Number fluctuations of cold spatially split bosonic objects

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Abstract

We investigate the number fluctuations of spatially split many-boson systems employing a theorem about the maximally and minimally attainable variances of an observable. The number fluctuations of many-boson systems are given for different numbers of lattice sites and both mean-field and many-body wave functions. It is shown which states maximize the particle number fluctuations, both in lattices and double-wells. The fragmentation of the states is discussed, and it is shown that the number fluctuations of some fragmented states are identical to those of fully condensed states.

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I. INTRODUCTION

Ultracold atoms offer the unique possibility to directly compare theoretical predictions about many-body physics with experiments. Many-body effects arise due to the interaction between particles and the external trapping potential. Of particular interest is the question about the nature of the quantum state present in a given system. For example, in double- and multi-well trapping geometries, the ground state is either fragmented or condensed, depending on the barrier height and the interaction strength [1–7]. For long-range interactions even the ground state in a single-well trap can be fragmented [8]. Apart from the fragmentation of the ground state, fragmentation of Bose-Einstein condensates (BECs) is also known to develop in nonequilibrium dynamics [9–18]. On the theoretical level, fragmentation manifests itself in the reduced density matrices of the system. While the reduced density matrices of a system of bosons themselves are not experimentally accessible, it is possible to draw conclusions about them from the measurement of experimentally accessible quantities, such as the particle number fluctuations.

Here, we would like to investigate the number fluctuations of several many-body states and their fragmentation. We focus on cold spatially split bosonic objects. Atom number fluctuations of fragmented and condensed systems have been investigated intensively both theoretically, see e.g. [1, 9, 14, 15, 19–22] and experimentally [18, 23–28], to name just a few. Here, we would like to elucidate the limits that quantum mechanics puts on number fluctuations of bosonic mean-field and many-body wave functions, and concentrate on their fragmentation. In particular, we find that some fragmented states cannot be distinguished by their number fluctuations from fully condensed superfluid states.

This paper is organized as follows. In Sec. II we discuss a theorem about the maximum variance of an observable. In Sec. III some basic definitions needed for the discussion of number fluctuations in multi-well traps are introduced. In Sec. IV we discuss the number fluctuations of two-mode many-boson states. In Sec. V we show how the previously obtained results can be generalized to BECs in multi-well traps and optical lattices. We summarize the results and conclude in Sec. VI.
II. MAXIMUM VARIANCE THEOREM

In this section we will prove a theorem about the maxima and minima of the variance of an observable. A more mathematically oriented proof can be found in Ref. [29].

Theorem 1. Let \( \hat{A} \) denote a hermitian operator and \( a_0 < \ldots < a_N \) a subset of its spectrum. Furthermore, let \( |\Psi\rangle \) be a wave function and

\[
|\Psi\rangle = \sum_{n=0}^{N} C_n |\Psi_n\rangle
\]

be an expansion of \( |\Psi\rangle \) in \( \hat{A} \)'s eigenstates with \( \sum_{n=0}^{N} |C_n|^2 = 1 \), where \( C_n |\Psi_n\rangle \) denotes the contribution of all degenerate eigenstates of \( \hat{A} \) to the eigenvalue \( a_n \). Then the variance of \( \hat{A} \)

\[
\Delta A^2 \equiv \langle \Psi | (\hat{A} - \langle \Psi | \hat{A} |\Psi\rangle)^2 |\Psi\rangle
\]

(2)

takes on its minimum, \( \Delta A^2_{\text{min}} = 0 \), for \( |\Psi\rangle \) is arbitrary. The maximum variance, \( \Delta A^2_{\text{max}} = \frac{1}{4} (a_N - a_0)^2 \) is obtained for \( |C_0|^2 = |C_N|^2 = 1/2 \).

