Variance of an anisotropic Bose-Einstein condensate

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Abstract

The anisotropy of a trap potential can impact the density and variance of a Bose-Einstein condensate (BEC) in an opposite manner. We exemplify this effect for both the ground state and out-of-equilibrium dynamics of structureless bosons interacting by a long-range inter-particle interaction and trapped in a two-dimensional single-well potential. We demonstrate that even when the density of the BEC is, say, wider along the $y$ direction and narrower along the $x$ direction, its position variance can actually be smaller and momentum variance larger in the $y$ direction than in the $x$ direction. This behavior of the variance in a many-particle system is counterintuitive. It suggests using the variance as a tool to characterize the strength of correlations along the $y$ and $x$ directions in a trapped BEC.

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I. INTRODUCTION

In quantum mechanics, the variance of an observable $\hat{o}\langle x \rangle$ for a particle described by the wave-packet $\psi(x)$ is often used to interpret and quantify the physical behavior of the particle [1]. For instance, a wider wave-packet has a larger position variance in comparison with a narrower wave-packet which has a smaller position variance. Physically, the two situations are associated, respectively, with de-localization and localization of the quantum particle. In other words, we are often used to infer the position (and momentum) variance from the shape of the density $|\psi(x)|^2$ of the particle. This intuitive or visual picture may vary in a system made of (many) interacting particles. It is the purpose of this work to demonstrate and investigate such many-body effects using Bose-Einstein condensates as an instrumental example.

Bose-Einstein condensates (BECs) made of ultracold atoms have attracted considerable attention [2–13]. On the theory side, many of the investigations to describe their properties have been performed using Gross-Pitaevskii (mean-field) theory, which assumes all bosons to reside in the same orbital. It is generally perceived that Gross-Pitaevskii theory properly describes the ground state as well as the out-of-equilibrium dynamics of (trapped) BECs in the infinite-particle limit, when the product of the number of particles times the scattering length (i.e., the interaction parameter) is constant. Indeed, there are rigorous results which prove (under certain conditions) that the energy per particle and density per particle of the many-boson system coincide in the infinite-particle limit with the respective Gross-Pitaevskii quantities, and that the bosonic system is 100% condensed [14–17], also see in this context [18, 19].

Despite the situation that BECs are 100% in the infinite-particle limit, and that their density per particle and energy per particle coincide with those computed by the Gross-Pitaevskii theory, the story does not end here. In [20, 21] we demonstrated that the variance of a many-particle operator and the uncertainty product of two many-particle operators can substantially deviate from those given by the Gross-Pitaevskii theory, even in the infinite-particle limit when the bosonic system is 100% condensed. Physically, these many-body effects are governed by the (often very small) number of depleted particles which, unlike the non-condensed fraction, does not vanish even in the infinite-particle limit. Mathematically, the difference between the predictions of the many-body and mean-field descriptions can
be tracked down to the subtlety of performing the infinite-particle limit only after (and not before) the many-particle operator is evaluated. In comparison with the variance of an operator of a single particle, the variance of many-particle operators is a much richer quantity, also see [22–25] in this context. At the bottom line, the many-body and mean-field wave-functions themselves differ at the infinite-particle limit and, consequently, their overlap is always smaller than one and can become arbitrarily small [19, 26].

In the present work we would like to investigate the intriguing possibilities which open up for the variance of a trapped BEC in two spatial dimensions, and in particular the connection between shape of the bosonic cloud (i.e., the density) and its position and momentum variance. Intermingled with the above is the investigation of the variance along the pathway from condensation to fragmentation of a trapped BEC. The latter is far away from the infinite-particle limit (where the bosonic system is 100% condensed) which was the focus of previous work [20, 21]. We mention that preliminary results in one spatial dimension were recently reported in [27]. The structure of the paper is as follows. In Sec. II we briefly discuss the variance in a many-body system and its computation from the wave-function of a trapped BEC. In Sec. III we present two detailed investigations, one of the ground state (Subsec. III A) and the second of the out-of-equilibrium dynamics following an interaction quench (Subsec. III B). Conclusions are put forward in Sec. IV. Finally, further details of the numerics and convergence are provided in the Appendix.

