Bose–Einstein condensation in a minimal inhomogeneous system

C Gaul1,2,3 and J Schiefele1

1 Departamento de Física de Materiales, Universidad Complutense, E-28040 Madrid, Spain
2 CEI Campus Moncloa, UCM-UPM, E-28040 Madrid, Spain
3 Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany

E-mail: cgaul@pks.mpg.de and jurgesch@ucm.es

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Abstract
We study the effects of repulsive interaction and disorder on bosons in a two-site Bose–Hubbard system, which provides a simple model of the dirty boson problem. By comparison with exact numerical results, we demonstrate how a straightforward application of the Bogoliubov approximation fails even to deliver a qualitatively correct picture. It wrongly predicts an increase of the condensate depletion due to disorder. We show that, in the presence of disorder, the noncommutative character of the condensate operator has to be retained for a correct description of the system. While these corrections to a simple meanfield Bogoliubov theory are usually small in extended systems, we show that care has to be taken when modeling small inhomogeneous Bose systems.

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(Some figures may appear in colour only in the online journal)

1. Introduction
The interplay of disorder and interaction in bosonic systems, known as the dirty boson problem [1], is responsible for the superfluid–insulator transition observed in many condensed-matter systems, like superfluid helium adsorbed on porous media [2, 3], high-$T_c$ superconductors [4], and light propagating in disordered media [5]. While disorder, giving rise to Anderson localization [6], can destroy the superfluid condensate and take the system to a Bose-glass phase [7, 8], weak repulsive interactions have instead a delocalizing effect. This competition has recently been studied experimentally with Bose gases of cold atoms in optical lattice potentials, where both the strength of interaction and disorder can be controlled experimentally [9, 10].
The aim of the present work is to study a minimal model of interacting bosons in a system of only two lattice sites, described by a Bose–Hubbard model (also known as Josephson junction or Lipkin–Meshkov–Glick model [11–13]) with the Hamiltonian

$$\hat{H} = -J(\hat{a}_{1}^{\dagger}\hat{a}_{2} + \hat{a}_{2}^{\dagger}\hat{a}_{1}) + \Delta(\hat{n}_1 - \hat{n}_2) + \frac{U}{2}(\hat{n}_1^2 + \hat{n}_2^2),$$

(1)

see figure 1. Here, $\hat{a}_j$ denotes bosonic operators, $\hat{n}_j = \hat{a}_j^{\dagger}\hat{a}_j$, and the parameters $J$, $U$, and $\Delta$ are hopping amplitude, on-site interaction, and tilt (or energy mismatch between the sites), respectively. In our toy model of the dirty boson problem, the tilt $\Delta$ represents an inhomogeneity or disorder [14]. Apart from being a prototype of disorder, Bose–Einstein condensates in double-well potentials are subject of current experimental investigation [15, 16], featuring interesting effects like self trapping and squeezing.

In the following, we seek to obtain more insight in the intricacies of the Bogoliubov approximation in inhomogeneous systems [17–25]. The Bogoliubov approximation is an efficient method for the perturbative treatment of weakly interacting Bose condensates; it brings the Hamiltonian to a form quadratic in quasi-particle operators [17]. These describe quantum fluctuations on top of the macroscopically occupied condensate mode. The Bogoliubov excitations can be associated with the Goldstone mode of the system due to spontaneously broken $U(1)$ symmetry [26]. The Bogoliubov approximation is valid for systems that approach a thermodynamic limit such that both the particle number and the volume of the system tend to infinity, while the ratio of the two remains a finite constant. If the volume of the system is constrained [27], additional finite-size effects play a role [28]. We show below that for our model with only two lattice sites, a naive application of the Bogoliubov approximation even fails to deliver a qualitative description of the system in the presence of disorder. Instead, we need to re-introduce the quantum character of the condensate mode to construct the $N$-particle wavefunction of the interacting groundstate. In this way, we obtain results that agree with the exact diagonalization of Hamiltonian (1) in the limit of large particle number. In contrast to extended disordered systems [23, 29], we find that the tilt $\Delta$ counteracts the depletion of the condensate due to interaction. This behavior only appears in small systems, and to put our findings into context, we provide and discuss some data on finite inhomogeneous systems with more than two sites in section 3.4.

