Fragmentation of phase-fluctuating condensates

Oleksandr V. Marchukov\textsuperscript{1,2} and Uwe R. Fischer\textsuperscript{1}

\textsuperscript{1}Center for Theoretical Physics, Department of Physics and Astronomy, Seoul National University, 08826 Seoul, Republic of Korea
\textsuperscript{2}School of Electrical Engineering, Faculty of Engineering, Tel Aviv University, 6997801, Tel Aviv, Israel

(Dated: October 10, 2017)

We study zero-temperature quantum phase fluctuations in harmonically trapped one-dimensional interacting Bose gases, using the self-consistent multiconfigurational time-dependent Hartree method. In a regime of mesoscopic particle numbers and moderate contact couplings, it is shown that the phase-fluctuating condensate is properly described as a fragmented condensate. In addition, we demonstrate that the spatial dependence of the amplitude of phase fluctuations significantly deviates from what is obtained in Bogoliubov theory. Our results can be verified in currently available experiments. They therefore provide an opportunity both to experimentally benchmark the multiconfigurational time-dependent Hartree method, as well as to directly observe, for the first time, the quantum many-body phenomenon of fragmentation in single traps.

I. INTRODUCTION

The standard paradigm of the weakly interacting Bose gas is Bogoliubov theory\cite{1}. A single orbital is occupied macroscopically, with a continuum of excitations existing on top of this condensate. On the other hand, in spatial dimension smaller than three, the absence of such a Bose-Einstein condensate (BEC) in infinitely extended homogeneous systems directly follows from the fundamental quantum statistical Bogoliubov inequality\cite{1}, as derived in\cite{2–4}. More recently, the advances in modern precision experiments using ultracold atomic gases have rekindled the interest in the coherence properties of low-dimensional quantum gases\cite{5,6}.

For finite systems, which are those actually realized in experiments with trapped Bose gases, the question of the existence of BEC in low dimensions is more intricate. For example, a one-dimensional (1D) BEC, at given interaction coupling and density, can exist up to a critical length of the condensate\cite{7,8}. Within the realm of Bogoliubov theory\cite{9,10}, its extension to quasicondensates\cite{11}, and the Luttinger liquid approach\cite{12}, phase fluctuations have been shown to gradually destroy off-diagonal-long-range-order (ODLRO) in finite 1D Bose-Einstein condensates, and to lead to a characteristic power law decay of correlation functions. These phase-fluctuating condensates have been probed in numerous experiments, initially in\cite{13,14}, and with increasing sophistication in recent years cf., e.g.,\cite{16–20}.

Our primary aim in what follows is to show that phase-fluctuating 1D condensates are properly to be described as fragmented condensates\cite{21,22} in a self-consistent many-body approach. The many-body correlations corresponding to fragmentation are not captured by mean-field theories, for which all excited modes are uncorrelated with each other and with the condensate. Fragmented condensates in 1D harmonic traps, on the other hand, must be described by a self-consistent theory which accommodates the correlations between all significantly occupied orbitals. Importantly, we reveal that this remains true even at very small degrees of fragmentation of the order of percent, and thus for moderate coupling constants and densities (particle numbers in the range $N = 10–100$). In particular, we show that, on the self-consistent level, the phase fluctuations develop a peak in position space, which is akin to what is observed for a pair of bosons in Monte Carlo simulations at infinitely large interactions and low densities in the Tonks-Girardeau limit\cite{24}. This peak is absent in Bogoliubov mean-field theory and its extension to larger coupling in Luttinger liquid theory\cite{12}. The fluctuation peak height is essentially proportional to the degree of fragmentation. In addition, the mean-field phase fluctuations saturate at large distances, while we find that they decrease again towards the condensate border. We take these facts as concrete evidence that inhomogeneous phase-fluctuating fragmented condensates in a harmonic trap must be described by self-consistent many-body solutions that go beyond hydrodynamic, local density, and Hartree-Fock type approximations.

The importance of many-body correlations between all modes in the phase-fluctuating regime which we reveal can be verified by current experiments\cite{16–20}. This facility of experimental access is in marked contrast to the large degrees of fragmentation necessary to observe significant density-density correlations\cite{25}. Our self-consistent many-body results therefore pave the way to study experimentally the many-body phenomenon of fragmentation in a single harmonic trap\cite{25}. They provide a benchmark to correlate theory and experiment in quantum many-body physics, and in principle to arbitrarily high order in the correlation functions\cite{18}.

II. MANY-BODY FORMALISM

In the interacting Bose gas, the (basis invariant) definition of BEC is due to Penrose and Onsager\cite{21}. It employs the position space single-particle density matrix
in its eigenbasis,

$$\rho^{(1)}(x, x') = \langle \hat{\psi}^\dagger(x) \hat{\psi}(x') \rangle = \sum_{i=1}^{M} N_i \varphi_i^*(x) \varphi_i(x'),$$  \hspace{1cm} (1)

where \( \hat{\psi}^\dagger(x) \) and \( \hat{\psi}(x) \) are bosonic creation and annihilation field operators, respectively. The angled brackets indicate quantum-statistical average over states; we work at zero temperature. Furthermore, \( \varphi_i(x) \) are the single-particle wavefunctions (called natural orbitals in this eigenbasis of \( \rho^{(1)}(x) \)), \( N_i \) are their occupation numbers, and \( M \) is the number of orbitals (in practice fixed to be a finite number by the available computational resources).