Proof. The normalization constraint \( \sum_{n=0}^{N} |C_n|^2 = 1 \) can be used to eliminate one of the \( N+1 \) coefficients \( C_n \) in Eq. (2). Without loss of generality, we choose the coefficient \( C_N \) and write \( |C_N|^2 = \frac{1}{2} \). For an extremum

\[
\frac{\partial \Delta A^2}{\partial C_n} = 0
\]

must hold which yields

\[
C_n (a_n - a_N) = 2C_n \sum_{m=0}^{N-1} |C_m|^2 (a_n - a_N)
\]

(4)

for \( n = 0, \ldots, N-1 \). The conditions \( \frac{\partial \Delta A^2}{\partial C_n} = 0 \) yield the complex conjugates of Eqs. (4). The set of Eqs. (4) have the solution \( C_n = 0 \) for \( n = 0, \ldots, N-1 \). In this case \( |C_N| = 1 \) and \( \Delta A^2 = 0 \), which is a minimum because \( \Delta A^2 \geq 0 \). Since the choice to eliminate the
coefficient $C_N$ was arbitrary, any state with $|C_n| = 1$ for $n ∈ 0, . . . , N$ minimizes $ΔA^2$ with the value $ΔA^2_{min} = 0$. This concludes the proof of the first part of Theorem 1.

Now suppose that $C_i ≠ 0$ for at least one $i ∈ 0, . . . , N − 1$, then it follows from Eqs. (4) that

$$a_i - a_N = 2 \sum_{m=0}^{N-1} |C_m|^2 (a_m - a_N). \tag{5}$$

In general Eq. (5) can only be fulfilled if $|C_i|^2 = 1/2$ and $C_m = 0$ for all $m ∈ 1, . . . , N − 1$ with $m ≠ i$. It then follows from the normalization condition that $|C_N|^2 = 1/2$. Since the choices $i$ and $N$ were arbitrary, the maximum variance condition is obtained for that pair of coefficients $(i, j)$ with $|C_i|^2 = |C_j|^2 = 1/2$ that maximizes $ΔA^2$. The maximum variance of $\hat{A}$ can therefore be written as

$$ΔA^2_{max} = \frac{1}{4} (a_j - a_i)^2. \tag{6}$$

Since the eigenvalues $a_n$ are ordered increasingly, the maximum value of $ΔA^2_{max}$ is obtained for the choice $i = 0$ and $j = N$, i.e. for $|C_0|^2 = |C_N|^2 = 1/2$. This concludes the proof of Theorem 1. \hfill \square

III. DEFINITIONS

In this section we briefly recall some definitions that will be useful for what follows. Let the operators $\hat{b}^\dagger_i$ and $\hat{b}_i$ denote the operators that create and annihilate a boson in the orbital $φ_i$ and fulfill the usual bosonic commutation relations $[\hat{b}_i, \hat{b}^\dagger_j] = δ_{ij}$. The number operator of the orbital $φ_i$ is $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$. For a permanent in which $N$ bosons reside in $s$ orbitals with $n_i$ bosons in the orbital $φ_i$ we use the shorthand notation

$$|1^{n_1}, 2^{n_2}, . . . , s^{n_s}\rangle = \frac{\hat{b}_1^{n_1} \hat{b}_2^{n_2} . . . \hat{b}_s^{n_s}}{\sqrt{n_1! n_2! . . . n_s!}} |0\rangle. \tag{7}$$

The most general wave function of $N$ identical bosons expanded in $s$ orbitals then reads

$$|Ψ\rangle = \sum_{n_1, . . . , n_s=0}^{N} C_{n_1 . . . n_s} |1^{n_1}, 2^{n_2}, . . . , s^{n_s}\rangle, \tag{8}$$

with $n_1 + . . . + n_s = N$. Furthermore, we write

$$\hat{Ψ}(x) = \sum_i \hat{b}_i φ_i(x) \tag{9}$$

for the bosonic field operator and $|\Psi\rangle$ for an $N$-boson wave function. Then $\hat{\rho}(x) = \hat{\Psi}^\dagger(x)\hat{\Psi}(x)$ is the operator of the single-particle density $\rho(x) = \langle \hat{\rho}(x) \rangle$. The first-order reduced density matrix (RDM) is defined as

$$\rho^{(1)}(x|x') = \langle \Psi|\hat{\Psi}^\dagger(x')\hat{\Psi}(x)|\Psi \rangle = \sum_i n_i^{(1)} \alpha_i^{(1)}(x)\alpha_i^{(1)*}(x')$$

and has eigenfunctions $\alpha_i^{(1)}(x)$ and eigenvalues $n_i^{(1)}$ which are known as natural orbitals and natural occupation numbers, respectively. Explicitly,

$$\int dx' \rho^{(1)}(x|x') \alpha_i^{(1)}(x') = n_i^{(1)} \alpha_i^{(1)}(x)$$

holds, where $n_1^{(1)} \geq n_2^{(1)} \geq \ldots$ is assumed and $\sum_i n_i^{(1)} = N$. If an eigenvalue $n_i^{(1)} = \mathcal{O}(N)$ exists the system is said to be condensed [30]. If there is more than one such eigenvalue, the BEC is said to be fragmented [31], see also [5–7]. The density fluctuations are given by

$$\Delta \rho^2(x) = \langle \hat{\rho}(x)^2 \rangle - \langle \hat{\rho}(x) \rangle^2.$$

