Interacting trapped bosons yield fragmented condensate states in low dimensions

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We investigate the level population statistics and degree of coherence encoded in the single-particle density matrix of harmonically trapped low-dimensional [quasi-one-dimensional (quasi-1D) or quasi-two-dimensional (quasi-2D)] Bose gases with repulsive contact interactions. Using a variational analysis, we derive fragmentation of the condensate in the weakly confining directions into two (quasi-1D) respectively three (quasi-2D) mutually incoherent macroscopic pieces, upon increasing a dimensionless interaction measure beyond a critical value. Fragmented condensate many-body states in low-dimensional systems therefore occur well before the thermodynamic limit of infinite extension is reached, in which phase fluctuations of the matter wave field create an infinite number of nonmacroscopic fragments.

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I. INTRODUCTION

Bose-Einstein condensation, the macroscopic occupation of one field operator mode (= single-particle orbital), ceases to exist in the thermodynamic limit of infinite extension in spatial dimension less or equal to two \cite{1, 2}, as a direct consequence of the Bogoliubov inequality \cite{2}. This so-called Hohenberg-Mermin-Wagner theorem has been argued also to hold for systems with a nonvanishing cross-section (quasi-1D) or a finite thickness (quasi-2D) \cite{4}. On the other hand, for a finite extension respectively radius of curvature along the cylinder axis or in the plane, condensation can persist \cite{5}. Low-dimensional Bose gases are nowadays routinely created by varying cloud aspect ratios in strongly anisotropic trapping geometries of magneto-optical or purely optical origin \cite{6-8}. While the very existence of condensates does not depend on interaction in the thermodynamic limit, the increasing dependence of their detailed dynamical and static properties on the interaction coupling when lowering the dimensionality has been demonstrated experimentally \cite{9, 10} as well as investigated theoretically \cite{11, 12}.

The search for fragmented condensate states of Bose gases, that is the macroscopic occupation of more than one field operator mode with no mutual coherence between them, has a long history, see, e.g., \cite{13, 14}. The obvious general difficulty in answering the rather delicate question whether a given system is coherent (a condensate) or fragmented consists in solving an interacting many-body problem, from which the single-particle density matrix follows. The latter, by definition \cite{13}, gives the degree of fragmentation versus that of any remaining coherence.

In the following, we shall show that fragmentation of condensates takes place well before the thermodynamic limit is reached in lower-dimensional Bose gases. We thus argue that interaction-induced fragmented phases, with only a few macroscopically occupied modes (termed fragmented condensates \cite{16}, exist before fragmentation into infinitely many incoherent pieces of nonmacroscopic size sets in, occurring when in the thermodynamic limit phase fluctuations destroy the condensate in the quasi-1D or quasi-2D low-dimensional regimes \cite{1, 2}.

We concentrate on the point where fragmentation sets in first, into two (quasi-1D) respectively three (quasi-2D trapping geometry) modes with no coherence between them, which may be described by the solution of a many-body problem essentially exactly solvable for any strength of interaction. Thus we demonstrate how the formalism laid down in \cite{17} leads to fragmentation of a scalar Bose gas in the weakly confining directions. It is stressed that for a trapped system positive interaction couplings lead to fragmentation above a critical value, counter to the expectation from the nontrapped thermodynamic continuum limit, where the physics is homogeneous and the Fock exchange term in the total energy is preventing fragmentation \cite{14}.

II. QUASI-1D TRAPPING GEOMETRY

We begin with the simple case of one excitation direction along the weakly confining (z) axis of a Bose gas in the quasi-1D limit. Assuming that only two (the energetically lowest) longitudinal modes are significantly occupied [that is, with macroscopic occupation numbers of \(O(N)\)], we restrict the expansion of the field operator to these two modes, \(\Psi(r) = \sum_{i=0,1} a_i \Psi_i(r)\); the modes are normalized to unity, \(\int d^3r |\Psi_i(r)|^2 = 1\).

The validity of the two-mode approximation on the mean-field level and in double-well traps has been discussed in \cite{18, 19}. In the following, we go beyond mean-field (solve for the full quantum solution) and consider a single trap, determining the interaction-dependent orbital parameters self-consistently by looking for the ground state variationally (see below). The two-mode...
approximation can then be expected to represent accurately the interacting many-body physics in a quasi-1D trapping setup for much larger values of the coupling constant than one would anticipate from a mean-field analysis with fixed orbitals [19].

Consider the interacting two-mode Hamiltonian

$$\hat{H} = \sum_{i=0}^{n} \epsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{A_1}{2} \hat{a}_i^\dagger \hat{a}_i \hat{a}_0 \hat{a}_0 + \frac{A_2}{2} \hat{a}_i^\dagger \hat{a}_i \hat{a}_1 \hat{a}_1 + \frac{A_3}{2} \hat{a}_i^\dagger \hat{a}_i \hat{a}_0 \hat{a}_0$$