The definition \[21\] states that if a subset of the eigenvalues \( N_i \) are “macroscopic,” i.e. some of the \( N_i/N \) remain finite in the large \( N \) limit, then the many-body state of the Bose gas is a simple or fragmented BEC when the cardinality of this subset is one or larger than one, respectively \[22\] \[23\]. We note that this formal definition must obviously remain somewhat vague where there is no thermodynamic limit of very large \( N \), but this does not usually lead to practical difficulties.

The Hamiltonian that we consider to address the many-body problem describes bosons interacting by a contact pseudopotential and placed in a harmonic trap:

$$H = \sum_{i=1}^{N} \left( \frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 x_i^2 \right) + g_{1D} \sum_{i>j} \delta(x_i - x_j).$$ \hspace{1cm} (2)

Here, \( x_i \) and \( p_i \) are 1D position and momentum operators of a given atom (or molecule) \( i \), respectively, \( \omega \) is the frequency of the trapping harmonic potential, \( N \) is the number of particles, \( m \) is their mass, and \( g_{1D} \) is the contact coupling. In order to establish the connection with experiment, one considers a 1D gas, i.e. the particles are trapped in a three-dimensional (3D) harmonic potential that is strongly anisotropic, with the transverse frequency being much larger than the axial one, \( \omega/\omega_\perp \ll 1 \), such that transverse motion is confined (frozen) to the ground state. The 1D coupling strength, \( g_{1D} \), is related to the 3D scattering length, \( a_{sc} \), by \( g_{1D} = 4\pi \hbar^2 a_{sc}/(\pi m l_\perp^2) \) far away from geometric scattering resonances, where \( l_\perp = \sqrt{\hbar/m \omega_\perp} \) is the transverse oscillator length \[24\].

The homogeneous quantum many-body problem corresponding to the Hamiltonian \[2 \] without harmonic trap (\( \omega = 0 \)) can be solved by Bethe ansatz, as was shown long ago by Lieb and Liniger \[28\]. On the other hand, for trapped (spatially confined) and thus generally inhomogeneous systems, the mathematical case most relevant to actual experiments, the exact solution is not known (except for the hard-core limit \[29\]). There are several numerical methods that are applicable to the present problem, such as, for example, density matrix renormalization group \[30\] \[31\] and quantum Monte Carlo methods \[32\]. Here, we used the multiconfigurational time-dependent Hartree (MCTDH) method for bosons \[33\] and, in particular, its implementation MCTDH-X \[34\]. This powerful method, long known in physical chemistry for distinguishable particles \[35\] \[36\], has since the advent of ultracold quantum gases proven its value for the study of the correlation properties of fragmented BECs cf., e.g., \[37\] \[40\], cf. Appendix A for a concise summary.

III. DEFINITION OF PHASE FLUCTUATIONS

Using the representation of the field operators \( \hat{\psi}(x) = e^{i \phi(x)} \sqrt{\rho(x)}, \hat{\psi}^\dagger(x) = \sqrt{\rho(x)} e^{-i \phi(x)} \), where \( \rho(x) \) is the particle density operator and \( \hat{\phi}(x) \) is a (hermitian) phase operator, the single-particle density matrix can be written in the form \( \rho^{(1)}(x, x') = \langle \sqrt{\rho(x)} e^{-i(\hat{\phi}(x) - \hat{\phi}(x'))} \sqrt{\rho(x')} \rangle \). It is well known that one should exercise care when defining the number and phase operators in this way, as thoroughly reviewed in Refs. \[47\] \[48\]; also see the coarse-graining procedure applied in \[11\]. We will use the definition above which coincides with the traditional Dirac approach \[48\], since we consider that particle density fluctuations are small, and to directly relate our results with previous work performed in \[9\] \[49\]. One then has

$$\langle \hat{\psi}^\dagger(x) \hat{\psi}(x') \rangle = \sqrt{\rho(x) \rho(x')} \exp \left[ -\frac{1}{2} \langle \delta \phi_{xx'}^2 \rangle \right],$$ \hspace{1cm} (3)

where \( \delta \phi_{xx'} = \hat{\phi}(x) - \hat{\phi}(x') \) is the phase difference operator and \( \rho(x) = \langle \hat{\psi}^\dagger(x) \hat{\psi}(x) \rangle \) is the mean local density; we neglected density fluctuations. Solving for \( \langle \delta \phi_{xx'}^2 \rangle \), we obtain a direct relation of mean-square phase fluctuations and single-particle density matrix in position space:

$$\langle \delta \phi_{xx'}^2 \rangle = -2 \ln \left[ \frac{\langle \hat{\psi}^\dagger(x) \hat{\psi}(x') \rangle}{\sqrt{\rho(x) \rho(x')}} \right].$$ \hspace{1cm} (4)

The above relation represents the definition of phase fluctuations within our analysis. Below, we aim to demonstrate that at mesoscopic numbers of particles trapped in a 1D harmonic oscillator potential with contact interaction, the mean-square phase fluctuations obtained by using self-consistent calculations differ significantly from mean-field results (cf., e.g., Refs. \[9\] \[49\]). Using the diagonalized form of the single-particle density matrix in Eq. \[1 \] one can rewrite Eq. \[4 \] as

$$\langle \delta \phi_{xx'}^2 \rangle = -2 \ln \left[ \frac{\sum_{i=1}^{M} N_i \varphi_i^*(x') \varphi_i(x)}{\sqrt{\rho(x) \rho(x')}} \right].$$ \hspace{1cm} (5)