2. Exact diagonalization

We work with a fixed particle number $N$. Then, the Hilbert space of (1) is $N + 1$-dimensional: $l$ particles on site 1 and $N - l$ particles on site 2, where $l$ runs from 0 to $N$. Numerically, it is
Figure 2. Coefficients \( c_l \) of the many-body wave function \( \langle 0 | = \sum c_l | l \rangle \) in the Fock basis for \( \Delta = 0, N = 7 \). \( |c_l|^2 \) gives the probability to find \( l \) particles on site 1. The gray diamonds connected by a dashed line show the noninteracting case of a pure condensate, where \( |c_l|^2 \propto \binom{N}{l} \), which coincides with the exact-diagonalization results and the analytic results from (22) in absence of interaction. Blue crosses and red dots show the exact numerical and the analytic results for \( UN/J = 2 \), respectively (symbols slightly displaced horizontally).

Figure 3. Number of non condensed particles \( \delta N \) as a function of the total particle number \( N \) for different values of \( UN/J \) and \( \Delta \). Blue crosses show results from the exact diagonalization. For large \( N \) these points converge to the analytical result given in (23) (dashed red lines).

It is straightforward to diagonalize the matrix \( H_{ll'} = \langle l | \hat{H} | l' \rangle \). Throughout this work, we consider zero temperature, so we take the eigenvector with the lowest energy and compute the one-body density matrix

\[
\rho_{ij} = \langle \hat{a}_i^\dagger \hat{a}_j \rangle.
\] (2)

According to Penrose and Onsager [30], the condensate mode is identified as the eigenstate of \( \rho \) with the largest eigenvalue \( N_0 \), and that eigenvalue is the population of the condensate. Conversely, the depletion of the condensate \( \delta N \) is the sum of all other eigenvalues. In the present case of only two sites, there is only the condensate and one other mode. Examples of the \( N \)-particle ground-state wavefunction are shown in figure 2, results for the depletion in figures 3 and 4.
3. Approximate analytical solution

At temperatures well below the transition to the condensed phase, it is convenient to separate
the bosonic operators $\hat{a}_j$ into condensate and noncondensate part

$$\hat{a}_j = f_j \hat{a}_0 + \delta \hat{a}_j. \quad (3)$$

In our discrete two-site system, the numbers $f_j$ with the normalization

$$|f_1|^2 + |f_2|^2 = 1 \quad (4)$$

are the analogue to the condensate wavefunction, i.e. a macroscopic number of particles in a
product state. For the sake of simplicity, we will assume $f_j$ to be real in the following.

3.1. Bogoliubov meanfield part

We assume a large number of atoms on each of the two sites, and continue by applying the
Bogoliubov approximation. It consists in substituting the operators $\hat{a}_0$ and $\hat{a}_0^\dagger$ with $\sqrt{N_0}$, where $N_0$ denotes the number of atoms in the condensed mode. Further assuming a small condensate
depletion with $N_0 \approx N$, we have

$$\hat{a}_j \approx \sqrt{N} f_j + \delta \hat{a}_j. \quad (5)$$

With this approximation, we will first determine an approximate form of the meanfield wave
function $f_j$, and bring the Hamiltonian (1) to a quadratic form in the fluctuation operators $\delta \hat{a}_j$. However, in section 3.3, we will show that for a correct description of the condensate depletion
and the system’s many-body wavefunction, it is essential to re-introduce the noncommutative
operator character of $\hat{a}_0$.

For technical reasons, we chose the grand-canonical frame $\hat{E} = \hat{H} - \mu \hat{N}$, $\hat{N} = \hat{n}_1 + \hat{n}_2$. We will always adjust the chemical potential $\mu$ as function of $J$, $U$, $\Delta$ and $N$ such that a given
particle number $N$ is kept fixed. The meanfield solution $f_j$ minimizes $E[\sqrt{N} f_j]$, i.e., the $f_j$
fulfill the the discrete Gross–Pitaevskii equation

$$- J f_2 + (\Delta + UN f_1^2 - \mu) f_1 = 0, \quad (6a)$$

$$- J f_1 + (-\Delta + UN f_2^2 - \mu) f_2 = 0. \quad (6b)$$
Together with the constraint (4), the meanfield problem is fully defined; \( f_1, f_2, \) and \( \mu \) are determined as functions of \( J, \Delta, \) and \( UN \). Introducing the population imbalance \( n = N(f_1^2 - f_2^2) \) and writing \( f_1^2 = \frac{1}{2}(1 + n/N) \) and \( f_2^2 = \frac{1}{2}(1 - n/N) \), \( J \) can be eliminated from (6a) and (6b), and one finds

\[
\frac{n}{N} = \frac{\Delta}{\mu - UN}. \tag{7}
\]