with the interaction coefficients $A_1 = V_{0000}$, $A_2 = V_{1111}$, $A_3 = V_{1101}$, $A_4 = V_{0101} + V_{0110}$, and $A_5 = V_{0011} + V_{0101} + V_{0110}$, where the interaction matrix elements are given by $V_{ijkl} = g \int d^3 r \psi_{i}^*(r) \psi_{j}^*(r) \psi_{k}(r) \psi_{l}(r)$. The contact interaction is assumed to be repulsive, $g = 4\pi a_s > 0$, with $a_s$ the $s$-wave scattering length (we put $\hbar = m = 1$, where $m$ is the boson mass); the single-particle energies $\epsilon_{i} \geq \epsilon_{0}$. The pair-exchange coefficients $A_3$ are real or complex numbers depending on the choice of modes ($A_1, A_2, A_4$ are always real by definition), and in general do not vanish in a spatially confined gas. The spatial basis dependence of the Hamiltonian stemming from the position dependence of the modes’ phase is contained in the values of the $A_3$, and is reflected in the correlation functions characterizing the response of the system to external perturbations. Global phase shifts, $\psi_{k}(r) \rightarrow e^{i\theta_k} \psi_{k}(r)$ with $\theta_k$ constants, as is well known, leave the correlation functions invariant.

We perform an expansion of the two-mode many-body wavefunction in a Fock basis,

$$|\Psi\rangle = \sum_{l=0}^{N} \psi_l |N-l,l\rangle,$$

so that $\psi_l$ is the probability amplitude for $l$ particles residing in the excited state [15]. The total density then is given by $\langle \Psi | \hat{\rho}(|r|) | \Psi \rangle = \sum_{l=0}^{N} \psi_{l}^2 \left[(N-l) \langle \rho_o (r) \rangle + l \langle \rho_1 (r) \rangle\right]$. 

Nonvanishing pair coherence, as defined by the expectation value $\frac{1}{2} \langle \Psi | \hat{a}_0^\dagger \hat{a}_0 \hat{a}_1 \hat{a}_1 + \hat{a}_1^\dagger \hat{a}_1 \hat{a}_0 \hat{a}_0 | \Psi \rangle = \text{Re} \left[ \sum_{l=0}^{N} d_l \psi_{l+1} \psi_{l+2} \right]$, where the pair-exchange coefficient

$$d_l = \sqrt{(l+2)(l+1)(N-l-1)(N-l)}$$

is enforced by energy minimization, and yields definite a value of $A_3$ and coherent pair oscillations between the two modes, with $A_3$ equal to their frequency. These coherent pair oscillations are thus in analogy to Josephson oscillations, which are due to an off-diagonal matrix element of the single-particle density matrix $\langle \Psi | \hat{a}_0^\dagger \hat{a}_1 | \Psi \rangle \propto N$, analogously represented by single-particle exchange terms of the form $-\frac{A_3}{2} \hat{a}_0^\dagger \hat{a}_1 + \text{h.c.}$ in the Hamiltonian, where $\Omega$ is the Josephson frequency.

Minimizing the energy with respect to the Fock state amplitudes $\psi_{l}$, the linear system to be solved reads

$$E\psi_l = \frac{A_3}{2} (d_l \psi_{l+2} + d_{l-2} \psi_{l-2}) + \epsilon_l \psi_l,$$

where $E = \langle \Psi | \hat{H} | \Psi \rangle$ is the total energy. The diagonal coefficient reads $\epsilon_l = \epsilon_0 (N-l) + \epsilon_l + \frac{1}{2} A_1 (N-l)(N-l-1) + \frac{1}{2} A_2 (l-1) + \frac{1}{2} A_3 (N-l)$. The above discrete equation connects the values of $\psi_{l}$ on $l$-sites” differing by two, and leads to alternating signs within the even and odd $l$ sectors of the $\psi_{l}$ when $A_3 > 0$, $\text{sign}(\psi_{l+2}) = -1$. As a result, $\text{sign}(\psi_{l+1}) = (\pm (-1)^l)$, the $\pm$ sign reflecting the initial condition on the $\psi_{l}$ [20]. This, then, leads to the destruction of first-order coherence defined by $g_1 = \frac{1}{2} \langle \psi_{l+1}^* \psi_{l} \rangle = \text{Re} \left[ \sum_{l=0}^{N} \psi_{l+1} \psi_{l} \sqrt{l(l+1)} \right]$, provided $A_1 + 2 A_2 + 3 A_3 - 4 A_4 > 0$ [17].

We take as the (real) modes the ground and first excited state oscillator modes along the cylinder axis

$$\psi_{0}(r,z) = \frac{1}{\sqrt{2\pi R_z}} \exp\left[-\frac{z^2}{2R_z^2} - \frac{r^2}{2l_z^2}\right],$$

$$\psi_{1}(r,z) = \frac{\sqrt{z}}{R_z} \psi_{0}(z),$$

where $R_z$ is a variational parameter for the orbital delocalization length away from the harmonic oscillator ground state in which $R_z \equiv l_z = l_z z^{-1/2}$, $\omega_z$, $\omega_z$, $\omega_{\perp}$ are the harmonic trapping frequencies in the $z$ and radial directions, respectively, where $l_z = \omega_z^{-1/2}$, $l_{\perp} = \omega_{\perp}^{-1/2}$ are the corresponding harmonic oscillator lengths. The transverse degrees of freedom are assumed to be frozen, so that the transverse part of the wave function is the harmonic oscillator ground state. The above choice for the modes leads to $A_3$ real and positive (note that generally $A_4 = 4 A_3$ for real modes and contact interaction).