In practice, $\Delta \rho^2(x)$ must be integrated over some finite region of space. If each orbital $\phi_i(x)$ is localized around $x = x_i$ and has little overlap with other orbitals, the integral of $\Delta \rho^2(x)$ over a region of space where $\phi_i(x)$ is not negligible can be approximated by

$$\Delta n_i^2 = \langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2.$$

The quantities $\Delta n_i^2$ are known as number fluctuations and will be discussed in the following.

**IV. TWO-MODE STATES**

Let us now investigate the number fluctuations and the fragmentation of some particular many-boson states constructed either from two localized modes, denoted $\phi_L$ and $\phi_R$ with $\phi_L(x) = \phi_R(-x)$ or their *gerade* and *ungerade* combinations, denoted $\phi_g(x) = \frac{1}{\sqrt{2}}[\phi_R(x) + \phi_L(x)]$ and $\phi_u(x) = \frac{1}{\sqrt{2}}[\phi_R(x) - \phi_L(x)]$. The particle number operator of the orbital $\phi_R$ can then be written as

$$\hat{n}_R = \hat{b}_R^\dagger \hat{b}_R = \frac{1}{2} \left( \hat{n}_g + \hat{n}_u + \hat{b}_g^\dagger \hat{b}_u + \hat{b}_u^\dagger \hat{b}_g \right).$$

Furthermore, if only two modes are available it follows from $\hat{n}_L = N - \hat{n}_R$ that

$$\Delta n_L^2 = \Delta n_R^2,$$

irrespective of the quantum state. We will therefore drop the site index in this section.
A. Many-body states

In recent theoretical work based on the time-dependent many-body Schrödinger equation it was shown that superpositions of macroscopic quantum states can be created by scattering an attractively interacting BEC from a barrier [13, 32]. The resulting state is known as a caton and has two dominant contributions in the basis of left and right localized orbitals. We idealize this caton state here by

$$|\Psi_{\text{cat}}\rangle = \frac{1}{\sqrt{2}} (|L_N\rangle + |R_N\rangle),$$  \hspace{1cm} (16)$$

which is also known as a NOON state, since it can be written as $\frac{1}{\sqrt{2}} (|N, 0\rangle + |0, N\rangle)$ using the conventional number state notation. For the state $|\Psi_{\text{cat}}\rangle$ we find that the number fluctuations are given by

$$\Delta n_{\text{cat}}^2 = N^2/4.$$  \hspace{1cm} (17)$$

Since $|0, N\rangle$ and $|N, 0\rangle$ are the eigenstates of $\hat{n}_R$ and $\hat{n}_L$, corresponding to their minimal and maximal eigenvalues, it follows from Theorem 1 that the state $|\Psi_{\text{cat}}\rangle$ is a state that maximizes the variance of $\hat{n}_R$ and $\hat{n}_L$. Note that any state of the form $\frac{1}{\sqrt{2}} (|L_N\rangle + \exp(i\theta)|R_N\rangle)$ leads to the same number fluctuations $\Delta n^2 = N^2/4$. The first-order RDM of such states has two macroscopic eigenvalues $n_1^{(1)} = n_2^{(1)} = N/2$, and thus the caton is a fragmented BEC that maximizes the number fluctuations. Thus, a measurement of the number fluctuations is insensitive to the relative phase $\theta$ between $|N, 0\rangle$ and $|0, N\rangle$.