With this, and by setting the determinant of the coefficient matrix of equations (6a) and (6b) to zero, one finds the quartic equation for the chemical potential

\[
(X - UN/2)^2(X^2 - J^2) - X^2\Delta^2 = 0, \tag{8}
\]

where \( X = \mu - UN/2 \). To leading order in \( \Delta \), this yields

\[
\mu = \frac{UN}{2} - J - \frac{\Delta^2}{2(J + UN/2)^2} + O(\Delta^4). \tag{9}
\]

Note that the negative shift of the chemical potential due to the ‘disorder’ \( \Delta \) is analogous to equation (15) of [22]. Via (7), the chemical potential determines the meanfield imbalance and the condensate wave function \( f_j \).

### 3.2. Bogoliubov noncondensate part

The meanfield wave function \( f_j \) has been obtained from the minimization of the meanfield energy functional. That means, the leading order of the relevant Hamiltonian \( F = \hat{E}[\hat{a}_j] - E[\sqrt{N}f_j] \) is quadratic in the quantum fluctuations:

\[
\hat{F} = \frac{1}{2} \sum_{i,j} \left( \delta \hat{a}_i, \delta \hat{a}_j \right) \left( D_{ij} B_{ij} \right) \left( \delta \hat{a}_j, \delta \hat{a}_i \right),
\]

\[
D = \left( \begin{array}{cc} 2Un_i + \Delta - \mu & -J \\ -J & 2Un_j - \Delta - \mu \end{array} \right), \quad B_{ij} = \delta_{ij}Un_j. \tag{10}
\]

Here, we find a typical feature of the Bogoliubov ansatz: equation (10) contains terms like \( Un_1\delta \hat{a}_1\delta \hat{a}_2 \), which destroy two particles, instead of destroying one particle and creating one particle. The particle number is not conserved, and implicitly we understand that missing particles have gone to the condensate mode.

In other words, the equations of motion mix creators and annihilators. This can be resolved by the Bogoliubov transformation to quasi-particles

\[
\hat{\beta}_\nu = u_\nu^* \delta \hat{a}_1 + u_\nu^* \delta \hat{a}_2 + v_\nu \delta \hat{a}_1^\dagger + v_\nu \delta \hat{a}_2^\dagger. \tag{11}
\]

Postulating \( i\hbar \hat{\beta}_\nu = [\hat{\beta}, \hat{F}] = \omega_\nu \hat{\beta}_\nu \) and comparing coefficients, we arrive at the Bogoliubov–de-Gennes equations [31]

\[
\sum_j \left[ \begin{array}{cc} D_{ij} & -B_{ij} \\ B_{ij} & D_{ij} \end{array} \right] - \omega_\nu \left( \begin{array}{c} 0 \\ \delta_{ij} \end{array} \right) \left( \begin{array}{c} u_{\nu j} \\ v_{\nu j} \end{array} \right) = 0. \tag{12}
\]

As the matrix in (12) is not Hermitian, we cannot expect the eigenvectors to be orthogonal. Rather, they fulfill the bi-orthogonality relation [28]

\[
(\omega_\nu - \omega_\nu^*) \sum_j (u_{\nu j}^* u_{\nu j} - v_{\nu j} v_{\nu j}) = 0. \tag{13}
\]

The matrix in (10) anticommutes with \( \left( \begin{array}{cc} 0 & k_j \\ 0 & 0 \end{array} \right) \). So, if \((u_{\nu 1}, u_{\nu 2}, v_{\nu 1}, v_{\nu 2})\) is an eigenvector with eigenvalue \( \omega_\nu \), then \((v_{\nu 1}, v_{\nu 2}, u_{\nu 1}, u_{\nu 2})\) is an eigenvector with eigenvalue \(-\omega_\nu \), which simply corresponds to \( \hat{\beta}_\nu^\dagger \). Thus, Bogoliubov modes occur in pairs.
A special mode \( v = 0 \) is found by setting \( u_{0j} = v_{0j} \). Then, (12) becomes the discrete Gross–Pitaevskii equation (6), such that \( u_{ij} = v_{ij} = f_{ij} \) and \( \omega_{00} = 0 \). The corresponding operator \( \hat{P} = \hat{P} \) is Hermitian. It can be interpreted as a kind of momentum associated to the Goldstone mode of the \( U(1) \) symmetry breaking of Bose–Einstein condensation [32]. There is a conjugate position \( \hat{Q} \) satisfying \( [\hat{Q}, \hat{P}] = i \). Since only one regular mode remains, we drop the index \( v = 1 \) and normalize \( \sum_{j} (|u_{j}|^2 - |v_{j}|^2) = 1 \), such that \( [\hat{\beta}, \hat{\beta}^\dagger] = 1 \). Both \( \hat{P} \) and \( \hat{Q} \) commute with \( \hat{\beta} \) and \( \hat{\beta}^\dagger \), and the operators \( \hat{\beta}, \hat{\beta}^\dagger, \hat{P}, \) and \( \hat{Q} \) form a complete set to express the \( \delta \hat{a}_j \) and \( \delta \hat{a}_j^\dagger \), such that the Bogoliubov Hamiltonian \( \hat{F} \) reads