The single-particle energies of the motion along $z$, occurring in the Hamiltonian [11] [the single-particle energy in the transverse direction is dynamically irrelevant], are $\epsilon_0 = \frac{\hbar^2}{4} R_z^2 \omega_z^2 + \frac{1}{4} l_z^2$ and $\epsilon_{1} = 3\epsilon_{0}$, while the interaction coefficients for these orbitals are $A_1 = U_0 = g/(R_z R_z^2 (2\pi)^{3/2})$, $A_1/A_2 = \{1, \frac{4}{3}, 2\}$. Analytical expressions for the ground-state distribution can be obtained when the absolute value of the Fock state amplitudes $|\psi(l)|$ is considered as a continuum variable [21]. In the continuum limit we have a Gaussian distribution for the absolute value of $\psi(l)$,

$$|\psi(l)| = \frac{1}{(\pi a_{osc}^2)^{1/4}} \exp\left[-\frac{(l - N - \hat{\gamma})^2}{2a_{osc}^2}\right],$$

where the effective oscillator length $a_{osc}^2 = \frac{\lambda_{osc}}{\sqrt{A_1 + A_2 + A_3 + A_4}}$ and the shift from a fully fragmented state centered at $l = \frac{N}{2}$ reads $\hat{\gamma} = \frac{N (A_1 - A_2) / 2 + \epsilon_{10}}{A_1 + A_2 + A_3 + A_4}$ [17]. The degree of fragmentation is in the two-mode model defined by $\hat{\gamma} = 1 - |\lambda_{0} - \lambda_{1}| / N$, where $\lambda_{0,1}$ are the two eigenvalues of the single-particle density matrix $\rho_{\mu\nu}^{(1)} = \langle \hat{a}_\mu^\dagger \hat{a}_\nu \rangle$, resulting in $(N_i = \langle \hat{n}_i \rangle = \langle \hat{a}_i^\dagger \hat{a}_i \rangle)$

$$\hat{\gamma} = 1 - \sqrt{\frac{1}{N^2} \left( N_0 N_1 - \langle \hat{a}_1^\dagger \hat{a}_1 \rangle^2 \right)},$$
Because in the present case first-order coherence \( \langle \hat{a}_1 \hat{a}_1 \rangle \) essentially vanishes \[20\], the fragmentation measure \( \mathcal{S} \) is simply determined by the mean occupation numbers of the two states. In the continuum limit, the degree of fragmentation is obtained to be \( \mathcal{S} = 1 - \frac{|\mathcal{A}|}{N/2} \). Two-mode fragmentation is therefore in this limit consistently obtained when \( a_{\text{osc}} \) is real as well as \( \mathcal{S} < N/2 \) holds, and is becoming maximal when \( \mathcal{S} = 0 \) \[17\].

The total energy is in the continuum limit \[15\] for the two-mode model \[1\] given by

\[
E = \frac{N^2}{4} A_3 \left( \frac{2}{a_{osc}^2} - 1 \right) + c_{N/2} - \frac{1}{2} \left( \frac{c_0 - c_N}{N^2} \right) a_{osc}^4 A_3 N^2. \tag{7}
\]

The relative values of the interaction coefficients \( A_i \) lead to \( a_{osc}^2 = \sqrt{\frac{2}{N}} \), which results in \( \frac{a_{osc}^2}{\lambda} = \frac{\pi}{3} + \frac{\pi}{2} N X - \frac{8 \pi}{3} X^2 \). The ratio \( X = c_0/(N A_1) = \frac{1}{6} A_1 \left( \frac{1}{A} + A^3 \right) \) is a measure of the ratio of single particle and interaction energies, where the dimensionless variational parameter is defined by \( \Lambda = R_z/l_z \). The shift reads \( \mathcal{S} = \frac{N}{6} (1 - 16 X) \), and the quantity

\[
G_1 = \frac{N g_{l_z}}{(2\pi)^3/2 l_z^3} = \frac{N g_{1D} l_z}{\sqrt{2\pi}} \tag{8}
\]
is a dimensionless measure of interaction strength. We used in the final expression on the right-hand side that the quasi-1D interaction strength reads \( g_{1D} = g/(2\pi l_z^3) = 2a_s/l_z^2 \) (valid when \( a_s \ll l_z \), i.e. away from geometric scattering resonances \[22\]), with dimension of inverse length. Note that \( G_1 \) linearly increases with increasing \( l_z \), indicating that single condensates cease to exist for \( l_z \) going to infinity for any particle number and at any finite interaction strength, which is in accordance with what we would expect from previous studies \[1\] \[2\] \[3\] \[22\].

The total energy obtained from solving the discrete many-body equations is to be minimized to obtain \( \Lambda = \Lambda(G_1) \). The analysis reveals that the numerically determined energy as a function of \( \Lambda \), for a given \( G_1 \), has only one, nonfragmented, minimum for small enough \( G_1 \) below a critical value, while above the latter, a second local minimum appears. The transition to a fragmented state, corresponding to the second minimum at a smaller (scaled) delocalization length \( \Lambda \), is discontinuous, and the degree of fragmentation jumps to a finite value, cf. Fig. \[1\].

Therefore, the phase transition between single condensate and fragmented condensate states obtained within the two-mode model \[1\] is of first order. Increasing the dimensionless interaction measure further, the nonfragmented local minimum gradually disappears (asymptomatically changing into a turning point), and only the fragmented minimum of the total two-mode energy remains (top curve in Fig. \[1\]).