We evaluate \[5 \] after finding the many-body ground state of the system using MCTDH-X \[24\]. For our calculations with \( N = 10 \) and \( N = 30 \), we used five available orbitals, \( M = 5 \), to ensure that there is no significant occupation in the highest orbitals. For a larger particle number, \( N = 100 \), we used four available orbitals, \( M = 4 \), due
TABLE I. Table of relative occupation numbers, \(n_i = N_i/N\) for \(N = 10\) and various couplings \(g_0\) [Eq. (6)].

| \(g_0\) | \(n_1\)  | \(n_2\)  | \(n_3\)  | \(n_4\)  | \(n_5\)  |
|---------|---------|---------|---------|---------|---------|
| 0.1     | 0.99875 | 0.00095 | 0.00022 | 0.00004 | 0.00002 |
| 0.5     | 0.98068 | 0.01338 | 0.00425 | 0.00119 | 0.00049 |
| 0.75    | 0.96611 | 0.02241 | 0.00788 | 0.00254 | 0.00105 |
| 1.0     | 0.95152 | 0.03087 | 0.01168 | 0.00418 | 0.00175 |

It is convenient to introduce a dimensionless, scaled interaction parameter

\[
g_0 = mg_{1D}/\hbar^2 = 4a_{sc}/l_{\perp}^2,
\]

where \(l = \sqrt{\hbar/m\omega}\) is the axial harmonic oscillator length. We considered the range \(g_0 = 0.1 - 1.0\), which even for our relatively small number of particles corresponds to the weakly-interacting Bose gas in the Thomas-Fermi regime [9]. This range of couplings is well within current experimental possibilities [16–20].

IV. RESULTS

The occupation numbers we obtain after convergence of the self-consistent equations has been reached, for \(N = 10\) and varying interaction strength \(g_0\), are given in Table I (for \(N = 30\) and \(N = 100\), cf. the discussion in Appendix B). We see that the degree of fragmentation, defined as the fraction of particles not being in the energetically lowest orbital, \(1 - n_1\), grows rapidly with interaction strength. However, for the \(g_0\) ranges we consider the fragmentation is still in the range of a few percent only. This, in turn, also represents a condition for our calculations, with a fixed number of orbitals \(M = 5\), to be reliable for the chosen range of \(g_0\).

In Fig. 1, we display surface plots of the mean-square quantum phase fluctuations \(\langle \delta \phi_{x,x'}^2 \rangle\) in the \(x-x'\) plane for three different values of dimensionless interaction strength. We see two very distinct bulges that emerge even for small interaction, which grow in size with increasing interaction strength. The detailed shape and fine structure of the bulges corresponds to the shape and weight of the different orbitals in the self-consistent solution for the quantum field. The emergence of the bulges has the direct interpretation of the loss of phase coherence between distant parts of the cloud by phase fluctuations. This phase-phase-correlations induced phenomenon is conjugate to the coherence loss indicated by density-density correlations which was discussed in [25].

Fig. 2 shows the dependence of the maximum value of phase fluctuations \(\Phi^2 := \max[\langle \delta \phi_{x,x'}^2 \rangle]\) (measured at the top of the bulges in Fig. 1), and of the degree of fragmentation \(1 - n_1\), as functions of the dimensionless interaction strength \(g_0\). We recognize a very smooth, almost linear dependence of both quantities on \(g_0\). The inset shows that their ratio slightly decreases with coupling strength (by about 15\% over the range of \(g_0\) investigated). We conjecture that this slight decrease is related to the increasing importance of density fluctuations contributing to the degree of fragmentation when one increases the coupling towards the boson-localized Tonks-Girardeau regime. The smooth dependence on \(g_0\) we get is expected from the fact that we observed in our
FIG. 2. Maximum value of mean-square phase fluctuations of (5) $\Phi^2 := \max[\langle \hat{\delta} \phi_{xx}^2 \rangle]$ (peak height in Fig. 1), and fragmentation degree, $1 - n_1$, where $n_1$ is the occupation number of the energetically lowest orbital, as function of interaction strength $g_0$, for $N = 10$. The inset shows the ratio of the maximum fluctuation $\Phi^2$ and fragmentation degree $1 - n_1$.

FIG. 3. The comparison of phase fluctuations $\langle \hat{\delta} \phi_{x0}^2 \rangle$, calculated in the hydrodynamic mean-field approach [19] (black solid line) and self-consistently with MCDTH using (3) (blue dashed line) for $N = 10$ and different interaction strengths: a) $g_0 = 0.1$, b) $g_0 = 0.5$, c) $g_0 = 0.75$ and d) $g_0 = 1.0$. The axial coordinate $x$ is scaled by the size of the gas cloud $R$.

simulations that the shape of the orbitals does not change drastically by increasing the interaction strength.

Hence, we obtain as an important result that in our regime of moderate couplings the degree of fragmentation $1 - n_1$ is a measure of the maximal strength of phase fluctuations. To gain further insight, in Fig. 3 we compare the phase fluctuations relative to the cloud center, $\langle \hat{\delta} \phi_{x0}^2 \rangle$, with those obtained from the hydrodynamical limit of Bogoliubov theory, which read [19]

$$\langle \hat{\delta} \phi_{x0}^2 \rangle_{\text{mf}} = \frac{\sqrt{2} g_0 l}{\pi R} \left( 2 \ln \left( \frac{R}{l} \right) - \text{Ci} \left( \frac{2 R |x|}{l^2} \right) + \text{Ci} \left( \frac{2 |x|}{R} \right) \right).$$

Here, $R$ is the total length of the cloud, calculated from the domain in which the density of the gas is not zero, and $	ext{Ci}(x) = -\int_{x}^{\infty} \cos(t) dt / t$ is the Cosine integral function.