This result should be compared to that of a caton state in the basis of the gerade and ungerade orbitals $\phi_g(x)$ and $\phi_u(x)$

$$|\Psi_{g/u,\text{cat}}\rangle = \frac{1}{\sqrt{2}} (|g_N\rangle + |u_N\rangle),$$  \hspace{1cm} (18)$$

which has exactly the same set of eigenvalues of the first-order RDM $n_1^{(1)} = n_2^{(1)} = N/2$, but much smaller number fluctuations which are given by

$$\Delta n_{g/u,\text{cat}}^2 = \frac{1}{4} N.$$  \hspace{1cm} (19)$$

Note that any state of the form $\frac{1}{\sqrt{2}} (|g_N\rangle + \exp(i\theta)|u_N\rangle)$ has the same fragmentation and number fluctuations as $|\Psi_{g/u,\text{cat}}\rangle$. Moreover, it is easy to see that also any state of the form $\cos(\theta)|g_N\rangle + \sin(\theta)|u_N\rangle$ has the same number fluctuations, $\Delta n^2 = N/4$. So far, no caton states have been reported in experiments. Equations (17) and (19) and the considerations
above clearly show that caton states cannot be characterized uniquely by their number fluctuations, or their fragmentation ratios alone.

B. Mean-field states

Spatially split mean-field states that have received a lot of attention are the soliton train states

\[ |\Psi_{st}^+\rangle = |g^N\rangle, \quad |\Psi_{st}^-\rangle = |u^N\rangle \]  

(20)

that describe spatially split, fully condensed BECs, i.e. condensates with \( n_1^{(1)} = N \). Soliton trains appear in the context of attractively interacting BECs within the framework of Gross-Pitaevskii theory. Interestingly, one finds for their number fluctuations

\[ \Delta n_{st}^2 = \frac{1}{4} N \]  

(21)

which is exactly the same result as for the \( |\Psi_{g/u\text{cat}}\rangle \) state. Similar to the case of caton states discussed above, also the state \( |u^N\rangle \) leads to \( \Delta n^2 = \frac{1}{4} N \). Thus, a measurement of the number fluctuations alone does not allow to distinguish between the states \( |\Psi_{g/u\text{cat}}\rangle \), \( |\Psi_{st}^+\rangle \) and \( |\Psi_{st}^-\rangle \). A simultaneous measurement of number fluctuations and fragmentation would be necessary to narrow down the number of possible states that the system was in.

Let us now turn to more general mean-field states. To this end we define parameterized two-mode operators

\[ \hat{a}_1(\theta) = \cos(\theta)\hat{b}_L + \sin(\theta)\hat{b}_R, \]
\[ \hat{a}_2(\theta) = -\sin(\theta)\hat{b}_L + \cos(\theta)\hat{b}_R \]  

(22)

which can annihilate bosons either in localized or delocalized orbitals depending on the value of \( \theta \), and compute the number fluctuations of the general mean-field state \( |\Psi_{MF}\rangle \) that can be constructed from the operators \( \hat{a}_1^\dagger \) and \( \hat{a}_2^\dagger \):

\[ |\Psi_{MF}\rangle = |a_1^n(\theta), a_2^{N-n}(\theta))\rangle. \]  

(23)

The number fluctuations of \( |\Psi_{MF}\rangle \) are given by

\[ \Delta n_{MF}^2 = \left[ \frac{N}{4} + \frac{n(N-n)}{2} \right] \sin^2(2\theta). \]  

(24)
The maximum of the number fluctuations $\Delta n_{MF}^2$ when considered as a function of $\theta$ and $n$ is given by

$$\max \Delta n_{MF}^2 = \frac{N^2}{8} + \frac{N}{4}$$

(25)

which is obtained for $n = N/2$ and $\theta = \pi/4$. For these values of $n$ and $\theta$ the wave function $|\Psi_{MF}\rangle$ becomes

$$|\Psi_{frag}\rangle = |g^{N/2}, u^{N/2}\rangle.$$  

(26)

The state $|\Psi_{frag}\rangle$ is a so called fragmenton state [11]. For attractively interacting BECs it was recently shown that soliton train states can quickly lose their coherence and become spatially split, fragmented objects, like the fragmenton state [17]. Just like the two caton states discussed above, fragmentons are fragmented BECs. The state $|\Psi_{frag}\rangle$ is two-fold fragmented with $n_1^{(1)} = n_2^{(1)} = N/2$. Interestingly, the number fluctuations of the fragmenton $|\Psi_{frag}\rangle$ has contributions $\propto N$ and $\propto N^2$, see Eq. (25). The minima of $\Delta n_{MF}^2$ are obtained for $\theta = 0, \pi/2, \ldots$ with $n \in 0, \ldots, N$ arbitrary. The corresponding states are known as number states or Fock states

$$|\Psi_{num}\rangle = |L^n, R^{N-n}\rangle$$

(27)

and have zero number fluctuations $\Delta n^2 = 0$. The fragmentation of number states depends on the number of particles in each localized orbital, and is given by $n_1^{(1)} = n$, $n_2^{(2)} = N - n$. This concludes our discussion of two-mode systems.