II. THEORY

We begin with the many-body Hamiltonian of \( N \) interacting bosons

\[
\hat{H}(\mathbf{r}_1, \ldots, \mathbf{r}_N; \lambda_0) = \sum_{j=1}^{N} \hat{h}(\mathbf{r}_j) + \sum_{j<k} \lambda_0 \hat{W}(\mathbf{r}_j - \mathbf{r}_k).
\]  

(1)

Here \( \hat{h}(\mathbf{r}) = -\frac{1}{2} \frac{\partial^2}{\partial r^2} + \hat{V}(\mathbf{r}) \) is the one-particle Hamiltonian where \( \hat{V}(\mathbf{r}) \) the trap potential and \( \hat{W}(\mathbf{r}_1 - \mathbf{r}_2) \) the inter-particle interaction of strength \( \lambda_0 \). Throughout this work \( \mathbf{r} = (x, y) \) is the position vector in two spatial dimensions and \( \hbar = m = 1 \).

In the time-independent part of our work, \( \hat{H}(\mathbf{r}_1, \ldots, \mathbf{r}_N; \lambda_0) \Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = E \Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \), we investigate the ground state of the bosons, where \( E \) is the energy and \( \Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \) normalized to unity. In the out-of-equilibrium part we solve the time-dependent Schrödinger equation, \( \hat{H}(\mathbf{r}_1, \ldots, \mathbf{r}_N; \lambda_0) \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; t) = i \frac{\partial \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; t)}{\partial t} \), for the
scenario where the system evolves following an interaction quench from \( \lambda_0 \) to \( \lambda'_0 \), with the initial condition \( \Psi(r_1, \ldots, r_N; 0) = \Phi(r_1, \ldots, r_N) \).

To analyze the many-body wave-function \( \Psi(r_1, \ldots, r_N; t) \) we use its reduced one-body and two-body density matrices [28–31]. The reduced one-body density matrix

\[
\rho^{(1)}(r_1, r'_1; t) = \int dr_2 \ldots dr_N \Psi^*(r'_1, r_2, \ldots, r_N; t)\Psi(r_1, r_2, \ldots, r_N; t) = \sum_j \frac{n_j(t)}{N} \alpha_j(r_1; t)\alpha_j^*(r'_1; t)
\]

is prescribed using the natural orbitals \( \alpha_j(r; t) \) and natural occupations \( n_j(t) \). We generally enumerate the occupation numbers in the order of non-increasing values. We call \( \sum_{j>1} n_j(t) \) the number of depleted particles (depletion in short) and \( \sum_{j>1} n_j(t) N \) the depleted fraction. The latter are used to define the degree of condensation of the interacting bosons [32]. The diagonal of the reduced one-body density matrix, \( \rho(r; t) = \rho^{(1)}(r, r; t) \), is referred to as the density. The diagonal part of the reduced two-body density matrix,

\[
\rho^{(2)}(r_1, r_2; r_1, r_2; t) = \int dr_3 \ldots dr_N \Psi^*(r_1, r_2, \ldots, r_N; t)\Psi(r_1, r_2, \ldots, r_N; t) = \sum_{jpkq} \frac{\rho_{jpkq}(t)}{N(N-1)} \alpha_j^*(r_1; t) \alpha_p^*(r_2; t) \alpha_k(r_1; t) \alpha_q(r_2; t),
\]

is expressed using the natural orbitals, where \( \rho_{jpkq}(t) = \langle \Psi(t)|\hat{b}_j^\dagger \hat{b}_p^\dagger \hat{b}_k \hat{b}_q|\Psi(t)\rangle \) and the creation \( \hat{b}_j \) (and annihilation) operators are associated with \( \alpha_j(r; t) \).

Using the density per particle and natural orbitals, the variance per particle of an operator \( \hat{A} = \sum_{j=1}^N \hat{a}(r_j) \) which is local in position space reads [20, 21]

\[
\frac{1}{N} \Delta_{\hat{A}}^2(t) = \frac{1}{N} \left[ \langle \Psi(t)|\hat{A}^2|\Psi(t)\rangle - \langle \Psi(t)|\hat{A}|\Psi(t)\rangle^2 \right] \equiv \Delta_{\hat{A},\text{density}}^2(t) + \Delta_{\hat{A},\text{MB}}^2(t),
\]

\[
\Delta_{\hat{A},\text{density}}^2(t) = \int dr \frac{\rho(r; t)}{N} a^2(r) - \left[ \int dr \frac{\rho(r; t)}{N} a(r) \right]^2,
\]

\[
\Delta_{\hat{A},\text{MB}}^2(t) = \frac{\rho_{1111}(t)}{N} \left[ \int dr |\alpha_1(r; t)|^2 a(r) \right] - (N-1) \left[ \int dr \frac{\rho(r; t)}{N} a(r) \right]^2 + \sum_{jpkq\neq1111} \frac{\rho_{jpkq}(t)}{N} \left[ \int dr \alpha_j^*(r; t) \alpha_k(r; t) a(r) \right] \left[ \int dr \alpha_p^*(r; t) \alpha_q(r; t) a(r) \right].
\]