The difference which manifests itself in Fig. 3 is evident: The mean-field result does, in particular, not capture the distinct phase fluctuation maximum in the middle of the cloud which is due to the self-consistently obtained precise shape of the orbitals, and has a tendency to overestimate the magnitude of phase fluctuations. Moreover, the mean-field phase fluctuations saturate to an asymptotic value at the edge of the cloud for mean-field. On the other hand, we obtain that, rather, the fluctuations decrease again towards the boundaries of the cloud. As a result, self-consistent many-body physics predicts potentially larger, more stable 1D condensates, because distant regions of the cloud tend to remain more phase-correlated than in mean field.

The emergence of the local phase-fluctuation maximum we observe within MCDTH is akin to the first-order correlation function dips obtained in Monte Carlo calculations for the Tonks-Girardeau limit of very strong interactions [24]. The self-consistent approach MCDTH, similarly, therefore contains many-body correlations between field-operator modes with spatially inhomogeneous modulus, which mean field and local density approximations, by their construction, do not describe.

V. DISCUSSION

To summarize, our primary result is twofold. First, that self-consistent many-body calculations for a 1D trapped Bose gas, performed with MCTDH-X, reveal that phase-fluctuating BECs are properly to be described as fragmented condensates containing many-body correlations between all significantly occupied orbitals. And, second, that the spatial dependence of phase fluctuations obtained via mean-field theory is both qualitatively and quantitatively different from the self-consistent one. As a corollary, we conclude that self-consistency is crucial for the accuracy and predictive power of many-body calculations, even when the degree of fragmentation is as small as on the level of percent. This is because 1D mean-field, despite its being reliable in the case of very large particle numbers and very weak couplings, does not describe the more subtle many-body correlations which develop for even moderate interaction strengths. Future work we envisage includes exploring the relevance of self-consistency to the large fragmentation regime, and thus its potential impact on the crossover location to the Tonks-Girardeau gas in a single harmonic trap [19, 20, 50].

Our results suggest a pathway to implement an experimental benchmark for MCTDH, by verifying its predictive power through readily accessible experimental...
[1] N. N. Bogoliubov, *Quantum and Classical Statistical Mechanics (Classics of Soviet Mathematics, Vol 2, Part 2)* (Gordon and Breach, New York, 1982).

[2] N. D. Mermin and H. Wagner, “Absence of Ferromagnetism or Antiferromagnetism in One- or Two-Dimensional Isotropic Heisenberg Models,” Phys. Rev. Lett. 17, 1133–1136 (1966).

[3] P. C. Hohenberg, “Existence of Long-Range Order in One and Two Dimensions,” Phys. Rev. 158, 383–386 (1967).

[4] L. Pitaevskii and S. Stringari, “Uncertainty principle, quantum fluctuations, and broken symmetries,” *Journal of Low Temperature Physics* 85, 377–388 (1991).

[5] C. J. Pethick and H. Smith, “Lower dimensions,” in *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, 2008) pp. 444–480.

[6] M. A. Cazalilla, R. Citro, T. Giamarchi, E. Orignac, and M. Rigol, “One dimensional Bosons: From Condensed Matter Systems to Ultracold Gases,” *Rev. Mod. Phys.* 83, 1405–1466 (2011).

[7] Uwe R. Fischer, “Existence of Long-Range Order for Trapped Interacting Bosons,” Phys. Rev. Lett. 89, 280402 (2002).

[8] Uwe R. Fischer, “Maximal length of trapped one-dimensional Bose-Einstein condensates,” *Journal of Low Temperature Physics* 138, 723–728 (2005).

[9] D. S. Petrov, G. V. Shlyapnikov, and J. T. M. Walraven, “Regimes of Quantum Degeneracy in Trapped 1D Gases,” Phys. Rev. Lett. 85, 3745 (2000).

[10] D. S. Petrov, G. V. Shlyapnikov, and J. T. M. Walraven, “Phase-Fluctuating 3D Bose-Einstein Condensates in Elongated Traps,” Phys. Rev. Lett. 87, 050404 (2001).

[11] Christophe Mora and Yvan Castin, “Extension of Bogoliubov theory to quasicondensates,” Phys. Rev. A 67, 053615 (2003).

[12] D. M. Gangardt and G. V. Shlyapnikov, “Stability and Phase Coherence of Trapped 1D Bose Gases,” Phys. Rev. Lett. 90, 010401 (2003).

[13] S. Dettmer, D. Hellweg, P. Rytty, J. J. Arita, W. Ertmer, K. Sengstock, D. S. Petrov, G. V. Shlyapnikov, H. Kreutzmann, L. Santos, and M. Lewenstein, “Observation of Phase Fluctuations in Elongated Bose-Einstein Condensates,” Phys. Rev. Lett. 87, 160406 (2001).

[14] D. Hellweg, L. Cacciapuoti, M. Kottke, T. Schulte, K. Sengstock, W. Ertmer, and J. J. Arita, “Measurement of the Spatial Correlation Function of Phase Fluctuating Bose-Einstein Condensates,” Phys. Rev. Lett. 91, 010406 (2003).