We obtain from the continuum limit Eq. \[7\] for the energy per particle in terms of \( G_1 \) and \( \Lambda \) the following polynomial equation, using that \( G_1 \omega_z/(N A_1) = \Lambda \),

\[
\frac{E}{N \omega_z} = \frac{7}{12} \left( \frac{1}{\Lambda^2} + \Lambda^2 \right) - \frac{1}{6 G_1} \left( \frac{1}{\Lambda^3} + 2 \Lambda + \Lambda^5 \right) + \frac{G_1}{3 \Lambda}. \tag{9}
\]

For large \( \Lambda \), we may approximate the above equation as \( \frac{E}{N \omega_z} \approx \frac{7 \Lambda^2}{12} - \frac{\Lambda^3}{6 G_1} + \frac{G_1}{3 \Lambda} \). The extrema equation is thus quadratic in \( \Lambda^3/G_1 \), so that \( \Lambda \) is scaling with \( G_1^{1/3} \) in this limit; the minimum solution describing a fragmented state is \( \Lambda^3 = \frac{4}{3} G_1 \) (the other solution does not describe a minimum, cf. Fig. \[1\] dashed line). Note that the large \( G_1 \) scaling \( \Lambda \propto (N a_z l_z^3)^{1/3} \) is identical to the single-condensate Thomas-Fermi scaling \[6\] [with a different prefactor]; the quantity \( X = \epsilon_0/(N A_1) \) asymptotes to 1/10 in this limit.

Evaluating in the large \( G_1 \) limit the difference between the fragmented energy minimum of \[9\] at \( \Lambda = (2G_1/5)^{1/3} \) and the energy obtained from a single condensate of all particles residing in the energetically lower mode, \( E_{gs} = \frac{1}{12} \Lambda^2 + \frac{\Lambda^3}{4} + \frac{\Lambda^5}{8} \), which has a minimum at \( \Lambda = G_1^{1/3} \), we get \[24\]

\[
\frac{\Delta E}{N \omega_z} = \frac{E_{gs}}{N \omega_z} - \frac{E}{N \omega_z} \approx 0.02 \times G_1^{2/3}. \tag{10}
\]

The energy difference between single condensate and

![FIG. 1. (Color online) Evolution (not to scale) of the energy landscape as a function of the variational parameter \( \Lambda \), with increasing dimensionless interaction measure, from bottom to top [the energy minima have additionally been shifted relative to each other for clarity]. Energy curves are from the full numerical solution of \[9\]. The continuum limit is indicated by the dashed curve for the energy curve close to criticality (second from the bottom), showing that the continuum limit energy, tending to negative infinity for large \( \Lambda \), does not describe the nonfragmented minima of the total energy, cf. Eq. \[9\]. Beyond a critical interaction measure, a new minimum corresponding to fragmentation appears (empty square), with a discontinuous jump from the nonfragmented minimum (circle) to a smaller \( \Lambda \) (third curve from the bottom). Increasing the interaction measure further, the nonfragmented minimum eventually completely disappears.](image-url)
fragmented condensate ground states is therefore very small around the transition point, increasing with the particle number like $N^{2/3}$.

We obtain in the continuum limit for the degree of fragmentation

$$\bar{\mathcal{S}}(G_1) = 1 - \frac{1}{3} \left( 1 - \frac{4}{3G_1} \right) \approx 1 - \frac{4}{3G_1} \frac{160^{1/3}}{3G_1^{4/3}},$$

(11)

where the last inequality represents the large $G_1$—large $\Lambda$ limit. The maximally achievable two-mode degree of fragmentation from this variational ansatz for the modes is thus 80%. We conclude that fragmentation of the condensate many-body state occurs for sufficiently strong interaction coupling at a given finite extent $R_\perp$ of the cloud, that is when

$$G_1 > (G_1)_c \approx 9.8$$

(12)

where the critical value $(G_1)_c$ for a fragmented minimum of the total energy to first appear, cf. Fig. has been determined from the full numerical solution of [3]. We display the continuum result for $\bar{\mathcal{S}} = \bar{\mathcal{S}}(G_1)$ obtained from the solution of Eq. (11), in Fig. (1). The system is for small interactions and densities ($G_1 = 1$) a single condensate and $\Lambda$ is close to unity; the slow increase of the optimal $\Lambda$ with $G_1$ additionally demonstrates that an ansatz incorporating only the two lowest harmonic oscillator states is a reasonably accurate approximation. For large shift (large $\Lambda$), the continuum description fails, and the full discrete coupled system of equations for $\psi$ in Eq. (3) has to be solved to find the optimal value of $\Lambda$. The result from the (exact) two-mode many-body wavefunction corresponding to the numerical solution of (3) is displayed together with the continuum limit in Fig. (2) where very good agreement is visible.