The first term, \( \Delta_{\hat{A},\text{density}}^2(t) \), describes the variance of \( \hat{a}(r) \) resulting from the density per particle \( \frac{\rho(r; t)}{N} \). The second term, \( \Delta_{\hat{A},\text{MB}}^2(t) \), collects all other contributions to the many-particle variance. \( \Delta_{\hat{A},\text{MB}}^2(t) \) is generally non-zero within a many-body theory, but is identically equal to zero within Gross-Pitaevskii theory. We remark that analogous expressions hold for operators which are local in momentum space.
III. RESULTS

Our system of choice is made of structureless bosons with harmonic inter-particle interaction trapped in a single-well anharmonic potential. Unlike models of particles interacting with harmonic inter-particle interaction and trapped in a harmonic trap, which have been extensively studied and can be solved analytically [33–47], the Schrödinger equation of the trapped BEC has no analytical solution in the present study, nor even the variance can be determined analytically, thus necessitating a numerical treatment.

For this, we have to employ a suitable many-body theoretical and computational approach. Such a many-body tool is the multiconfigurational time-dependent Hartree (MCTDH) for bosons (MCTDHB) method [48, 49] which has been extensively used in the literature [50–67]. For further documentation of MCTDHB see [68–70], and for its benchmarks with an exactly-solvable model [71] (and [72]). MCTDHB can be seen as the indistinguishable-particle bosonic daughter of MCTDH [73–76].

A. Statics

We investigate the variance along the pathway from condensation to fragmentation of the ground state of trapped bosons [77–81]. Fragmentation of BECs has drawn much attention, see, e.g., [82–90]. In particular for structureless bosons with a long-range interaction in a single trap, the ground state has been shown to become fragmented when increasing the inter-particle repulsion [58, 91–95]. Figs. 1, 2, and 3 below collect the results.

The one-body Hamiltonian in (1) is \( \hat{h}(x, y) = -\left( \frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} \frac{\partial^2}{\partial y^2} \right) + \frac{(x^2 + (1-\beta)y^2)^2}{4} \), where the degree of anisotropy is \( \beta \). The inter-particle interaction is harmonic and repulsive, \( \lambda_0 \hat{W}(x_1 - x_2, y_1 - y_2) = -\lambda_0 [(x_1 - x_2)^2 + (y_1 - y_2)^2] \), \( \lambda_0 > 0 \). Fig. 1 depicts snapshots of the density per particle of \( N = 10 \) bosons for three interaction strengths \( \lambda_0 = 0.01, 0.10, \) and \( 0.20 \) [the interaction parameters are \( \Lambda = \lambda_0(N-1) = 0.09, 0.9, \) and \( 1.8, \) respectively] and three degrees of anisotropy \( \beta = 0\% \) (isotropic), \( 10\% \), and \( 20\% \). We follow the changes in the ground state. The density broadens as the interaction is increased. For the isotropic trap, see the upper row Fig. 1a,b,c, the density remains, of course, rotationally symmetric and eventually a torus-like shape emerges. For the anisotropic traps, the density splits into two clouds, see the middle row Fig. 1d,e,f and lower row Fig. 1g,h,i. The more anisotropic
FIG. 1. (Color online) Anisotropy of the variance in the ground state. Shown is the density per particle of $N = 10$ bosons for the interaction strengths $\lambda_0 = 0.01$, 0.10, and 0.20 (left to right columns) and trap anisotropies $\beta = 0\%$ (isotropic), 10%, and 20% (upper to lower rows). Increasing the interaction strength the ground state changes its shape and the reduced one-body density matrix fragments, see Fig. 2. In the upper row, panels (a), (b), and (c), the system is isotropic and naturally the position variances in the $y$ and $x$ directions are equal. In the middle row, panels (d), (e), and (f), and lower row, panels (g), (h), and (i), the system is anisotropic and, as the density in the $y$ direction becomes wider than the density in the $x$ direction, the respective variances surprisingly behave in an opposite manner. That is, the variance in the $y$ direction becomes smaller than that in the $x$ direction, see Fig. 3. This many-body phenomenon, where the anisotropy of the position variance behaves in an opposite manner to the anisotropy of the density, is hence counterintuitive. The results are obtained for $M = 10$ time-adaptive (self-consistent) orbitals. See the text for further discussion. The quantities shown are dimensionless.
is the trap, the more split is the ground-state density for a given interaction parameter.