V. LATTICE STATES

A. General lattice states

We will now generalize the discussion to lattices with $s$ sites, denoted $i = 1, 2, \ldots, s$ and corresponding localized orbitals $\phi_i(x)$. First, we will prove that the maximum number fluctuations in an $s$-site lattice are identical to those of a two-mode system, namely $\max \Delta n_i^2 = N^2/4$. For simplicity, we begin with a lattice of $s = 3$ sites. The ansatz wave function, Eq. (8), then reads

$$|\Psi_3\rangle = \sum_{n_1,n_2,n_3=0}^N C_{n_1,n_2,n_3} |1^{n_1}, 2^{n_2}, 3^{n_3}\rangle,$$

(28)
with \(n_1 + n_2 + n_3 = N\) and \(\sum_{n_1,n_2,n_3} |C_{n_1n_2n_3}|^2 = 1\). We define
\[
|\mathcal{C}_{n_1}|^2 \equiv \sum_{n_2=0}^{N-n_1} |C_{n_1,n_2,N-n_1-n_2}|^2
\] (29)
and note that \(\sum_{n_1=0}^{N} |\mathcal{C}_{n_1}|^2 = 1\). The variance \(\Delta n_1^2\) of \(\langle \hat{n}_1 \rangle\) can then be written as
\[
\Delta n_1^2 = \langle (\hat{n}_1 - \langle \hat{n}_1 \rangle)^2 \rangle = \sum_{n_1=0}^{N} |\mathcal{C}_{n_1}|^2 n_1^2 - \left( \sum_{n_1=0}^{N} |\mathcal{C}_{n_1}|^2 n_1 \right)^2.
\] (30)

Analogous to our proof of Theorem 1, it follows that for a three-site lattice the maximum number fluctuations are \(\Delta n_1^2 = N^2/4\), obtained for \(|\mathcal{C}_{n_1}|^2 = 1\) for any \(n_1 \in 1, \ldots, N\). Similarly, the minimum number fluctuations are \(\Delta n_1^2 = 0\), obtained for \(|\mathcal{C}_{n_1}|^2 = 1/2\). Thus, we recover the same values for the minimum and maximum number fluctuations as in the case of two lattice sites, see Sec. IV. For a lattice with \(s\) sites the same reasoning applies if \(|\mathcal{C}_{n_1}|^2\) is redefined as the sum over all absolute value squares of coefficients with exactly \(n_1\) bosons at lattice site \(i = 1\) [see Eq. (34) below]. Thus, we find
\[
\max \Delta n_i^2 = \frac{N^2}{4}, \quad \min \Delta n_i^2 = 0,
\] (31)
for the absolute maximum and minimum number fluctuations for lattices with \(s\) sites.

In the present calculation no assumption was made about the symmetry of the wave function. Hence, states that maximize the number fluctuations \(\Delta n_i^2\) will generally have different number fluctuations at different lattice sites. This can easily be seen by noticing that, e.g., the state \(\frac{1}{\sqrt{2}}(|N,0,0\rangle + |0,0,N\rangle\rangle\) has number fluctuations \(\Delta n_1^2 = N^2/4\) at the first, but \(\Delta n_2^2 = 0\) at the second lattice site. States that maximize number fluctuations and possess the symmetry of the lattice will be treated next.

**B. Symmetry restricted lattice states**

We will now require that all lattice sites be equivalent with mean occupation \(\langle \hat{n}_i \rangle = N/s\). Since all sites are assumed to be equivalent we will drop the site index from now on. As before, we begin with \(s = 3\) lattice sites. It is easy to see that the three-site lattice caton
\begin{align}
|\Psi_{cat-3}\rangle &= \frac{1}{\sqrt{3}} \left( |1^N\rangle + |2^N\rangle + |3^N\rangle \right) \\
\text{has mean occupation } \langle \hat{n} \rangle &= \frac{N}{3} \quad \text{and number fluctuations} \\
\Delta n_{cat-3}^2 &= \frac{2}{9} N^2
\end{align}
for all three sites. Its number fluctuations are slightly less than the maximal possible value \( \Delta n^2 = N^2/4 \), and we will now show that these are also the maximum number fluctuations under the constraint of equivalent sites.