\[
\hat{F} = \omega (\hat{\beta}^\dagger \hat{\beta} + 1/2) + \alpha \hat{P}^2/2, \tag{14}
\]

with the Bogoliubov frequency \( \omega \) and the parameter \( \alpha \), which determines the diffusion of the condensate phase [32]. For \( \Delta = 0 \), one finds the usual Bogoliubov dispersion \( \omega^{(0)} = \sqrt{2J(UN + 2J)} \) and the inverse mass term \( \alpha^{(0)} = UN \). Both quantities are even functions of \( \Delta \); the quadratic corrections are calculated in the appendix, (A.14) and (A.21).

### 3.3. Many-body wavefunction and condensate depletion

To construct an explicit expression for the many-body wavefunction, it is necessary to go back to the original definition (3) of the field operator \( \hat{a}_i \). It then follows from the bosonic commutation relation \( [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \) that the operators \( \delta \hat{a}_i \) and \( \delta \hat{a}_i^\dagger \) obey the commutation relations

\[
[\delta \hat{a}_i, \delta \hat{a}_j^\dagger] = \delta_{ij} - f_{ij}^* f_{ji} \delta \hat{a}_i \delta \hat{a}_j^\dagger = \delta_{ij} - f_{ij}^* f_{ji} = \delta_{ij}, \tag{15}
\]

where the last equality defines the projection operator \( \delta_{ij} \). It is this very projection to the space orthogonal to the condensate wavefunction that is used in number-conserving Bogoliubov approaches [33–35]. Within the naive approach of (5), the relation (15) would be \( [\delta \hat{a}_i, \delta \hat{a}_j^\dagger] \approx \delta_{ij} \). The additional term in (15) includes the fact that the number of condensate particles rather than the total number of particles should appear in the Gross–Pitaevskii equation (6) [36]. In particular, removing the fluctuations proportional to the condensate removes number fluctuations and the phase-diffusion term \( \alpha \hat{P}^2/2 \) in the Hamiltonian (14).

In the ground state \( |C_N\rangle \) of the noninteracting system, all \( N \) particles occupy the condensate state,

\[
|C_N\rangle = \frac{1}{\sqrt{N!}} (\hat{a}_0^\dagger)^N |0\rangle,
\]

where \( |0\rangle \) is the no-particle state or physical vacuum. The effect of pairwise particle interaction is to deplete this condensate mode and to populate the excitation mode. Thus, the lowest state of the interacting system—the Bogoliubov vacuum denoted by \( |0\rangle \)—consists of a superposition of states, each with a different number \( p \) of pairs of particles excited out of the condensate:

\[
|0\rangle = Z \sum_{p=0}^{N/2} (2^p p!)^{-1} (\delta \hat{a}_i^\dagger A_{ij} \delta \hat{a}_j^\dagger)^p |C_{N-2p}\rangle, \tag{16}
\]

where summation over repeated indices is implied. The symmetric matrix \( A_{ij} \) and the normalization constant \( Z \) in the ansatz (16) can be determined from the condition \( \hat{\beta} |0\rangle = 0 \).

We refer the reader to [28] for details of the calculation. With the abbreviations \( \Pi_i^* \equiv \delta_{ij} \mu_i^*, \Pi_i \equiv \delta_{ij} \nu_i^*, \) and \( \alpha_{ij} \equiv \delta_{ik} A_{kl} \delta_{lj} \), it results in

\[
\alpha_{ij} = -\Pi_i^* \Pi_j^\dagger / \beta, \tag{17}
\]
with $\beta = \bar{\pi}_1 \bar{\pi}_1^\dagger + \bar{\pi}_2 \bar{\pi}_2^\dagger$ and
\[
Z^{-2} = \exp \left\{ \sum_{p=1}^{N/2} \frac{\text{Tr}[(\bar{\Lambda}^\dagger \bar{\Lambda})^p]}{2p} \right\}.
\]
(18)

Equation (16) together with (17) and (18) yields an explicit representation of the interacting ground state $|0\rangle$.