Along side the changes in the shape of the ground-state density, the reduced one-particle density of the ground state fragments [58, 91–95]. Depending on the anisotropy of the trap and strength of the interaction, the ground state evolves from nearly fully condensed, for $\lambda_0 = 0.01$ and $\beta = 0\%$, to almost fully two-fold fragmented, for $\lambda_0 = 0.20$ and $\beta = 20\%$, see Fig. 2 and discussion below. The more anisotropic is the trap, the more fragmented is the ground state for a given interaction parameter. It is interesting to follow the ‘correlation diagram’ of the occupation numbers [see (2)] for $\lambda_0 = 0.20$. Degenerate occupation numbers for the isotropic trap ($n_2, n_3$ and $n_4, n_5$ for $\beta = 0\%$) split when the anisotropy sets in, and together with the non-degenerate occupation numbers ($n_1$ and $n_6$ for $\beta = 0\%$) essentially merge to pairs ($n_1, n_2$ and $n_3, n_4$ and $n_5, n_6$ for $\beta = 20\%$) when the fragmentation is full, see Fig. 2.

We now move to the central quantity of interest – the variance. Fig. 3 depicts the many-particle position variance per particle, $\frac{1}{N} \Delta^2_{\hat{X}}$, and momentum variance, $\frac{1}{N} \Delta^2_{\hat{P}}$, of the ground state for the interaction strengths $\lambda_0 = 0.01$, 0.10, and 0.20 and anisotropies of the trap $\beta = 0\%$, 10\%, and 20\% discussed above. Generally, enlarging the anisotropy of the trap (in our case along the y-axis) enlarges the area available for the trapped interacting bosons. For the weakest interaction, $\lambda_0 = 0.01$, the position variance along the y-axis increases monotonically, and that along the x-axis hardly changes, see the upper two curves in Fig. 3a. Side by side, the momentum variance along the y-axis decreases monotonically, whereas that along the x-axis decreases very mildly, see the lower two curves in Fig. 3b. These are compatible with the shapes of the density, see the left column Fig. 1a,d,g, and with the occupation numbers, see Fig. 2, indicating that the systems are essentially fully condensed $[\frac{\hat{n}_1}{N} > 0.99(9)$ for all three anisotropies].

Already for $\lambda_0 = 0.10$, changing the anisotropy of the trap leads to a different behavior of the variance. At 10\% anisotropy, where the system is somewhat depleted with $\frac{\hat{n}_1}{N} > 0.92$, the position variance along the y-axis slightly increases and that along the x-axis hardly changes. Accidentally, the momentum variance along both directions are approximately equal (and slightly increase). At 20\% anisotropy the position variance along both directions are incidentally approximately equal (and decrease), and the momentum variance along the y-axis is larger than that along the x-axis (both increase). The system is now already two-fold fragmented with $\frac{\hat{n}_4}{N} = 0.73$ and $\frac{\hat{n}_5}{N} = 0.26$. Looking at the shapes of the density in
FIG. 2. (Color online) Occupation numbers $n_j/N$ for $N = 10$ bosons with interactions of different strengths, and in traps of different anisotropies, throughout the pathway from condensation to fragmentation of the ground state. The three largest occupation numbers for $\lambda_0 = 0.01$ (blue curves with stars) computed with $M = 3$ time-adaptive (self-consistent) orbitals and the six largest occupations numbers for $\lambda_0 = 0.10$ (green curves with boxes) and $\lambda_0 = 0.20$ (red curves with circles) computed with $M = 10$ orbitals (actual data are marked by symbols, the curves are to guide the eye). Fragmentation of the ground state with increasing interaction strength and anisotropy of the trap is demonstrated, see the text for further discussion. Also plotted by the black curves with the same palette of symbols are the results obtained by including the next ‘filled shell’ of orbitals, namely, $M = 6$ and $M = 15$, respectively. It is seen that the results with $M = 3$ and $M = 6$ orbitals for the weakest interaction, and the results with $M = 10$ and $M = 15$ orbitals for the stronger interactions lie atop each other. The quantities shown are dimensionless.

In the middle column Fig. 1b,e,h, we observe the effects of the depletion and more visibly of the fragmentation on the variance. The many-body term of the variance becomes dominant over the density term of the variance [see (4)] in the ground state of the system.