III. QUASI-2D TRAPPING GEOMETRY

Consider now a cylindrically symmetric trap, with an infinite continuum of excitation directions in real space, that is, in all radial directions. A crucial difference to the quasi-1D case is the topology, resulting in an angular quantum number $m_\phi$. Furthermore, the lowest ($m_\phi = \pm 1$) azimuthal excitation modes of the cylindrically symmetric harmonic oscillator are lower in energy than the radial excitations. The harmonic oscillator ground state in radial as well as transverse directions and the two lowest excited states along the azimuthal direction are given by

$$\psi_0(r,z) = \frac{1}{\sqrt{\pi^{3/2} R_\perp^2 l_z}} \exp \left[ -\frac{r^2}{2R_\perp^2} - \frac{z^2}{2l_z^2} \right],$$

$$\psi_\pm(r,\phi,z) = \frac{r}{R_\perp} \exp[\pm i\phi] \psi_0,$$

(13)

and are thus the three lowest-lying single-particle states.

![Figure 2](image_url)

**FIG. 2.** (Color online) Optimal value of the variational parameter $\Lambda$, and degree of fragmentation $\bar{\mathcal{S}}$ (inset), both as a function of the dimensionless measure of interaction strength $G_1$, in the quasi-1D trapping geometry. Numerical solutions of the discrete set of many-body equations (3) are depicted by blue circles (nonfragmented energy minima), and by red squares, respectively, the larger describing the energy minima at which fragmentation occurs, cf. Fig. The solution in the continuum limit of Eq. (11) is shown for the fragmented state by the black solid line. The number of particles is $N = 500$.

A. Two-mode approximation

We first investigate whether fragmentation occurs between the ground state and a (coherent) superposition of the left- and right-circulating azimuthal waves $\psi_+, \psi_-$. We shall consider below the full three-mode problem of taking all three states in (13) into account, and will show that in the continuum limit the corresponding predictions become essentially identical to those of the simpler two-mode model, which we discuss here to most clearly elucidate the primary differences to the quasi-1D trapping geometry.

We consider an equal-weight coherent superposition for the excited state wavefunction (such that it has angular momentum zero like the ground state),

$$\psi_1 = \frac{1}{\sqrt{2}} (\psi_+ + \psi_-)$$

$$= \sqrt{\frac{2}{\pi^{3/2} R_\perp^2 l_z}} r \cos \phi \exp \left[ -\frac{r^2}{2R_\perp^2} - \frac{z^2}{2l_z^2} \right],$$

(14)

and evaluate the coefficients parametrizing the two-mode Hamiltonian [1]. We obtain $A_1 = g / ((2\pi)^{3/2} R_\perp^4 l_z) \equiv V_0 \equiv \frac{G_\perp}{4\pi A}$ and $A_1/A_1 = \{1, \frac{3}{4}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \} \sim (1, 2, 2, 2, 2, 2)$ with $\Lambda = R_\perp/l_z$; the ratios of the interaction coefficients are therefore identical to the quasi-1D case. We furthermore have $c_0 = \frac{1}{2R_\perp^2} + \frac{1}{2} \omega_z^2 l_z^2$ and $\epsilon_1 = 2\omega_z$. The result for the shift is $\mathcal{S} = \frac{N g}{4\pi A} (1 - 8X)$, with $X = \frac{c_0}{\epsilon_1} = 1 + \frac{\Lambda^3}{20\pi^2}$. The dimensionless interaction measure now is defined to be

$$G_2 = \frac{Ng}{(2\pi)^{3/2} l_z} = \frac{Ng_{2D}}{2\pi}.$$

(15)
It involves \( g_{2D} = g/(\sqrt{2\pi l_z}) \), the quasi-2D coupling constant when \( l_z \gg a_s \), i.e., away from geometric scattering resonances [24]. Observe that the dimensionless interaction strength \( G_2 \) here is independent of the harmonic oscillator length, in marked distinction to its 1D counterpart \( G_1 \) in [5]. This independence characterizes the 2D trapped case as marginal [3], in the sense that for any finite trapping length (nonzero trapping frequency), single condensates persist as long as the interaction coupling is sufficiently small. Physically, this corresponds to the fact that the usual logarithmic divergence of (the integral of) phase fluctuations in two spatial dimensions [2], is cut off by the trapping.

The calculation then proceeds along the same lines as in the quasi-1D case and, again using [14], we have \( E/NA_1 = \frac{N}{2} + \frac{\delta}{2}NX - \frac{4N}{3}X^2 \). The continuum limit energy expression has a form analogous to Eq. (9), using the relation \( G_{2\omega_{\perp}}/(NA_1) = \Lambda^2 \),

\[
\frac{E}{N\omega_{\perp}} = \frac{5}{9}\left( \frac{1}{\Lambda^2} + \Lambda^2 \right) - \frac{1}{6G_2}\left( \frac{1}{\Lambda^2} + 2\Lambda^2 + \Lambda^6 \right) + \frac{G_2}{3\Lambda^3}.
\]

Note, however, the different power law dependence on \( \Lambda \) in the interaction terms.

The minimum equation obtained by differentiating (16) with respect to \( \Lambda \) now is solvable analytically; it is a quadratic equation in \( \Lambda^4 \), yielding

\[
(A_{2m})^4 = \frac{1}{6}\left( 5G_2 - 2 \sqrt{16 - 80G_2 + (G_2)^2} \right)
\]

at the fragmented energy minimum. The large \( G_2 \) scaling \( \Lambda \propto (N\alpha_s/l_z)^{1/4} \) is, like in the quasi-1D setup, identical to the single-condensate Thomas-Fermi scaling [4]; the quantity \( X = \epsilon_0/(NA_1) \) asymptotes here to 1/3. In the large \( G_2 \) limit the energy difference between the fragmented energy minimum of (16) and the energy minimum of \( E_{gs} = \frac{1}{7}(1/\Lambda^2 + \Lambda^2) + G_2/(2\Lambda^2) \) [again assuming all particles to be in the energetically lower mode, i.e., that the many-body state is a simple condensate or equivalently a \( l = 0 \) Fock state], at \( \Lambda = G_2^{1/4} \), is given by \( \Delta E = E_{gs} - \frac{E}{G_2} \approx 0.002 \times G_2^{1/2} \). The energy difference between condensate and fragmented ground states thus increases more slowly than in the quasi-1D case with the dimensionless interaction measure, cf. Eq. (10).