Accordingly, the $N$-body wavefunction in configuration space can be written in the form
\[
\Psi(i_1, \ldots, i_N) \equiv N^{1/2} \langle 0 | \hat{a}_{i_1}, \ldots, \hat{a}_{i_N} | 0 \rangle = Z \sum_{p=0}^{N/2} \chi_p(i_1, \ldots, i_N),
\]
(19)

where $\chi_p$ is the part of the wavefunction with exactly $p$ pairs of particles excited out of the condensate:
\[
\chi_p(i_1, \ldots, i_N) = \left[ \frac{(N-2p)!}{N!} \right]^{1/2} \sum \mathcal{A}_{i_1i_2} \cdots \mathcal{A}_{i_{2p+1}i_{2p}} \times f_{i_{2p+1}} \cdots f_{i_N}. \]
(20)

For each pair of noncondensate particles occupying the sites $i$ and $j$, there is a factor $\mathcal{A}_{ij}$ from (16), for each condensate particle at site $i$ a factor $f_i$. The sum in (20) runs over the $N![(N-2p)!/2p!]^{-1}$ distinct ways of choosing $p$ different pairs from the $N$ variables $\{i_1, \ldots, i_N\}$. With (19) and (20), we obtain
\[
\rho_{ij} = N \sum_{i_2, \ldots, i_N} \Psi(i_1, i_2, \ldots, i_N) \Psi^\dagger(i_j, i_2, \ldots, i_N) = N_0 f_i f_j + \bar{\pi}_i \bar{\pi}_j^\dagger
\]
(21)

for the one-body density matrix, where $N_0 = N - |ar{\pi}_1|^2 - |ar{\pi}_2|^2$.

To compare the interacting ground state (16) with the results of exact diagonalization, we need to expand the wave function (19) in the Fock basis ($l$ bosons on the left and $N-l$ bosons on the right site):
\[
|0\rangle = \sum_{l=0}^{N} c_l |l\rangle, \quad c_l = \binom{N}{l}^{1/2} \Psi(1, \ldots, 1, 2 \ldots 2). \]
(22)

Figure 2 shows an example for $N = 7$ particles, i.e., with $0 \leq p \leq 3$ pairs in (19). For moderate interaction $U \ll J$, the agreement with data from the exact diagonalization is good despite of the small number of particles. Compared to the noninteracting case, the amplitudes for large $l$ and large $N-l$ are suppressed, i.e., the interacting system disfavors particles to cluster on one of the sites.

The density matrix (21) allows us to calculate the condensate depletion
\[
\delta N = N - N_0 = |ar{\pi}_1|^2 + |ar{\pi}_2|^2.
\]
(23)

In figure 3, $\delta N$ is shown as a function of $N$. For large $N$, the numeric results obtained by exact diagonalization converge to the value given by (23). Note that for $\Delta = 0$, we have $f_j = 1/\sqrt{2}$.

Equation (15) becomes $\bar{\delta} = \left( \begin{array}{cc} 1 & -1 \\ -1 & 1 \end{array} \right) / 2$, and with $v_1 = -v_2$, we arrive at $\bar{\pi}_j = v_j$. Hence in this case,
\[
\lim_{\Delta \to 0} \delta N = |v_1|^2 + |v_2|^2 = \delta N_{\text{Bg}},
\]
(24)

that is, the condensate depletion is correctly described within the simple Bogoliubov approximation of section 3.2. However, for $\Delta \neq 0$, this is not the case: figure 4 shows the condensate depletion as a function of the tilt $\Delta$. While $\delta N$ of (23) (red line) matches well with the results of the exact diagonalization (symbols), $\delta N_{\text{Bg}}$ (gray dashed line) does not even qualitatively match the functional form of $\delta N(\Delta)$, and the Bogoliubov approximation $\hat{a}_0 \to N_0$, resulting in $[\delta \hat{a}_i, \delta \hat{d}_j] = \delta_{ij} \to \delta_{ij}$, is not valid.
3.4. Systems of more than two sites

