\bar{\mu}}{U} T \right].
\]

We see clearly now that the already mentioned naive past assumptions about constant values of the amplitudes in this phase model have no justification in reality. The coefficients \( \epsilon_1 \) and \( \epsilon_2 \) have complex structures, even though we dropped the lattice dependence, leaving in only the coordination number \( z \). We also note that \( \epsilon_2 \), which comes from the DIT term, is temperature dependent.

**B. Transformation to \( S = 1 \) pseudospin**

Assuming the on-site two-particle interaction is strong, which is a reasonable condition for this model, we can ignore the complex term in Eq. [59], getting

\[
\mathcal{Z} = \int D\phi \left\{ e^{-\int_0^\beta d\tau \sum_i \frac{\partial}{\partial \phi_i(\tau)} \left( \phi_i(\tau) \right)^2} \times e^{-\int_0^\beta d\tau \left[ -\sum_{\langle i,j \rangle} \left( \epsilon_2 e^{-i2\phi_{ij}(\tau') + \epsilon_1 e^{i\phi_{ij}(\tau')}} \right) \right]} \right\}.
\]

This simplification excludes the accurate description of the properties of the system with chemical potential variation. The partition function corresponds to the following phase hamiltonian:

\[
\hat{H} = -4U \sum_i \left( \frac{1}{i \partial \phi_i} \right)^2 - \sum_{\langle i,j \rangle} \epsilon_1 \cos \left( \phi_i - \phi_j \right) + \sum_{\langle i,j \rangle} \epsilon_2 \cos \left[ \frac{1}{2} \left( \phi_i - \phi_j \right) \right],
\]

The two interaction terms give rise to two different ordered phases, represented by two order parameters:

\[
\Psi_{\phi} \equiv \langle e^{i\phi} \rangle,
\]

\[
\Psi_{2\phi} \equiv \langle e^{i2\phi} \rangle.
\]

\( \Psi_{\phi} \) is the superfluid order parameter, known from the pure BH model; \( \Psi_{2\phi} \) corresponds to the phenomenon of bosonic pair tunneling.
1. Pure Bose-Hubbard mapping

The matrix elements of the phase operator in its own basis are
\[
\langle k | N(\phi) | m \rangle = \int_{0}^{2\pi} \frac{d\phi}{2\pi} e^{-ik\phi} \left( \frac{1}{i} \frac{\partial}{\partial \phi} \right) e^{im\phi} = m \delta_{k,m}. \tag{69}
\]

The other operators needed can be derived from Eq. [22], giving
\[
\langle k | \cos \phi | m \rangle = \int_{0}^{2\pi} \frac{d\phi}{2\pi} e^{-i(k-m)\phi} \cos \phi = \frac{1}{2} \left( \delta_{k-m-1,0} + \delta_{k-m+1,0} \right), \tag{70}
\]
\[
\langle k | \sin \phi | m \rangle = \frac{i}{2} \left( \delta_{k-m-1,0} - \delta_{k-m+1,0} \right). \tag{71}
\]

For spin $S = 1$, $k$, $m$ are limited to the lowest-energy states: $-1, 0, 1$. We have assumed that $U \rightarrow \infty$, which in particular means that $k_B T / U$ is small, and
\[
N(\phi) = S_\phi, \tag{72}
\]
\[
\cos \phi = \frac{1}{\sqrt{2}} S_x, \tag{73}
\]
\[
\sin \phi = \frac{1}{\sqrt{2}} S_y. \tag{74}
\]

First, we only transform the first two terms of the Hamiltonian to:
\[
\mathcal{H} = U \sum_i N_i^2 - \sum_{\langle i,j \rangle} \varepsilon_j \cos (\phi_i - \phi_j) = U \sum_i \langle S_i^x \rangle^2 - \frac{1}{2} \sum_{\langle i,j \rangle} \langle S_i^x S_j^x + S_i^y S_j^y \rangle. \tag{75}
\]