The results for $\lambda_0 = 0.20$ are even more prominent. First, despite the fact that the density broadens along the $y$-axis while the anisotropy is enlarged, the position variance decreases (in both directions, but more mildly in the $x$ direction). Moreover and in an opposite manner, the $y$-axis position variance is smaller than that along the $x$-axis, see lower two curves in Fig. 3a, although the density along the $y$-axis is much broader than that along the $x$-axis, see the right column Fig. 1c,f,i. The behavior of the momentum variance is in line with the above many-body effects. The momentum variance along the $y$-axis is
FIG. 3. (Color online) (a) Position variance per particle $\frac{1}{N} \Delta^2_{X}$ and $\frac{1}{N} \Delta^2_{Y}$ and (b) momentum variance $\frac{1}{N} \Delta^2_{P_X}$ and $\frac{1}{N} \Delta^2_{P_Y}$ for $N = 10$ bosons in traps of different anisotropies and for interactions of different strengths throughout the pathway from condensation to fragmentation of the ground state. The magenta curves and symbols are for quantities along the $x$ direction and the cyan curves and symbols are for quantities along the $y$ direction (actual data are marked by symbols, the curves are to guide the eye). Crosses are data for $\lambda_0 = 0.01$ (computed with $M = 3$ orbitals), and boxes are for $\lambda_0 = 0.10$ and circles for $\lambda_0 = 0.20$ (computed with $M = 10$ orbitals). Anisotropy of the variance is demonstrated, see the text and Fig. 1 for further discussion. Also plotted by the black curves with the same palette of symbols are the results obtained by including the next ‘filled shell’ of orbitals, namely, $M = 6$ and $M = 15$, respectively. It is seen that the results with $M = 3$ and $M = 6$ orbitals for the weakest interactions, and the results with $M = 10$ and $M = 15$ orbitals for the stronger interactions practically lie atop each other. The quantities shown are dimensionless.
larger than that along the x-axis, i.e., opposite to the shape of the density. Furthermore, the momentum variance increases monotonously along the y direction, but first decreases and than increases along the x direction. The occupation numbers, \( \frac{n_1}{N} = 0.49(5) \) and \( \frac{n_2}{N} = 0.49 \) for \( \beta = 10\% \) and \( \frac{n_1}{N} \approx 0.5 \) and \( \frac{n_2}{N} \approx 0.5 \) for \( \beta = 20\% \), signify that the system becomes essentially fully two-fold fragmented. Again and more pronouncedly, the many-body term of the variance is dominant over the density term of the variance [see (4)] when the ground state is fragmented.

Let us recapitulate. As a two-dimensional isotropic anharmonic trap is stretched along the y direction, the density basically broadens in that direction. The long-range interaction causes the system to fragment. Then, the position variance decreases and the momentum variance increases, unlike from what one could anticipate by just examining the shape of the density. On top of that, we find that, although the density of the cloud is anisotropic, here it is broader along the y-axis than along the x-axis, the position variance along the y direction is smaller than that along the x direction. Correspondingly, the momentum variance along the y direction is larger than that along the x direction. We stress that this is contrary to what one would expect by just examining the shape of the two-dimensional density. All in all, these are intriguing many-body effects in the ground state of a fragmented trapped BEC.

**B. Dynamics**

The counter-intuitive properties of the position and momentum variances discussed in Subsec. IIIA are associated with the larger depleted fraction and more pronounced fragmentation of the ground state of a finite Bose system. The natural question to ask is whether such or similar effects can occur in larger systems. In the present subsection we shall demonstrate that the answer is positive and concentrate on an out-of-equilibrium scenario. We thereby keep in mind that we are en route the limit of an infinite number of particles where the depletion per particle of the system diminishes to zero.

The one-body Hamiltonian is again \( \hat{h}(x, y) = -\left( \frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} \frac{\partial^2}{\partial y^2} \right) + \frac{\{(x^2 + (y^1 - y_2)^2)^2\}}{4} \), where the degree of anisotropy is \( \beta = 0\%, 10\%, \) and \( 20\% \), and the inter-particle interaction is harmonic and repulsive, \( \lambda_0 \hat{W}(x_1 - x_2, y_1 - y_2) = -\lambda_0 [(x_1 - x_2)^2 + (y_1 - y_2)^2] \), \( \lambda_0 > 0 \). We consider the smallest interaction parameter from the above ground-state study, \( \Lambda = \lambda_0 (N - 1) = 0.09 \),
but take a hundred times larger number of interacting bosons, $N = 1000$. The system is prepared in the ground state of the trap. The initial depletion fraction is accordingly a hundred times smaller $[\frac{n_1(0)}{N} > 0.9999(9)]$ for each of the three anisotropies $\beta = 0\%$, $10\%$, and $20\%$ than for the corresponding cases with $N = 10$ bosons in Subsec. III A. The initial densities per particle look just like the left column Fig. 1a,d,g.