In order to put our results on the tilted doublewell system in context with extended disordered systems, we are going to have a brief look at larger inhomogeneous systems with \( L \) sites. Here, we restrict ourselves to the numerical solution within Bogoliubov theory, which consists in solving the generalization of the discrete Gross–Pitaevskii equation (6) by imaginary time evolution [37] and a subsequent diagonalization of the non-Hermitian Bogoliubov–de-Gennes problem (12). We then select the \( L - 1 \) modes with positive eigenvalues \( \omega_{\nu} \), normalize them according to

\[
\sum_j (|u_{\nu j}|^2 - |v_{\nu j}|^2) = 1,
\]

project out the condensate mode and compute the condensate depletion

\[
\delta N = \sum_{\nu} |\bar{v}_{\nu j}|^2.
\]

Some results are shown in figure 5. In the three-site system shown in figure 5(a), we see that in the case where we tilt the whole system, the behavior is similar to the two-site system: the depletion \( \delta N \) (solid red/lower) diminishes monotonically as an even function of the tilt \( \Delta \), while the naive prediction (dashed) increases initially. The case of a barrier on the middle site (blue/upper) is different. For a repulsive barrier \( \Delta > 0 \), the depletion \( \delta N \) increases, but for an attractive well in the middle, it decreases. The latter case is similar to the tilted two-site and three-site systems: the bosons condense on the site with the lowest on-site energy, and excitations to neighboring sites are energetically suppressed. In a more extended system of, say, 12 sites with moderate disorder, as shown in figure 5(b), such condensation in a single site becomes unlikely. Although the dependence on the particular realization of disorder is still very strong in a 12-site system, the general behavior of a disordered system is already visible: the depletion increases roughly quadratically with the disorder strength \( \Delta \) [23]. Note that in this case the difference between the proper Bogoliubov result and the naive one has already become very small compared to the cases of \( L = 2 \) and \( L = 3 \) in figures 4 and 5(a).

4. Summary and discussion

While either disorder or interaction alone tend to diminish the phase coherence in extended bosonic systems, the numerical calculations in [14] found the—at first glance
counterintuitive—result that a combination of the two can actually enhance coherence in a two-site model. In the present work, we observe this behavior in the variation of the condensate depletion with the disorder parameter $\Delta$. Figure 4 shows how an increase in $\Delta$ restores the condensate population, counteracting its depletion by repulsive interaction. However, as illustrated in section 3.4, this mechanism only works in very small systems with a limited number of sites and not for one-dimensional random potentials in general [38].

One can intuitively understand the behavior of the minimal two-site model in the limit of very strong tilt $\Delta$, where the left site becomes energetically inaccessible and all particles are on the right. Then, the one-body density matrix has only one non-zero entry $\rho_{22} = N$, which is the only non-zero eigenvalue, and the depletion vanishes. Because of the lack of other degrees of freedom for the bosons to go to, it is questionable, of course, to name this state of our toy model a Bose–Einstein condensate at all. In general, the mechanism that leads to a decrease of condensate depletion as a function of the tilt is the accumulation of bosons on a single site with strongly attractive potential.

We showed how, although both condensate population and total particle number can be assumed large, a naive application of the Bogoliubov approximation to the two-site system is not valid. The problems occur because a thermodynamic limit cannot be defined due to the fixed size of the system [28]. By explicit construction of the $N$-particle ground state, we showed that the usual Bogoliubov wavefunctions $u$ and $v$ appear in a modified form $\tilde{u}$, $\tilde{v}$ in the one-body density matrix of our system: they have to be corrected by terms proportional to $[\hat{a}_0, \hat{a}_0^\dagger]$. In extended systems, these terms are multiplied with the inverse volume of the system, which renders them negligible in the thermodynamic limit [28].

Our comparison with exact numerical results reveals that the Bogoliubov description, which—by definition—neglects the noncommutative character of the condensate operator $\hat{a}_0$, fails to describe the two-site system in the presence of disorder. Therefore, a careful description of the interacting condensate particles is mandatory to capture the interplay between interaction and disorder within small inhomogeneous Bose systems.

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Appendix. Analytical solution of the Bogoliubov–de-Gennes equation

In this appendix, we solve the Gross–Pitaevskii equation (6a), (6b) and the Bogoliubov–de-Gennes problem (12) perturbatively for weak tilt $\Delta$. We use $UN/2$ as energy scale; in particular, we define the dimensionless Bogoliubov frequency $w = 2\omega/UN$. The dependence on the dimensionless parameter $y := 2J/UN$ is treated exactly. We expand all quantities as $\mu = \mu^{(0)} + \delta \mu^{(1)} + \delta^2 \mu^{(2)} + \cdots$, where $\delta = 2\Delta/(UN + 2J)$ is the small parameter, which is the dimensionless smoothed tilt potential [39].