The two-mode fragmentation measure gives

\[
F(G_2) = 1 - \frac{1}{3} \left| 1 - \frac{4(1 + \Lambda^2)}{G_2} \right| \approx \frac{4}{9} - O\left( \frac{1}{G_2} \right) \tag{18}
\]

The maximally achievable two-mode degree of fragmentation from the ansatz [13] is thus 44%. Fragmentation takes place when the dimensionless coupling (cf. Fig. 3 where we compare numerical and continuum limit analytical results for the fragmentation)

\[
G_2 > (G_2)_c \approx 80. \tag{19}
\]

Due to the independence of \( G_2 = \sqrt{2/\pi} N\alpha_s/l_z \) on the trapping in the plane, condensate fragmentation in quasi-2D obtains at fixed transverse trapping solely because of an increase of the combination \( N\alpha_s \).

### B. Three-mode approximation

We now consider all three modes in (13) as the independent field operator modes, \( \hat{\Psi}(r) = \sum_{i=0,\pm} a_i \hat{\Psi}_i(r) \). A significant simplification takes place in the Hamiltonian due to the exact vanishing of the pair-exchange coefficients involving two particles of the same mode \( \pm \) and the single-particle ground state owing to the cylindrical symmetry of the excitation modes. The remaining pair-exchange process is between a pair of counter- and co-propagating azimuthal excitations and the ground state. The Hamiltonian then reads

\[
\hat{H} = \sum_{i=0,\pm} \epsilon_i \hat{n}_i + \frac{B_1}{2} \hat{n}_0(\hat{n}_0 - 1) + \sum_{j=\pm} \frac{B_2}{2} \hat{n}_j(\hat{n}_j - 1) + \frac{B_3}{2} \hat{n}_0 [\hat{n}_+ + \hat{n}_-] + \frac{B_4}{4} \hat{\Psi}_0^\dagger \hat{\Psi}_0^\dagger \hat{\Psi}_+ \hat{\Psi}_- + \text{h.c.} \tag{20}
\]

The interaction coefficient \( B_1 = 2\pi g \int r dr dz \psi_0^2 = g/((2\pi)^{3/2}R_{\perp}^2 l_z) \), and

\[
B_1 = \frac{G_{2\omega_{\perp}}}{NA_1}, \quad B_i/B_1 = \left\{ \frac{1}{2}, 2, 2 \right\} \tag{21}
\]

The single-particle energies are \( \epsilon_0/\omega_{\perp} = \frac{\delta}{2\Lambda} + \frac{B_1}{2} \Lambda^2 \) and \( \epsilon_{\pm} = \epsilon_- = 2\epsilon_0 \). We evaluate the total energy in the
three-state Fock basis, with the following ansatz for the state vector
\[ |\Psi \rangle = \sum_{l,l'} \psi_{l,l'} |N - l - l', l, l'\rangle, \tag{22} \]
that is with the probability amplitudes \( \psi_{l,l'} \) for \( l \) and \( l' \) particles being in the co- and counterpropagating modes,

\[ \langle \Psi | \hat{H} | \Psi \rangle = \sum_{l,l'=0}^{N} |\psi_{l,l'}|^2 \left[ \epsilon_0 N + (\epsilon_1 - \epsilon_0)(l + l') + \frac{B_1}{2} (N - l - l')(N - l' - l' - 1) + \frac{B_2}{2} [l(l - 1) + l'(l' - 1)] \right. \\
\left. + \frac{B_3}{2} (N - l - l')(l + l') + \frac{B_4}{2} l |l| + \frac{B_5}{4} d_{l,l'} \psi_{l+1,l'}^* \psi_{l+1,l'+1} + \text{h.c.} \right. \tag{23} \]

where the pair-exchange coefficient here reads \( d_{l,l'} = \frac{B_3}{2} (N - l - l')(l + l') \), and only diagonal coupling terms occur in \( l\) and \( l'\)

\[ \psi_{l,l'} \equiv \psi_{l,l+k} \equiv \psi_{k}^l \text{ and also the matrix elements } c_{l,l'}, d_{l,l'}; \text{ then, we note that only diagonal coupling terms occur in } \langle \Psi | \hat{H} | \Psi \rangle, \text{ i.e.} \]
\[ E \psi_{l,l'} = c_{l,l'} \psi_{l,l'} + \frac{B_3}{4} d_{l,l'} \psi_{l+1,l'} + \frac{B_3}{4} d_{l-1,l'} \psi_{l-1,l'} \tag{24} \]