If $T = 0$, we have at this point a model analogous to the pure BH model, as well as to the QPM Hamiltonian. Applying a mean field approximation: $\langle S_i^\mu \rangle = 0$;
\[
S_i^x S_j^x \approx \langle S_i^x \rangle \langle S_j^x \rangle + \langle S_i^y \rangle \langle S_j^y \rangle - \langle S_i^x \rangle \langle S_j^y \rangle, \tag{76}
\]
we arrive at the following Hamiltonian:
\[
\mathcal{H} = U \langle S_i^x \rangle^2 - \frac{1}{2} \varepsilon_i \langle S_i^x \rangle^2 = J \left[ U \langle S_i^x \rangle^2 - \langle S_i^x \rangle \langle S_i^\phi \rangle \right], \tag{77}
\]
where $J = \frac{1}{2} \varepsilon_i$ and $\Psi_\phi$ is the superfluid order parameter.

2. Adding the double interaction

We define the bilinear superexchange terms:
\[
Q_i = \langle S_i^x \rangle^2 - \langle S_i^\mu \rangle^2, \tag{78}
\]
\[
Q_i^{xy} = 2 S_i^y S_i^\mu, \tag{79}
\]
and perform a mean field approximation
\[
\langle Q_i \rangle = Q_i + \langle Q_i \rangle - \langle Q_i \rangle \tag{80}
\]
Assuming $\langle Q_i \rangle = 0$, the full mean field pseudospin Hamiltonian is
\[
\mathcal{H} = U \langle S_i^x \rangle^2 - \frac{1}{2} \varepsilon_i \langle S_i^x \rangle^2 - \frac{1}{4} \delta_x^2 (\langle Q_i \rangle^2) = J \left[ \frac{U}{J} \langle S_i^x \rangle^2 - \langle S_i^x \rangle \langle S_i^\phi \rangle - \frac{J_2}{J} \langle Q_i \rangle \langle Q_i \rangle \right], \tag{81}
\]
where
\[
J = \frac{1}{2} \varepsilon_1, \quad \tag{82}
\]
\[
J_2 = \frac{1}{4} \varepsilon_2. \quad \tag{83}
\]

We define the system’s free energy per site as [21]
\[
f = \frac{1}{2} \left( J \Psi_\phi^2 + J_2 \Psi_{2\phi}^2 \right) - \frac{1}{\beta} \ln Z. \tag{84}
\]

The two order parameters, Eq. [67] and Eq. [68] then minimize the free energy, and their values can be calculated from the following self-consistent equations:
\[
\frac{\partial f}{\partial \Psi_\phi} = 0, \quad \frac{\partial f}{\partial \Psi_{2\phi}} = 0, \tag{85}
\]
which in this case are
\[
1 = \frac{4J \tanh \frac{\beta/2}{\sqrt{(U - J_2 \Psi_{2\phi})^2 + 4J^2 \Psi_{2\phi}^2}}}{\sqrt{(U - J_2 \Psi_{2\phi})^2 + 4J^2 \Psi_{2\phi}^2}} \left[ X + 2 \right], \tag{86}
\]
\[
\Psi_{2\phi} = \frac{U}{J_2 - 4J} + \frac{4J}{4J - J_2} \frac{1}{2 + X}, \tag{87}
\]
where
\[
X = \frac{e^{-\beta \frac{U + 3J_2 \Psi_{2\phi}}{U - J_2 \Psi_{2\phi}}}}{\cosh \left( \frac{\beta/2}{\sqrt{(U - J_2 \Psi_{2\phi})^2 + 4J^2 \Psi_{2\phi}^2}} \right)} \tag{88}
\]

The critical line equations in Eqs. [86] and [87] allow us to obtain phase diagrams for any chosen parameters of the on-site interaction $U$, the chemical potential $\mu$, the temperature $T_C$ (so labelled to avoid confusion with the density-induced tunneling parameter), the pure BH hopping $t$ and the density-induced tunneling amplitude $T$.