At $t = 0$ the interaction parameter is suddenly quenched to twice its value $\Lambda' = \lambda'_0(N - 1) = 0.18$. We ask what the out-of-equilibrium dynamics of the system would be like. Figs. 4 and 5 collect the results. A complementary and comparative investigation for $N = 10$ bosons and the same interaction-quench scenario is presented in the Appendix.

Following the quench of the interaction, the density performs breathing oscillations [94, 96, 97], i.e., its widths along the $y$ and $x$ directions varies in time. Furthermore, since the interaction is repulsive and at $t = 0$ suddenly increased, the density first expands at short times, i.e., the cloud initially broadens both along the $y$ and $x$ directions.

We have performed the calculations of the out-of-equilibrium dynamics both at the Gross-Pitaevskii level ($M = 1$) and at the many-body level ($M = 3$). The two-dimensional time-dependent many-body density per particle, $\frac{n(r,t)}{N}$, essentially coincides with the corresponding mean-field density. This is quite reasonable and expected due to the initial marginal depletion fraction $[\frac{n_1(0)}{N} > 0.9999(9)]$ which remains very small throughout the evolution of the BEC in time, see below. As far as the condensed fraction is considered, the system remains essentially fully condensed, also see [21, 27] for respective out-of-equilibrium studies in a one-dimensional trap.

In Fig. 4 the time-dependent many-particle position variance per particle, $\frac{1}{N}\Delta^2_X(t)$ [panels (a), (b), and (c)], and momentum variance, $\frac{1}{N}\Delta^2_P(t)$ [panels (d), (e), and (f)], are shown. The many-body and mean-field results are compared for each of the three trap anisotropies $\beta = 0\%$, $10\%$, and $20\%$. In Fig. 5 the total number of depleted particles outside the condensed mode [$\alpha(r,t)$ natural orbital] are shown as a function of time. The systems are essentially fully condensed with only a fraction of a single particle being depleted.

We start by analyzing the out-of-equilibrium dynamics in the isotropic trap, see Fig. 4a,d. The results and discussion are to assist one in analyzing the dynamics in the anisotropic traps. For the isotropic trap, the quantities along the $y$ and $x$ directions, of course, coincide. Both the many-body and mean-field variances vary in time in an oscillatory manner. However, there are a couple of clearly visible differences. The first, is that the mean-field variances
FIG. 4. (Color online) Anisotropy in the breathing dynamics following an interaction quench. Shown and compared are the many-body results for $N = 1000$ bosons using $M = 3$ time-adaptive orbitals and the mean-field results (equivalent to $M = 1$). (a),(b),(c) The time-dependent many-particle position variance per particle, $\frac{1}{N} \Delta^2 \hat{X}(t)$ and $\frac{1}{N} \Delta^2 \hat{Y}(t)$, and (d),(e),(f) the momentum variance, $\frac{1}{N} \Delta^2 \hat{P}_X(t)$ and $\frac{1}{N} \Delta^2 \hat{P}_Y(t)$, following an interaction quench from $\Lambda = \lambda_0 (N - 1) = 0.09$ to 0.18 at $t = 0$ are plotted. For the isotropic system, panels (a),(d), the quantities along the $y$ and $x$ directions are, of course, equal. For the anisotropic systems, panels (b),(e) and (c),(f), the time-dependent position variance in the $y$ and $x$ directions do not cross each other at the mean-field level, and similarly the momentum quantities, signifying that the position (momentum) density in the $y$ direction is always wider (narrower) than that in the $x$ direction. This, however, is no longer the case at the many-body level: A system whose position (momentum) density along the $y$ direction is wider (narrower) than that along the $x$ direction can actually have a smaller (larger) position (momentum) variance along this direction. Here, two such systems are visually discernible.
oscillate with a rather constant amplitude, whereas the many-body variances oscillates with a (slowly) growing amplitude. The latter can be attributed to the (slowly) growing amount of depleted particles, see Fig. 5, albeit less than one tenth of a particle is outside the condensed mode! Indeed, the variance is a highly sensitive probe of correlations even when the system is practically condensed [20, 21]. The second difference, is the opposite dynamical behavior of the variances at short times when computed at the many-body and Gross-Pitaevskii levels. Despite the expansion of the cloud at short times, the time-dependent position variance increases and momentum variance decreases, implying that the many-body contributions to the variance $\Delta^2_{\hat{x},MB}(t) = \Delta^2_{\hat{y},MB}(t)$ and $\Delta^2_{\hat{p}_x,MB}(t) = \Delta^2_{\hat{p}_y,MB}(t)$ are opposite in sign with respect to and dominate the mean-field terms $\Delta^2_{\hat{x},density}(t) = \Delta^2_{\hat{y},density}(t)$ and $\Delta^2_{\hat{p}_x,density}(t) = \Delta^2_{\hat{p}_y,density}(t)$. This is an appealing time-dependent many-body effect taking place in macroscopic Bose systems.