where the superscript \( k \) runs from 0 to \( N \), thereby restricting the corresponding \( l \in \{0, \ldots, N/2 - [k/2]\} \). The symmetry of the eigenvalue problem with respect to the exchange of \( l \) and \( l' \) justifies the reduction to \( l \leq l' \) that has been implicitly performed by choosing the ranges of \( k \) and \( l \). Hence all states at a given \( k \neq 0 \) are at least twofold degenerate. The above reformulation of \( \langle \Psi | \hat{H} | \Psi \rangle \) elucidates that different values of \( k \) belong to uncoupled equations and thus allows us to study the lower dimensional problems \( \langle \Psi | \hat{H} | \Psi \rangle \) independently. In matrix language, this observation can be understood as a particular ordering of the \( (l, l') \) indices, such that the eigenvalue problem decomposes into a block diagonal matrix, with each of the \( N + 1 \) blocks corresponding to a symmetric tri-diagonal matrix for a given \( k \) by Eq. \( \langle \Psi | \hat{H} | \Psi \rangle \) and with block sizes

\[ N/2 + 1 - [k/2], \text{ where the square brackets indicate the next larger integer.} \]

In the large \( N \) limit, we again apply the continuum limit \( \int \) to \( \langle \Psi | \hat{H} | \Psi \rangle \), respecting the alternating signs for even and odd values of \( l \) in the \( \psi_{k}^l \), which occur due to the repulsive pair-exchange coupling \( B_3 > 0 \), cf. the corresponding distribution in the quasi-1D case, Eq. \( \langle \Psi | \hat{H} | \Psi \rangle \). Taking the continuum limit yields

\[ -\frac{1}{2m_0} \Delta |\psi_k|^2 + \frac{1}{2} m_0 \Omega^2 (l - \mathcal{G})^2 |\psi_k| = (E - E_0) |\psi_k| \tag{26} \]

with inverse mass coefficient of the harmonic oscillator analogy \( 1/m_0 = \frac{G_2 \omega_+}{8N^2 \Lambda^2} \sqrt{(N - k)^2(N + 3k)} \), the effective frequency

\[ \Omega = \frac{G_2 \omega_+}{\sqrt{2N\Lambda^2}} \sqrt{k^2 + N^2 - \frac{8k^3}{N + 3k} - \frac{\sqrt{(N - k)^2(N + 3k)}}{4}} \tag{27} \]

and the shift of the \( |\psi_k(l)| \) distribution from \( l = N/4 \),

\[ \mathcal{G} = \frac{\omega_+}{m_0 \Omega^2} \left[ \frac{G_2 \omega_+}{\Lambda^2 N} \left( \frac{1}{4} (k + N) + k \sqrt{\frac{N - k}{N + 3k}} \right) \right. \\
\left. + \frac{1}{\Lambda^2} + \Lambda^2 \right]. \tag{28} \]

Finally, the \( l \) independent (but \( k \) dependent) energy shift reads

\[ E_0 = \frac{\omega_+}{4\Lambda^2} \left[ \frac{G_2}{8N} \left( 15N^2 - 2kN - 5k^2 \right) \right. \\
\left. + (1 + \Lambda^4) (3N + k) - \frac{1}{m_0} - \frac{1}{2} m_0 \Omega^2 \mathcal{G}^2. \tag{29} \]

In these expressions, we have substituted the matrix elements \( B_{i} \) with their values obtained from the variational ansatz in \( \langle \Psi | \hat{H} | \Psi \rangle \), and the corresponding single-particle energies \( \epsilon_i \).

The full ground state energy in this limit reads \( E = \Omega/2 + E_0 \) and its variational minimum at \( \Lambda_{3m} \) can be
solved for analytically. We do not display the very lengthy resulting expression here. The Taylor expansion around \( k/N = 0 \) reads, cf. the expression for the two-mode case in \([14]\),

\[
\Lambda_{3m} = \Lambda_{2m} + \frac{G_2}{12G_>} \left( 448 - 151G_2 + 56G_> \right) \left( \frac{k}{N} \right)^2 \quad + O \left( \frac{k}{N} \right)^3
\]  

(30)

with \( G_> = \sqrt{16 - 80G_2 + (G_2)^2} \).

Exactly as in the quasi-2D two mode case, at the transition point where \( G_> \) becomes real, given by \((G_2)_c\) in \([19]\), the continuum limit becomes valid, and matches the newly appearing minimum of the numerical solution of the eigenvalue problem \([26]\). We then precisely recover the two-mode energy in the limit \( N \to \infty \) for \( k = 0 \). This is a nontrivial result, because the corresponding states in the Fock basis do not coincide. Examining the resulting energy minimum at \( \Lambda_{3m} \), we observe a monotonous increase with the eigenvalue index \( k \) and can hence justify focussing only on minimal energy solutions for states around \( k \). Below, we discuss the effects of quasi degenerate states for small \( k \) whose occurrence can be understood in the continuum limit by showing that

\[ \partial_k E_{\text{min}}(k)|_{k=0} = 0. \]

For finite particle numbers, comparing the ground-state energies for the three- and two-mode ansätze, we find that the three-mode model yields a slightly lower energy at \( k = 0 \), of order \( 0.001\omega_\perp \) per particle for particle numbers of order \( N \sim 10^4 \), further decreasing with increasing \( N \) and asymptotically approaching zero due to the identity of the energies in the continuum limit.