[15] S. Richard, F. Gerbier, J. H. Thywissen, M. Hugbart, P. Bouyer, and A. Aspect, “Momentum Spectroscopy of 1D Phase Fluctuations in Bose-Einstein Condensates,” Phys. Rev. Lett. 91, 010405 (2003).

[16] S. Hofferberth, I. Lesanovsky, T. Schumm, A. Imambekov, V. Gritsev, E. Demler, and J. Schmiedmayer, “Probing quantum and thermal noise in an interacting many-body system,” Nature Physics 4, 489–495 (2008).

[17] S. Manz, R. Bucker, T. Betz, Ch. Koller, S. Hofferberth, I. E. Mazets, A. Imambekov, E. Demler, A. Perrin, J. Schmiedmayer, and T. Schumm, “Two-point density correlations of quasicondensates in free expansion,” Phys. Rev. A 81, 031610 (2010).

[18] Thomas Schweiger, Valentin Kasper, Sebastian Erne, Igor Mazets, Bernhard Rauer, Federica Cataldi, Tim Langen, Thomas Gasenzer, Jurgen Berges, and Jorg Schmiedmayer, “Experimental characterization of a quantum many-body system via higher-order correlations,” Nature 545, 323–326 (2017).

[19] Thibaut Jacquin, Julien Armijo, Tarik Berrada, Karen V. Kheruntsyan, and Isabelle Bouchoule, “Sub-Poissonian Fluctuations in a 1D Bose Gas: From the Quantum Quasicondensate to the Strongly Interacting Regime,” Phys. Rev. Lett. 106, 230405 (2011).

[20] Bess Fang, Aisling Johnson, Tommaso Roscilde, and Isabelle Bouchoule, “Momentum-Space Correlations of a One-Dimensional Bose Gas,” Phys. Rev. Lett. 116, 050402 (2016).

[21] Oliver Penrose and Lars Onsager, “Bose-Einstein Condensation and Liquid Helium,” Phys. Rev. 104, 576–584 (1956).

[22] Anthony J. Leggett, “Bose-Einstein condensation in the alkali gases: Some fundamental concepts,” Rev. Mod. Phys. 73, 307–356 (2001).

[23] Erich J. Mueller, Tin-Lun Ho, Masahito Ueda, and Gordon Baym, “Fragmentation of Bose-Einstein condensates,” Phys. Rev. A 74, 033612 (2006).

[24] A. Minguzzi, P. Vignolo, and M. P. Tosi, “High-momentum tail in the Tonks gas under harmonic confinement,” Physics Letters A 294, 222–226 (2002).

[25] Myung-Kyun Kang and Uwe R. Fischer, “Revealing Single-Trap Condensate Fragmentation by Measuring Density-Density Correlations after Time of Flight,” Phys. Rev. Lett. 113, 140404 (2014).

[26] Philipp Bader and Uwe R. Fischer, “Fragmented Many-Body Ground States for Scalar Bosons in a Single Trap,” Phys. Rev. Lett. 103, 060402 (2009).

[27] Maxim Olschanski, “Atomic Scattering in the Presence of an External Confinement and a Gas of Impenetrable Bosons,” Phys. Rev. Lett. 81, 938 (1998).

[28] Elliott H. Lieb and Werner Liniger, “Exact Analysis of an Interacting Bose Gas. I. The General Solution and the accessible in current experiments as well [54, 55].

VI. ACKNOWLEDGMENTS

We thank Axel Lode and Marios Tsatsos for their help with the MCTDH method as well as with the application of the MCDTH-X package. This research was supported by the NRF Korea, Grant No. 2014R1A2A2A01006535.
Ground State," Phys. Rev. 130, 1605–1616 (1963).

[29] A. G. Volosniev, D. V. Fedorov, A. S. Jensen, M. Valiente, and N. T. Zinner, “Strongly interacting confined quantum systems in one dimension,” Nature Communications 5, 5300 (2014).

[30] Steven R. White, “Density matrix formulation for quantum renormalization groups,” Phys. Rev. Lett. 69, 2863–2866 (1992).

[31] Karen Hallberg, “New Trends in Density Matrix Renormalization,” Adv. Phys. 55, 477–526 (2006).

[32] Brian M. Austin, Dmitry Yu. Zubarev, and William A. Lester, “Quantum Monte Carlo and Related Approaches,” Chemical Reviews 112, 263–288 (2012).

[33] Ofir E. Alon, Alexej I. Streltsov, and Lorenz S. Cederbaum, “Multi-configurational time-dependent Hartree method for bosons: Many-body dynamics of bosonic systems,” Phys. Rev. A 77, 033613 (2008).

[34] A. U. J. Lode, M. Tsatsos, and E. Fasshauer, “MCTDH-X: The time-dependent multiconfigurational Hartree for indistinguishable particles software,” http://ultracold.org.

[35] H.-D. Meyer, U. Manthe, and L. S. Cederbaum, “The multi-configurational time-dependent Hartree approach,” Chemical Physics Letters 165, 73–78 (1990).

[36] H.-D. Meyer, F. Gatti, and G. A. Worth, eds., Multi-dimensional Quantum Dynamics: MCTDH Theory and Applications (John Wiley & Sons, 2009).

[37] Ofir E. Alon and Lorenz S. Cederbaum, “Pathway from Condensation via Fragmentation to Fermionization of Cold Bosonic Systems,” Phys. Rev. Lett. 95, 140402 (2005).

[38] Kaspar Sakmann, Alexej I. Streltsov, Ofir E. Alon, and Lorenz S. Cederbaum, “Exact Quantum Dynamics of a Bosonic Josephson Junction,” Phys. Rev. Lett. 103, 220601 (2009).