IV. RESULTS

Below are some exemplary diagrams obtained with use of Eqs. [86] and [87]. First of all, Fig. [ ] shows the
dependence of the single and pair order parameters on the normalized temperature $T/T_{C_1}$. The normalization is taken as $T_{C_1}$, which is the critical temperature connected to the single bosonic condensation phase transition, which separates the single $\Psi$ and pair $\Psi_{2\phi}$ superfluid phase. We have chosen parameter values for which phase separation can be clearly seen. This is the most interesting observation we have made so far: not only are there two separate, coexisting superfluid phases in this model; pair condensation also occurs independently of single-particle condensation. We can also see that even though a mean field approximation was used in the later stages of pseudospin mapping, the system retained enough information that we were able to expose phenomena that eluded mean-field-only-based approaches. Interestingly, the pair condensation survives at higher temperatures than single bosonic condensation, even as we change the density of the particles and the energy scales. In the range of parameters where $t/T < 1$ (pair energy scales are higher) we see that the single particle condensation is almost suppressed and energy fluctuations are enormous, but pretty narrow in the temperature range. This is contrary to the opposite case, when $t/T > 1$, where one can see a strong single superfluid phase and a well established and separated pair condensed fraction. We note that there is no region with only $\Psi \neq 0$ and the phase transitions are lambda-like, already observed experimentally.

Although normalization was taken to clarify the amplitude of the energy calculations, we now move forward without it to observe the actual temperature dependence of the thermodynamic function Fig. [2]. What occurs is an interesting phenomenon. Although higher values of DIT energy give rise to higher critical temperatures of the single condensation $T_{C_1}$, it simultaneously suppresses the superfluid phase, providing a strong response in the pair sector. On the other hand, in the opposite regime, the pair superfluid phase ceases to exist, providing support for the pure BH model superfluidity with an increase in value of the critical temperature $T_{C_1}/U$. If we take the value of the DIT equal $T/U = 0.009$, the critical temperature $T_{C_1}$ of the single particle condensation becomes approximately seven times larger; for $T/U = 0.003$, it is almost twice as large.
Figure 2. Upper diagram: comparison of the specific heat versus temperature dependence for the opposite choice of the single and pair energy scales $t/U > 1$ left peaks and $T/t < 1$ - right respectively. Bottom diagram: impact of the density induced therm on single boson condensation $T_C^s$ for the choice parameter from left plot ($\mu/U = 1.42$).

V. SUMMARY

In this work we have presented an analytical study of the density-induced tunneling Bose-Hubbard model. We utilized methods known for their high accuracy in order to receive a fuller picture than mean field theory could provide, considering the model within a path integral formulation of quantum mechanics and applying the U(1) quantum rotor method. Those methods allowed us to rewrite the effective action, and, by extension, the Hamiltonian, as phase-only, to map it onto a $S = 1$ pseudospin model and from that obtain critical line equations.

Thanks to the quantum rotor method, which has proved its accuracy in other systems, and especially its preservation of multi-particle correlations, we have managed to shed light on the existence of a previously unconfirmed pair superfluid phase at finite temperatures in the density-induced tunneling BH model. What’s more, we have shown that, for certain parameter values, this phase occurs exclusively where single-particle condensation does not. Despite the complications caused by DIT, we managed to obtain the specific heat and observe regions where energy fluctuations are highest and (in accordance with order parameters) accurately point out the phase transitions. These phases we recognized as the usual Bose condensation and an additional, previously unaccounted for, bosonic pair condensation at finite temperatures. We conclude from our analysis that there are different ways in which DIT impacts the pure BH system. For large values of the density-induced amplitude, the critical temperature of single particle condensation is higher and the specific heat has a sharp peak (well known lambda behavior). For lower values of the tunneling amplitude (ie. less than the tunneling amplitude for pure BH), the peak in the thermodynamic function is broader. Of course, the results shown in this work call for experimental confirmation, but, once confirmed, could potentially introduce a new branch of thought in optical lattice-related research.

The analytical framework established in this paper can serve as a foundation for the analysis of any number of properties of the density-induced tunneling BH model, as well as its modifications, such as external magnetic fields, particle mixtures or various lattice geometries beyond the simple cubic lattice here considered. We plan to make use of this framework in future research.

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