The continuum limit, as well as numerical experiments for finite \( N \) thus justify taking the minimal energy solution of the \( k = 0 \) problem as the global ground state, which amounts to taking the state with equally populated counterclockwise and clockwise circulating single-particle modes. However, we note that because of the similarity in structure for the eigenvalue problems of neighbouring values of \( k \), the difference of the minimal energy eigenvalues per particle corresponding to different \( k \) is of order \( \omega_\perp/N \). For large particle numbers, we thus expect quasi-degeneracy of the eigenvalues located around \( k = 0 \), because they then become arbitrarily closely spaced.

To study the consequences on fragmentation, we consider the one-particle density matrix whose off-diagonal elements are given by

\[
\rho_{+-} = \sum_{l,l'} \sqrt{l(l+1)} \psi_{l,l'}^* \psi_{l-1,l'+1},
\]

\[
\rho_{0+} = \sum_{l,l'} \sqrt{(N-l-l')(l+1)} \psi_{l,l'}^* \psi_{l+1,l'},
\]

\[
\rho_{0-} = \sum_{l,l'} \sqrt{(N-l-l')(l'+1)} \psi_{l,l'}^* \psi_{l,l'+1},
\]

(31)

and introduce a generalized fragmentation measure for three modes

\[
\mathfrak{F}(G_2) = 1 - \left| \frac{1}{4} + \frac{1 - G_2/4 + \Lambda_{3m}}{G_2} \right| \approx \frac{1}{3} - O \left( \frac{1}{G_2} \right).
\]

(32)

and has its asymptotic maximum value 33% at large \( G_2 \gg (G_2)_c \), see also the inset of Fig.\([4]\).

In the quasi-degenerate case of large \( N \) we expect many neighbouring low lying \( k \) states to be occupied, leading for any small perturbation to a mixing of different \( k \) states away from \( k = 0 \), and to nonvanishing off-diagonals \([31]\). Hereby coherence is established, and a nonfragmented ground state in terms of the three-mode single-particle density matrix and the corresponding fragmentation measure is obtained. On the other hand, superposition of many modes of different \( k \) leads to a (coherently superposed) excited state of zero angular momentum [taking into account both degenerate sectors corresponding to \( l \leq l' \) and \( l' \leq l \)], and we are then led back to two-mode fragmentation between ground state and the

![Figure 4](image-url)
coherently superposed excited state. This is due to the fact shown in section III A, namely that the two-mode fragmented state is always lower in energy than a single condensate above a critical $G_2$ given by (11).

IV. DISCUSSION AND CONCLUSIONS

We considered harmonically trapped low-dimensional gases and found by a variational analysis that they split from a single macroscopically occupied field operator mode in the weakly confining direction (the condensate) into two (quasi-1D trapping) respectively three (quasi-2D trapping) such macroscopically occupied modes with no remaining phase coherence between them, upon increasing a dimensionless measure of interaction strength beyond a critical value. We have furthermore demonstrated that due to the symmetry of the matrix equations for the state vector amplitudes, three-mode fragmentation is highly susceptible to decay into a two-mode fragmented state in the quasi-2D isotropic trapping geometry.

The results obtained represent, then, to the best of our knowledge the first example of ground-state fragmented scalar condensates in a single trap, and implement the result of (17) in a physically realistic situation. They imply that the quasi-1D and quasi-2D condensates decay into fragmented condensates of a few macroscopically occupied modes for a sufficiently large interaction energy, with the quasi-1D condensates, as could be expected, being significantly more fragile. By way of a numerical example for the quasi-1D situation, trapping frequencies of $\omega_{\perp}/2\pi = 3.5\,\text{Hz}$ and $\omega_{\parallel}/2\pi = 360\,\text{Hz}$ (used in the magnetic trapping setup of (6)) correspond to a ratio $l_{\perp}/l_{\parallel} \simeq 10$. For $^{23}\text{Na}$, we have $l_{\perp} \simeq 1\,\mu\text{m}$. For $a_s \simeq 2.8\,\text{nm}$, the number of atoms driving $G_1$ above its critical value is only of order $N_c \sim 500$. This raises the interesting question what was actually observed in the experiment (4), where the quoted particle numbers are of order $N \sim 10^4$ for the quasi-1D setup. While the threshold to the first onset of fragmentation seems surprisingly low, one should note that the energy difference separating fragmented and nonfragmented condensate states is very small close to the threshold, Eq. (10), the energy barriers between the two states being even smaller, cf. Fig. 1.

In order to observe the (zero temperature) transition point itself, extremely low temperatures would therefore be required. Fragmented condensates become energetically clearly preferred over single condensates at experimentally accessible thermal fluctuation levels only at significantly higher values of the dimensionless interaction measures, and therefore at much higher particle numbers for given trapping frequencies. Another possibility to increase the interaction measures and to obtain fragmented condensate states is to increase the coupling constant itself (16).

We have shown that fragmented condensate states in low-dimensional systems can be obtained well before the thermodynamic limit of infinite extension. While the degree of fragmentation depends on the (number of variational) modes chosen for a particular trapping setup as well as the applied fragmentation measure, the occurrence of few-mode condensate fragmentation for interacting bosonic gases should be a rather generic feature of their many-body physics. Few-mode fragmentation is owed to the confined nature of the system and a sufficiently strong and positive pair-exchange coupling between the bosonic modes.

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