We now turn to the anisotropy of the variance in the $y$ and $x$ directions during the breathing dynamics, see Fig. 4b,c,e,f. When the trap becomes anisotropic, the time-dependent quantities along the $y$ direction ‘split’ from the quantities along the $x$ direction. Since the
isotropic trap is made anisotropic by a stretch along the $y$-axis, the ‘base line’ of the position variance along the $y$ direction is shifted up to higher values, and the ‘base line’ of the momentum variance along the $y$ axis is shifted down to lower values, at least as far as the (initial conditions and) short-time dynamics is concerned. Obviously, this shift is larger for 20% anisotropy than for 10% anisotropy, compare Fig. 4b,e and Fig. 4c,f. All in all, one can anticipate from (the geometry of the trap and) the shape of the density the anisotropy of the time-dependent position and momentum variances, at least for short times. This result extends what is found in Subsec. IIIA for the ground-state of an essentially fully-condensed system.

But the geometrical picture of the anisotropy of the variance emerging at short times changes in time. At the mean-field level, the position variances in the $y$ and $x$ directions (which are different in the anisotropic trap) oscillate with a rather constant amplitude. Consequently, they do not cross each other, indicating that during the breathing dynamics the cloud’s density remains wider along the $y$ direction than along the $x$ direction. The corresponding momentum variances also oscillate with a rather constant amplitude and, therefore, do not cross each other as well. This implies that during the dynamics the momentum density of the cloud stays narrower along the $y$ direction than along the $x$ direction.

At the many-body level, on the other hand, the variances along the $y$ and $x$ directions oscillate with a (slowly) growing amplitudes. Therefore, at a certain point in time the $y$ and $x$ position variances must cross each other for the first time. Similarly, the $y$ and $x$ momentum variances must also cross at some point in time. The smaller the anisotropy, the earlier is this time, compare Fig. 4b,e for $\beta = 10\%$ and Fig. 4c,f for $\beta = 20\%$. Thus, the presence of even the slightest time-dependent depletion leads to a large influence on the time-dependent variance at the many-body level: The anisotropy of the variance for a whole time intervals is opposite to the anisotropy of the density. Then, a simple analysis shows that $\Delta_{\hat{x},MB}(t) - \Delta_{\hat{y},MB}(t) > \Delta_{\hat{x},density}(t) - \Delta_{\hat{y},density}(t) > 0$ and $\Delta_{\hat{p}_y,MB}(t) - \Delta_{\hat{p}_x,MB}(t) > \Delta_{\hat{p}_y,density}(t) - \Delta_{\hat{p}_x,density}(t) > 0$.

We have repeated the investigation of the out-of-equilibrium scenarios for a system of $N = 10$ bosons and the same interaction parameters. The results are collected in the Appendix, see Fig. 6 and 7. The similarity of the out-of-equilibrium results for the same interaction parameter and different numbers of particles ($N = 1000$ bosons in the present
subsection, \( N = 10 \) in the Appendix), together with analogous behavior in the dynamics of larger systems in one-dimensional traps \([21, 27]\), provide, in our opinion, strong evidences that the effects of the anisotropy of the time-dependent position and momentum variances in essentially fully-condensed BECs persist in the limit of an infinite number of particle.

All in all, we have discussed two out-of-equilibrium effects associated with the variance during the breathing dynamics of essentially-condensed trapped bosons. At short times, it is the decrease (increase) of the position (momentum) variance in contrast to the increase (decrease) of the width of the position (momentum) density. At longer times, it is the opposite behavior of the anisotropy of the variances in position and momentum spaces when computed at the mean-field and many-body levels.