With (7) and (9), the perturbative solution of the meanfield problem (6a), (6b) reads

$$\begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} f^{(0)} + \delta f^{(1)} + \delta^2 f^{(2)} + \cdots \\ f^{(0)} - \delta f^{(1)} + \delta^2 f^{(2)} + \cdots \end{pmatrix},$$

(A.1)

$$f^{(0)} = 1/\sqrt{2}, \quad f^{(1)} = -f^{(0)}/2, \quad f^{(2)} = -f^{(0)}/8.$$  

(A.2)
Next, we come to the perturbative solution of the Bogoliubov–de-Gennes equations (12). The first orders of the matrices $d = 2D/UN$ and $b = 2B/UN$ read

$$d^{(0)} = (1 + y) I - y\sigma_z, \quad b^{(0)} = I,$$

(A.3)

$$d^{(1)} = -(1 - y)\sigma_z, \quad b^{(1)} = -\sigma_z,$$

(A.4)

$$d^{(2)} = y/2 I, \quad b^{(2)} = 0.$$

(A.5)

We observe that even orders commute with $\sigma_z$, whereas odd orders anti-commute. This results in the following expansion of the Bogoliubov mode:

$$\omega = \omega^{(0)} + \delta^2 \omega^{(2)} + \cdots,$$

(A.6)

\[
\begin{pmatrix}
  u_1 \\
  u_2 \\
  v_1 \\
  v_2
\end{pmatrix} =
\begin{pmatrix}
  u^{(0)} + \delta u^{(1)} + \delta^2 u^{(2)} + \cdots \\
  -u^{(0)} + \delta u^{(1)} - \delta^2 u^{(2)} + \cdots \\
  v^{(0)} + \delta v^{(1)} + \delta^2 v^{(2)} + \cdots \\
  -v^{(0)} + \delta v^{(1)} - \delta^2 v^{(2)} + \cdots
\end{pmatrix}.
\]

(A.7)

At each order, the problem reduces to a $2 \times 2$ problem, which is conveniently expressed in terms of the matrix

$$M_k = \begin{pmatrix} d_{11} \pm d_{12} & -(b_{11} \pm b_{12}) \\ b_{11} \pm b_{12} & -(d_{11} \pm d_{12}) \end{pmatrix}.$$

(A.8)

The zeroth order consists in diagonalizing the matrix $M^{(0)}_-$, which yields

$$w^{(0)} = 2\sqrt{y(1+y)},$$

(A.9)

$$\begin{pmatrix} u^{(0)} \\ v^{(0)} \end{pmatrix} = \frac{1}{\sqrt{2\sqrt{(1 + 2y + w^{(0)})^2 - 1}}} \begin{pmatrix} 1 + 2y + w^{(0)} \\ 1 \end{pmatrix}.$$ (A.10)

The first-order equation is of the form

$$\begin{pmatrix} M^{(0)}_+ - w^{(0)} \end{pmatrix} \begin{pmatrix} u^{(1)} \\ v^{(1)} \end{pmatrix} = -M^{(1)}_- \begin{pmatrix} u^{(0)} \\ v^{(0)} \end{pmatrix},$$

(A.11)

and is easily solved by inverting the matrix on the left-hand side:

$$\begin{pmatrix} u^{(1)} \\ v^{(1)} \end{pmatrix} = \frac{1}{4y(1+y)} \begin{pmatrix} y - (1 - y)w^{(0)} & y + w^{(0)} \\ y - w^{(0)} & y + (1 - y)w^{(0)} \end{pmatrix} \begin{pmatrix} u^{(0)} \\ v^{(0)} \end{pmatrix}.$$ (A.12)

The solution of the second order,

$$\begin{pmatrix} M^{(0)}_+ - w^{(0)} \end{pmatrix} \begin{pmatrix} u^{(2)} \\ v^{(2)} \end{pmatrix} = -M^{(2)}_- (u^{(0)}, v^{(0)}; u^{(0)}, v^{(0)}) + M^{(1)}_- \begin{pmatrix} u^{(1)} \\ v^{(1)} \end{pmatrix}$$