[39] Axel U. J. Lode, Kaspar Sakmann, Ofir E. Alon, Lorenz S. Cederbaum, and Alexej I. Streltsov, “Numerically exact quantum dynamics of bosons with time-dependent interactions of harmonic type,” Phys. Rev. A 86, 063606 (2012).

[40] Alexej I. Streltsov, “Quantum systems of ultracold bosons with customized interparticle interactions,” Phys. Rev. A 88, 041602 (2013).

[41] Uwe R. Fischer, Axel U. J. Lode, and Budhadipta Chatterjee, “Condensate fragmentation as a sensitive measure of the quantum many-body behavior of bosons with long-range interactions,” Phys. Rev. A 91, 063621 (2015).

[42] Shachar Klaiman and Ofir E. Alon, “Variance as a sensitive probe of correlations,” Phys. Rev. A 91, 063613 (2015).

[43] Shachar Klaiman and Lorenz S. Cederbaum, “Overlap of exact and Gross-Pitaevskii wave functions in Bose-Einstein condensates of dilute gases,” Phys. Rev. A 94, 063648 (2016).

[44] M. C. Tsatsos, M. J. Edmonds, and N. G. Parker, “Transition from vortices to solitonic vortices in trapped atomic Bose-Einstein condensates,” Phys. Rev. A 94, 023627 (2016).

[45] Kaspar Sakmann and Mark Kasevich, “Single-shot simulations of dynamic quantum many-body systems,” Nature Physics 12, 451–454 (2016).

[46] Axel U. J. Lode and Christoph Bruder, “Fragmented Superradiance of a Bose-Einstein Condensate in an Optical Cavity,” Phys. Rev. Lett. 118, 013603 (2017).

[47] P. Carruthers and Michael Martin Nieto, “Phase and Angle Variables in Quantum Mechanics,” Rev. Mod. Phys. 40, 411–440 (1968).

[48] Robert Lynch, “The quantum phase problem: a critical review,” Phys. Rep. 256, 367–436 (1995).

[49] Tin-Lun Ho and Michael Ma, “Quasi 1 and 2d Dilute Bose Gas in Magnetic Traps: Existence of Off-Diagonal Order and Anomalous Quantum Fluctuations,” Journal of Low Temperature Physics 115, 61 (1999).

[50] Note that [37] has treated this crossover to “fermionization” (that is, the one-dimensional localization of hard-core bosons), however within a double well.

[51] Kang-Soo Lee and Uwe R. Fischer, “Truncated many-body dynamics of interacting bosons: A variational principle with error monitoring,” International Journal of Modern Physics B 28, 1550021 (2014).

[52] Uwe Manthe, “The multi-configurational time-dependent Hartree approach revisited,” The Journal of Chemical Physics 142, 244109 (2015).

[53] Jayson G. Cosme, Christoph Weiss, and Joachim Brand, “Center-of-mass motion as a sensitive convergence test for variational multimode quantum dynamics,” Phys. Rev. A 94, 043603 (2016).

[54] M. Gring, M. Kuhnert, T. Langen, T. Kitagawa, B. Rauer, M. Schreitl, I. Mazets, D. Adu Smith, E. Demler, and J. Schmiedmayer, “Relaxation and Prethermalization in an Isolated Quantum System,” Science 337, 1318–1322 (2012).

[55] T. Langen, R. Geiger, M. Kuhnert, B. Rauer, and J. Schmiedmayer, “Local emergence of thermal correlations in an isolated quantum many-body system,” Nature Physics 9, 640–643 (2013).

Appendix A: Multiconfigurational time-dependent Hartree method

We present, for the sake of being self-contained, here a brief description of the multiconfigurational time-dependent Hartree (MCTDH) method that we use for our self-consistent many-body calculations. The method has been generalized to apply for all indistinguishable particles [34]; here, we focus on bosons. For more detailed reviews and examples see Refs. [33] [35] [36].
A system of $N$ interacting bosons is described by using the time-dependent Schrödinger equation

$$
\sum_{i=1}^{N} \hat{h}(x_i; t) + \sum_{i>j} \hat{W}(x_i - x_j) \right) \Psi(x_1, \ldots, x_N; t) = i\hbar \frac{\partial \Psi}{\partial t},
$$

(A1)

where $\hat{h}(x_i; t) = \frac{p_i^2}{2m} + V(x_i)$ is the one-body Hamiltonian, with $m$ as mass of the particles, $x_i$ and $p_i$ as position and momentum operators of a given boson $i$, and $V(x_i)$ as the potential energy. The term $\hat{W}(x_i - x_j)$ is the pairwise particle interaction operator. The many-body wavefunction, $\Psi(x_1, \ldots, x_N; t)$, in the MCTDH formulation is expressed by the following ansatz

$$
|\Psi\rangle = \sum_{\{\vec{N}\}} C_{\vec{N}}(t)|\vec{N}; t\rangle,
$$

(A2)

where the basis $|\vec{N}; t\rangle$ consists of all possible symmetrized wavefunction products of $N$ particles (permanents) distributed over $M$ single-particle functions (orbitals), where $\vec{N} = (N_1, N_2, \ldots, N_M)$ and $N_1 + N_2 + \cdots + N_M = N$, i.e. $N_j$ represents the occupation of the orbital $j$, and $C_{\vec{N}}(t)$ are the time-dependent expansion coefficients. The basis size equals $(N+M-1)!/(N!M-1)!$, i.e. the total number of distributions of $N$ particles among $M$ orbitals. In the language of second quantization, the permanents can be written as

$$
|\vec{N}; t\rangle = \frac{1}{\sqrt{N_1!N_2!\cdots N_M!}} (b_{1}^\dagger (t))^{N_1} (b_{2}^\dagger (t))^{N_2} \cdots (b_{M}^\dagger (t))^{N_M} |\text{vac}\rangle.
$$