As an ansatz for the wave function on the lattice we use Eq. (32). Let us focus again on the number fluctuations on one, say the first, of the \( s \) equivalent lattice sites and define the quantities
\begin{equation}
|C_{n_1}|^2 \equiv \sum_{n_2=0}^{N-n_1} \cdots \sum_{n_{s-1}=0}^{N-n_1-\cdots-n_{s-1}} |C_{n_1,\ldots,n_1-\cdots-n_{s-1}}|^2.
\end{equation}
The requirement of mean occupation \( N/s \) on all lattice sites can be written as
\begin{equation}
\sum_{n_i=0}^{N} |C_{n_i}|^2 n_i - \frac{N}{s} = 0
\end{equation}
for \( i = 1, \ldots, s \). Using the equivalence of all sites, we can focus on the first lattice site, and after dropping the site index the problem reduces to finding the extremum of the functional
\begin{align}
\tau[\{C_n\}, \{\overline{C}_n\}] &= \sum_{n=0}^{N} |C_n|^2 n^2 - \left( \sum_{n=0}^{N} |C_n|^2 n \right)^2 \\
&\quad - \mu \left( \sum_{n=0}^{N} |\overline{C}_n|^2 n - \frac{N}{s} \right)
\end{align}
where the normalization \( \sum_{n=0}^{N} |C_n|^2 = 1 \) is used. This normalization constraint can be used to eliminate \( |\overline{C}_n|^2 \) in Eq. (36), giving
\begin{align}
\tau &= \sum_{n=0}^{N-1} |\overline{C}_n|^2 (N-n)^2 - \left( \sum_{n=0}^{N-1} |\overline{C}_n|^2 (N-n) \right)^2 \\
&\quad + \mu \left( \sum_{n=0}^{N-1} |\overline{C}_n|^2 (N-n) - \frac{s-1}{s} N \right).
\end{align}
For an extremum \( \partial \tau / \partial C_n^* = 0 \) must hold, i.e.
\begin{equation}
0 = \left[ (N-n)^2 - 2(N-n) \left( \frac{s-1}{s} N \right) + \mu (N-n) \right] \overline{C}_n
\end{equation}
for \( n = 0, \ldots, N-1 \). If \( \overline{C}_n = 0 \) for \( n = 0, \ldots, N-1 \), Eqs. (38) are satisfied, but it follows from the normalization that \( |\overline{C}_N|^2 = |C_{N,0,\ldots,0}|^2 = 1 \), i.e. the ansatz wave function, Eq. (8),
reduces to \(|N, 0, \ldots, 0\rangle\). Not all sites are equivalent in the state \(|N, 0, \ldots, 0\rangle\) and therefore there is no solution with \(C_n = 0\) for \(n = 0, \ldots, N - 1\). Thus at least one \(|C_n|^2\) must be nonzero for \(n = 1, \ldots, N - 1\). Assuming one particular nonzero \(C_n\), Eq. (38) puts the constraint

\[ \mu = N \frac{s - 2}{s} + n \]  

for each value of \(n \in 1, \ldots, N - 1\) on \(\mu\). Obviously, this constraint can only be satisfied for at most one \(n\). Thus, solutions to Eqs. (38) must be of the form \(C_n \neq 0\) and \(C_N \neq 0\), and the normalization constraint becomes \(|C_n|^2 + |C_N|^2 = 1\). Likewise, the requirement of mean occupation \(N/s\) reads \(N/s = |C_n|^2 n + |C_N|^2 N\). The two conditions can be combined to express \(|C_N|^2\) and \(|C_n|^2\) as

\[ |C_N|^2 = \frac{1}{s} \frac{N - sn}{N - n}, \]
\[ |C_n|^2 = 1 - \frac{1}{s} \frac{N - sn}{N - n} \]

which in turn can be used to express \(\Delta n^2 = |C_n|^2 n^2 + |C_N|^2 N^2 - (|C_n|^2 n + |C_N|^2 N)^2\) after some algebra as

\[ \Delta n^2 = -n \frac{s(s - 1)N}{s^2} + \frac{s - 1}{s^2} N^2. \]  

The maximum of \(\Delta n^2\) as a function of \(n\) is obtained for \(n = 0\) with

\[ \max \Delta n^2 = \frac{s - 1}{s^2} N^2. \]  