IV. CONCLUSIONS

We have investigated in the present work the variance of the position and momentum many-particle operators of structureless bosons interacting by a long-range inter-particle interaction and trapped in a two-dimensional single-well anharmonic potential. In the first investigation, that of the pathway from condensation to fragmentation of the ground state, we find out that, although the density of the cloud is broader along the y-axis than along the x-axis, the position variance can behave in an opposite manner, namely, be larger along the x-axis than along the y-axis. Similarly, the momentum variance can be larger along the y-axis than along the x-axis. This opposite anisotropy of the variance with respect to the density is a counterintuitive many-body effect that emerges when the ground-state of the bosonic system is fragmented.

In the second study, that of the out-of-equilibrium breathing dynamics of a BEC, we find out that, already when a fraction (even a tenth) of a boson is depleted, qualitative differences between the many-body and mean-field variances arise. Explicitly, the time-dependent many-body position variance can show opposite behavior of the anisotropy between the y-axis and x-axis with respect to the mean-field quantities, despite the system being essentially fully condensed. Corresponding results hold for the time-dependent many-body momentum variance in comparison with the mean-field quantities.

Both the ground-state and out-of-equilibrium scenarios suggest a wealth of effects emanating from the many-body term of the variance both in position and momentum spaces in
interacting trapped many-boson systems, in two spatial dimensions. The anisotropy of the variance advocates that it can be used to characterize the strength of correlations along the $y$ and $x$ directions in the system. We have seen that such many-body effects encoded within the variance do not necessarily match with the information that can be extracted based on the shape of system’s density. This is in sharp contrast to the text-book example of a single particle discussed in the introduction.

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**Appendix A: Further computational details and convergence**

The multiconfigurational time-dependent Hartree for bosons (MCTDHB) method [48, 49, 68–70, 76] is used in the present work to compute the ground-state and out-of-equilibrium properties of trapped bosons in two spatial dimensions interacting by a long-range inter-particle interaction. The maximal configurational space are 501 501 for $N = 1000$ bosons and $M = 3$ orbitals and 1 961 256 for $N = 10$ bosons and $M = 15$ orbitals. We use the numerical implementation in the software packages [98, 99]. To obtain the ground state we propagate the MCTDHB equations of motion in imaginary time [71, 81]. For the computations the many-body Hamiltonian is represented by $128^2$ exponential discrete-variable-representation grid points (using a Fast-Fourier Transform routine) in a box of size $[-10, 10] \times [-10, 10]$. Convergence of the occupation numbers (depletion) and the position and momentum variance with increasing number of ‘filled shells’, namely, $M = 3, 6, 10,$ and 15 time-adaptive orbitals, is demonstrated for $N = 10$ bosons in Figs. 2 and 3 for the ground state [20] and in Figs. 6 and 7 for the out-of-equilibrium breathing dynamics [21],
FIG. 6. (Color online) Convergence of the time-dependent many-particle position variance per particle, $\frac{1}{N} \Delta X^2(t)$ and $\frac{1}{N} \Delta Y^2(t)$ [panels (a), (b), and (c)], and the momentum variance, $\frac{1}{N} \Delta P_X^2(t)$ and $\frac{1}{N} \Delta P_Y^2(t)$ [panels (d), (e), and (f)], with the number of time-adaptive orbitals $M$ used in the MCTDHB computations for systems consisting of $N = 10$ bosons in traps of anisotropies $\beta = 0\%$, 10\%, and 20\% following an interaction quench from $\Lambda = \lambda_0(N-1) = 0.09$ to 0.18 at $t = 0$. Compare to Fig. 4. It is found that the results with $M = 3$ accurately describe the physics and the results with $M = 6$ and $M = 10$ orbitals lie atop each other. The quantities shown are dimensionless.
FIG. 7. (Color online) Convergence of the total number of depleted particles with the number of time-adaptive orbitals $M$ used in the MCTDHB computations for systems consisting of $N = 10$ bosons following an interaction quench from $\Lambda = \lambda_0(N-1) = 0.09$ to $0.18$ at $t = 0$, see Fig. 6. It is found that the results with $M = 3$ accurately describe the physics and the results with $M = 6$ and $M = 10$ orbitals lie atop each other. Compare to Fig. 5. The quantities shown are dimensionless.

also see in this context [100]. It is found that the results are nicely converged.

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