(A3)

The operator $b_{j}^\dagger (t)$ is the time-dependent bosonic creation operator, and $|\text{vac}\rangle$ is the vacuum state. Clearly, the ansatz is exact if $M \to \infty$, that is if we consider the full Hilbert space of the problem. In practice, this is however not possible due to the unavoidable computational constraints for any nontrivial (that is, two-body interacting) problem, however for large enough $M$, i.e., when the occupation of the highest orbitals is negligible, the many-body function (A2) represents a numerically exact solution of time-dependent many-body Schrödinger equation.

In order to calculate the expansion coefficients $C_{\vec{N}}(t)$ and orbitals $\{|\varphi_j(x_i; t)\rangle, \ j = 1, \ldots, M\}$, one applies the Dirac-Frenkel variational principle to the action

$$
S([C_{\vec{N}}(t)], \{|\varphi_j(x_i; t)\rangle\}) = \int dt \left[ \langle \Psi | \hat{H} - i\hbar \frac{\partial}{\partial t} | \Psi \rangle - \sum_{j,k=1}^{M} \mu_{jk}(t) (\langle \varphi_j | \varphi_k \rangle - \delta_{jk}) \right],
$$

(A4)

where $\mu_{jk}(t)$ are time-dependent Lagrange multipliers, ensuring that the orbitals remain orthonormal. The variational procedure gives the equations of motion

$$
i\hbar \frac{\partial C(t)}{\partial t} = H(t) C(t),
$$

$$
i\hbar \frac{\partial |\varphi_j\rangle}{\partial t} = \hat{P} \left[ \hat{h} |\varphi_j\rangle + \sum_{k,s,q,j,l=1}^{M} \rho_{jk}^{-1} \rho_{k\text{slot}} \hat{W}_{sl} |\varphi_q\rangle \right],
$$

(A5)

that can be solved numerically in order to obtain the many-body wavefunction $\Psi(x_1, \ldots, x_N; t)$. Here, $C(t)$ is the column vector that consists of all possible expansion coefficients $C_{\vec{N}}(t)$, $H(t)$ is a matrix composed of matrix elements of the time-dependent Hamiltonian in the corresponding basis $|\vec{N}; t\rangle$, $\hat{W}_{sl} = \int \int dx dx' \varphi_s^*(x) W(x - x') \varphi_l(x')$ are the local interaction potentials, $\hat{P} = 1 - \sum_{k'=1}^{M} |\varphi_k'\rangle \langle \varphi_k'|$ is a projection operator, and $\rho_{jk}$ and $\rho_{k\text{slot}}$ are the matrix elements of the one-body and two-body density matrices, respectively.

The system of coupled equations in Eqs. (A5) is to be solved both for the orbitals and expansion coefficients together. This constitutes the notion of self-consistency in inhomogenous quantum many-body systems of interacting bosons we employ throughout the paper.
Appendix B: MCDTH Results for larger particle numbers

Here, we discuss the results of our calculations with an increased number of particles, \( N = 30 \) and \( N = 100 \). The main features are qualitatively very similar to the \( N = 10 \) case. Tables II and III shows the relative occupation numbers of the orbitals. Note that the energy shift due to the interactions is proportional to the number of particles, i.e. for the same value of the numerical parameter \( g_0 \) the actual interaction differs for systems with a different number of particles. That explains the slight increase in the fragmentation degree for the systems with larger particle numbers we report below. The degree of fragmentation \( 1 - n_1 \) is again not large, but not negligible even for relatively weak interaction.

| \( g_0 \) | \( n_1 \) | \( n_2 \) | \( n_3 \) | \( n_4 \) |
|---|---|---|---|---|
| 0.1 | 0.99694 | 0.00220 | 0.00064 | 0.00015 | 0.00006 |
| 0.5 | 0.97256 | 0.01633 | 0.00698 | 0.00277 | 0.00016 |
| 0.75 | 0.95917 | 0.02303 | 0.01067 | 0.00473 | 0.00136 |
| 1.0 | 0.94785 | 0.02843 | 0.01381 | 0.00653 | 0.00337 |

TABLE II. Table of relative occupation numbers, \( n_i = N_i/N \) for \( N = 30 \), and various dimensionless couplings \( g_0 \), which are defined in Eq. (6) of the main paper.

| \( g_0 \) | \( n_1 \) | \( n_2 \) | \( n_3 \) | \( n_4 \) |
|---|---|---|---|---|
| 0.1 | 0.99503 | 0.00334 | 0.00113 | 0.00044 |
| 0.5 | 0.97889 | 0.01192 | 0.00622 | 0.00297 |
| 0.75 | 0.97360 | 0.01433 | 0.00808 | 0.00398 |
| 1.0 | 0.96983 | 0.01595 | 0.00946 | 0.00477 |

TABLE III. Table of relative occupation numbers, \( n_i = N_i/N \) for \( N = 100 \), and various dimensionless couplings \( g_0 \), which are defined in Eq. (6) of the main paper. Note that due to the technical challenges we used \( M = 4 \) number of orbitals for these calculations.