Substituting \(n = 0\) in Eqs. (40) we find that the maximum particle number fluctuations for states with equivalent lattice sites are obtained for

\[ |C_0|^2 = \frac{s - 1}{s}, \quad |C_N|^2 = \frac{1}{s}. \]

Let us now return to the three-site lattice caton state, given in Eq. (32). By setting \(s = 3\) in Eq. (42) and comparing the result to Eq. (33), we find that \(|\Psi_{\text{cat}}\rangle\) is a state that maximizes the particle number fluctuations under the constraint that all three sites are equivalent. Note that also states with nonzero relative phases between the components of \(|\Psi_{\text{cat}}\rangle\) would lead to the same number fluctuations, but the sites would generally not be equivalent then. More generally, we find for the \(s\)-site caton state

\[ |\Psi_{\text{cat}}\rangle = \frac{1}{\sqrt{s}} \left( |1^N\rangle + |2^N\rangle + \ldots + |s^N\rangle \right) \]  

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that the number fluctuations are given by
\[ \Delta n_{\text{cat}}^2 = \frac{s - 1}{s^2} N^2. \] (45)

This means that \( s \)-site caton states maximize the number fluctuations under the constraint that all sites are equivalent, see Eq. (42).

Let us now discuss \( s \)-site mean-field states. In case that \( N/s \) is integer, it is easy to see that the Mott insulating state
\[ |\Psi_{MI}\rangle = |1^{N/s}, 2^{N/s}, \ldots, s^{N/s}\rangle \] (46)
is a lattice state with equivalent sites that minimizes the number fluctuations with \( \Delta n_{MI}^2 = 0 \). Therefore, the complete range of number fluctuations under the constraint of equivalent sites is
\[ 0 \leq \Delta n^2 \leq \frac{s - 1}{s^2} N^2. \] (47)

Lastly, we define \( \hat{b}^\dagger_g = \frac{1}{\sqrt{s}} (\hat{b}_1^\dagger + \ldots + \hat{b}_s^\dagger) \) and discuss the superfluid lattice state
\[ |\Psi_{sf}\rangle = |g^N\rangle. \] (48)
The ground state of noninteracting bosons in a lattice potential is of this form and its number fluctuations are given by
\[ \Delta n_{sf}^2 = N \frac{s - 1}{s^2}. \] (49)

By comparison with Eq. (47) it becomes clear that the superfluid state \( |\Psi_{sf}\rangle \) is about in the middle of the range of possible number fluctuations. It is fully condensed and hence its first order RDM has only one macroscopic eigenvalue, \( n^{(1)}_1 = N \), i.e. there is no fragmentation. The state \( |\Psi_{sf}\rangle \) is by far the most intensively studied state and concludes our investigation here.

VI. CONCLUSIONS

We have studied the number fluctuations and the fragmentation of various many-boson states, focusing on ultracold spatially split systems. Number fluctuations are a key quantity in determining the state of a quantum system. We have shown that there is a great indeterminacy if number fluctuations are considered alone. Additional observables will have to be considered to allow for conclusive results, e.g. the fragmentation. For an overview of the obtained results please see Table I.
Table I. Number fluctuations and fragmentation of different spatially split bosonic objects. Given are the number of sites over which the object is distributed, the largest eigenvalue of the first-order reduced density matrix $n_1^{(1)}$, the number fluctuations $\Delta n^2$ and the maximally obtainable number fluctuations $\text{max} \Delta n^2$. Only objects for which all sites are equivalent are shown.

| Object         | # sites | $n_1^{(1)}$ | $\Delta n^2$ | $\text{max} \Delta n^2$ |
|----------------|---------|-------------|---------------|--------------------------|
| Caton          | 2       | $N/2$       | $N^2/4$       |                          |
| g/u Caton      | 2       | $N/2$       | $N/4$         | $N^2/4$                  |
| Soliton trains | 2       | $N$         | $N/4$         |                          |
| Fragmenton     | 2       | $N/2$       | $N^2/8 + N/4$ |                          |
| Lattice caton  | $s$     | $N/s$       | $N^2(s - 1)/s^2$ |                    |
| Mott-insulator | $s$     | $N/s$       | 0             | $N^2(s - 1)/s^2$         |
| Superfluid     | $s$     | $N$         | $N(s - 1)/s^2$ |                          |

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