(A.13)

is less trivial, because the matrix on the left-hand side is not invertible, since its eigenvectors $(u^{(0)}, v^{(0)})$ and $(u^{(0)}, v^{(0)})'$ have eigenvalues 0 and $-2w^{(0)}$, respectively. In order to solve (A.13), we expand the second order in terms of the zeroth order: $(u^{(2)}, v^{(2)}) = a^{(2)}(u^{(0)}, v^{(0)}) + c^{(2)}(v^{(0)}, u^{(0)})$. Then, we solve for the three unknowns $w^{(2)}$, $a^{(2)}$, and $c^{(2)}$ by multiplying (A.13) from the left with $(u^{(0)}, -v^{(0)})$, $(v^{(0)}, -u^{(0)})$, and by employing the normalization condition to second order:

$$w^{(2)} = 4y(2y - 1)u^{(0)}v^{(0)}$$

(A.14)

$$c^{(2)} = \frac{-1}{8(1+y)}, \quad a^{(2)} = -\sqrt{|u^{(1)}|^2 - |v^{(1)}|^2}. $$

(A.15)

Remarkably, the renormalization of the Bogoliubov frequency $\omega = wUN/2$ can be either positive or negative, (A.14).
Condensate depletion. Finally, we combine the previous results (A.7), (A.10), (A.12), and (A.15) to compute the amplitudes \( \bar{\gamma}_j \), which are needed for the depletion (23), up to second order. \( \bar{\eta} \) and \( \bar{\gamma}_j \) are expanded the same way as \( u_j \) and \( v_j \) in (A.7), with \( \bar{\eta}^{(0)} = v^{(0)} \), \( \bar{\eta}^{(1)} = v^{(1)} - \xi^{(1)} f^{(0)} \), \( \bar{\eta}^{(2)} = v^{(2)} - \xi^{(1)} f^{(1)} \), with \( \xi^{(1)} = 2(f^{(0)} v^{(1)} + v^{(0)} f^{(1)}) \). Finally, we arrive at

\[
\delta N^{(0)} = 2|\bar{\gamma}^{(0)}|^2 = \frac{1}{2w^{(0)}[1 + 2y + w^{(0)}]},
\]

\[
\delta N^{(2)} = -\frac{3}{8} \frac{1}{(1 + y)w^{(0)}}.
\]

Thus, the initial change of the depletion is negative for all \( y = 2J/UN \) and scales quadratically with the tilt.

The second order of the (wrong) naive Bogoliubov depletion turns out to have the same functional form as (A.17): \( \delta N_{\text{NS}}^{(2)} = 2[|\bar{\gamma}^{(1)}|^2 + 2|\bar{\gamma}^{(0)}|^2] = -\delta N^{(2)}/3 \), but is positive.

Zero mode. In order to transform the Hamiltonian (10) from fluctuations \( \delta \hat{a}_j \) and \( \delta \hat{a}^\dagger_j \) to the Bogoliubov quasiparticle \( \hat{\theta}, \hat{\theta}^\dagger \) and the self-adjoined zero mode \( \hat{P} = \sum_j f_j (\delta \hat{a}_j + \delta \hat{a}^\dagger_j) \), we also need the conjugate variable \( \hat{Q} \), which is determined by

\[
\{ \hat{Q}, \hat{P} \} = i, \quad \{ \hat{Q}^\dagger, \hat{P} \} = 0.
\]

This is achieved by the ansatz \( \hat{Q} = \sum_{j} \gamma_j (i \delta \hat{a}_j - i \delta \hat{a}^\dagger_j) \), where the amplitudes \( \gamma_j \) are expanded in the same way as \( \delta \) as the amplitudes \( f_j \) in (A.1). From the conditions (A.18), we determine

\[
\gamma^{(0)} = \frac{1}{4 f^{(0)}}, \quad \gamma^{(1)} = -\frac{\nu^{(1)} + \nu^{(1)}}{\nu^{(0)} + \nu^{(0)}} \gamma^{(0)},
\]

\[
\gamma^{(2)} = -4 \gamma^{(0)} [\gamma^{(0)} f^{(2)} + \gamma^{(1)} f^{(1)}].
\]

Then, we can express the operators \( \delta \hat{a}_j \) and \( \delta \hat{a}^\dagger_j \) in terms of \( \hat{\theta}, \hat{\theta}^\dagger, \hat{P}, \) and \( \hat{Q} \), which indeed brings the Hamiltonian (10) to the form given in (14). We have already determined the Bogoliubov frequency \( \omega = UNw/2 \) above in (A.9) and (A.14). Similarly, we determine the inverse mass parameter \( \alpha \):

\[
\alpha = UN \left[ 1 + \frac{8 \Delta^2 J}{(UN + 2J)^2} + \cdots \right],
\]

which is positive for all values of \( J/UN \). The numerical solution of the Bogoliubov–de-Gennes equation shows that \( \alpha \) tends to \( 2UN \) for strong tilt \( \Delta \).

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