In Fig. 7 we show surface plots of the mean-square of quantum fluctuations \( \langle \delta \phi_{xx'}^2 \rangle \) in the \( x - x' \) plane for various values of the dimensionless interaction strength \( g_0 \). Bulges of a similar geometric shape to the \( N = 10 \) case emerge, cf. Fig. 1 since the shape of the correlations is dictated by the geometry of the trapping potential and single-particle orbitals. Fig. 8 shows the dependence of the maximum value of mean-square phase fluctuations \( \Phi^2 := \max[\langle \delta \phi_{xx'}^2 \rangle] \) and fragmentation degree \( 1 - n_1 \), as a function of dimensionless coupling \( g_0 \). We see that \( \Phi^2 \) grows slightly slower for \( N = 30 \) than for \( N = 10 \), but remains a smooth and almost linear function of \( g_0 \), cf. Fig. 2. Finally, Fig. 6 displays the comparison of the MCTDH calculations with the hydrodynamic limit of Bogoliubov theory \( 49 \). As for \( N = 10 \), cf. Fig. 3, the results are qualitatively different for the mean-field and MCTDH calculations. This is to be expected, since we still consider a relatively small number of particles.

Similarly, qualitatively comparable results are also obtained when \( N = 100 \). In Fig. 7 we show surface plots of the mean-square of quantum fluctuations as in Figs. 1 and 4. The aim here is to demonstrate that the effects described in the main text also appear for a larger (by one order of magnitude), experimentally attainable, number of particles. Note that for the Fig. 7 we used a smaller number of orbitals, \( M = 4 \), due to the increased numerical demand. Note also that the existence of additional local maxima, which can already be observed in Fig. 4, is more prominent for the larger system \( N = 100 \). That is to be expected, since in the large \( N \) limit the mean-field results should be reproduced. We argue that Figs. 8 and 9 support this claim. As in Fig. 8 we plot the maximum value of mean-square phase fluctuations, \( \Phi^2 := \max[\langle \delta \phi_{xx'}^2 \rangle] \), and fragmentation degree, \( 1 - n_1 \), as functions of the interaction strength, \( g_0 \). We can see a tendency to saturation for both, and especially for \( \Phi^2 \). In Fig. 9 we again compare our numerical results to the mean-field calculations. It is clear that the discrepancy between the results remains even for larger number of particles. However, the peak in phase fluctuations that is very prominent for \( N = 10 \) becomes less so, and it is not unreasonable to suspect that for an even larger number of particles the hydrodynamic mean-field calculations will be reproduced by the MCTDH method. Still, it remains obviously a challenging computational task, if one is to include a reasonable number of natural orbitals in the calculation for large \( N \).
FIG. 4. Mean-square quantum phase fluctuations $\langle \delta \phi^2 \rangle$ for $N = 30$ and varying interaction strength: a) $g_0 = 0.1$, b) $g_0 = 0.5$, and c) $g_0 = 1.0$. The maxima along the off-diagonals, $x' = -x$, correspond to the fact that the gas becomes phase-uncorrelated in distant regions of the cloud.
FIG. 5. Maximum value of mean-square phase fluctuations of (5) $\Phi^2 := \max[\langle \delta\phi_x^2 \rangle]$ (peak height in Fig. 4), and fragmentation degree, $1 - n_1$, where $n_1$ is the occupation number of the energetically lowest orbital, as function of interaction strength $g_0$, for $N = 30$. The inset shows the ratio of the maximum fluctuation $\Phi^2$ and fragmentation degree $1 - n_1$.

FIG. 6. The comparison of phase fluctuations $\langle \delta\phi_x^2 \rangle$, calculated in the hydrodynamic mean-field approach [49] (black solid line) and self-consistently with MCDTH using (5) (blue dashed line) for $N = 30$ and different interaction strengths: a) $g_0 = 0.1$, b) $g_0 = 0.5$, c) $g_0 = 0.75$ and d) $g_0 = 1.0$. The axial coordinate $x$ is scaled by the size of the gas cloud $R$. 
FIG. 7. Mean-square quantum phase fluctuations $\langle \delta \phi^2 \rangle_{x,x'}$ for $N = 100$ and varying interaction strength: a) $g_0 = 0.1$, b) $g_0 = 0.5$, and c) $g_0 = 1.0$. The maxima along the off-diagonals, $x' = -x$, correspond to the fact that the gas becomes phase-uncorrelated in distant regions of the cloud.
FIG. 8. Maximum value of mean-square phase fluctuations of $\Phi^2 := \max[\langle \hat{\delta}\phi_{x0}^2 \rangle]$ (peak height in Fig. 7), and fragmentation degree, $1 - n_1$, where $n_1$ is the occupation number of the energetically lowest orbital, as function of interaction strength $g_0$, for $N = 100$. The inset shows the ratio of the maximum fluctuation $\Phi^2$ and fragmentation degree $1 - n_1$.

FIG. 9. The comparison of phase fluctuations $\langle \hat{\delta}\phi_{x0}^2 \rangle$, calculated in the hydrodynamic mean-field approach [49] (black solid line) and self-consistently with MCDTH using (5) (blue dashed line) for $N = 100$ and different interaction strengths: a) $g_0 = 0.1$, b) $g_0 = 0.5$, c) $g_0 = 0.75$ and d) $g_0 = 1.0$. The axial coordinate $x$ is scaled by the size of the gas cloud $R$. 