Uncertainty product of an out-of-equilibrium Bose-Einstein condensate

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Abstract. The variance and uncertainty product of the position and momentum many-particle operators of structureless bosons interacting by a long-range inter-particle interaction and trapped in a single-well potential are investigated. In the first example, of an out-of-equilibrium interaction-quench scenario, it is found that, despite the system being fully condensed, already when a fraction of a particle is depleted differences with respect to the mean-field quantities emerge. In the second example, of the pathway from condensation to fragmentation of the ground state, we find out that, although the cloud's density broadens while the system's fragments, the position variance actually decreases, the momentum variance increases, and the uncertainty product is not a monotonous function but has a maximum. Implication are briefly discussed.

1. Introduction

Bose-Einstein condensates (BECs) made of ultracold trapped bosonic atoms have become a vast ground to study interacting quantum systems [1-12]. There has been a substantial theoretical interest in BECs, and ample studies have been made to describe their static and dynamic properties using Gross-Pitaevskii theory. The time-dependent Gross-Pitaevskii equation governs a mean-field theory which assumes that all bosons are described by a single time-dependent one-particle function throughout the evolution of the BEC in time. It is generally accepted that Gross-Pitaevskii theory adequately describes the ground state and out-of-equilibrium dynamics of BECs in the limit of an infinite number of particles and at constant interaction parameter (i.e., when the product of the number of particles times the scattering length is kept fixed). Here, mathematically rigorous results exist and show that, under certain conditions, the energy per particle and density per particle of the many-boson system coincide in this limit with the Gross-Piteavekii results and that the system is 100% condensed [13-16].

Whereas a condensate fraction of 100% implies that the number of depleted (non-condensed) particles divided by the total number of particles vanishes in the infinite-particle limit, the former is always non-zero in an interacting many-boson system. This observation has motivated us recently to look at properties of BECs which depend on the number of depleted particles rather than the condensate fraction. In [17, 18] we showed, for the ground state as well as for an out-of-equilibrium BEC, that even in the infinite-particle limit when the BEC is 100% condensed, the variance of a many-particle operator and the uncertainty product of two such operators can differ from those predicted by the Gross-Pitaevskii theory. The existence of many-body effects beyond those predicted by Gross-Pitaevskii theory stems from the necessity of performing the

infinite-particle limit only after a many-particle quantum mechanical observable is evaluated and not prior to its evaluation. Unlike the variance of operators of a single particle [19], the variance and uncertainty product of many-particle operators is more involved, also see [20-22] in this context. It has furthermore been shown that the overlap of the exact and Gross-Pitaevskii wave-functions of a trapped BEC in the limit of an infinite number of particles is always smaller than unity and may even become vanishingly small [23].

The purpose of the present work is to build on and go beyond [17, 18] in two directions, first, by studying the variance and uncertainty product of trapped bosons with a long-range inter-particle interaction and, second, when the system is no longer condensed. The structure of the paper is as follows. In Sec. 2 we briefly discuss a general theory for the many-body variance and uncertainty product of an out-of-equilibrium trapped BEC. In Sec. 3 we present two applications, for the breathing dynamics of a trapped BEC (Subsec. 3.1) and for the pathway from condensation to fragmentation of the ground state of trapped interacting bosons (Subsec. 3.2). Concluding remarks are put forward in Sec. 4. Numerical and convergence details are collected in the Appendix.

2. Theoretical Framework

Consider the many-body Hamiltonian of N interacting bosons in a trap $V(\mathbf{r})$,

$$\hat{H}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \sum_{j=1}^{N} \left[-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{r}_j^2} + \hat{V}(\mathbf{r}_j) \right] + \sum_{j<k} \lambda_0 \hat{W}(\mathbf{r}_j - \mathbf{r}_k). \tag{1}$$

Here, $\hbar = m = 1$, and $\hat{W}(\mathbf{r}_1 - \mathbf{r}_2)$ is the inter-particle interaction with λ_0 its strength.

The system evolves in time according to the time-dependent Schrödinger equation,

$$\hat{H}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; t) = i \frac{\partial \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; t)}{\partial t}, \tag{2}$$

where the wave-function $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; t)$ is normalized to unity. Typically, the system is initially prepared in the ground state of the trap $V(\mathbf{r})$, $\hat{H}(\mathbf{r}_1, \ldots, \mathbf{r}_N)\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = E\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$, where E is the ground-state energy and $\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ normalized to unity.

In what follows we employ the reduced one-body and two-body density matrices of $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; t)$ [24-27]. The reduced one-body density matrix is given by

$$\frac{\rho^{(1)}(\mathbf{r}_1, \mathbf{r}_1'; t)}{N} = \int d\mathbf{r}_2 \ldots d\mathbf{r}_N \, \Psi^*(\mathbf{r}_1', \mathbf{r}_2, \ldots, \mathbf{r}_N; t) \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N; t) =$$
$$= \sum_j \frac{n_j(t)}{N} \alpha_j(\mathbf{r}_1; t) \alpha_j^*(\mathbf{r}_1'; t). \tag{3}$$

The quantities $\alpha_j(\mathbf{r}; t)$ are the so-called natural orbitals and $n_j(t)$ their respective occupations which are time dependent and used to define the degree of condensation in a system of interacting bosons [28]. The density of the system is simply the diagonal of the reduced one-body density matrix, $\rho(\mathbf{r}; t) = \rho^{(1)}(\mathbf{r}, \mathbf{r}; t)$.

We express in what follows quantities using the time-dependent natural orbitals $\alpha_j(\mathbf{r}; t)$. The diagonal part of the reduced two-body density matrix is given by

$$\frac{\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1, \mathbf{r}_2; t)}{N(N-1)} = \int d\mathbf{r}_3 \ldots d\mathbf{r}_N \, \Psi^*(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N; t) \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N; t) =$$
$$= \sum_{jpkq} \frac{\rho_{jpkq}(t)}{N(N-1)} \alpha_j^*(\mathbf{r}_1; t) \alpha_p^*(\mathbf{r}_2; t) \alpha_k(\mathbf{r}_1; t) \alpha_q(\mathbf{r}_2; t), \tag{4}$$

where the matrix elements are $\rho_{jpkq}(t) = \langle\Psi(t)|\hat{b}_j^\dagger\hat{b}_p^\dagger\hat{b}_k\hat{b}_q|\Psi(t)\rangle$, and the creation and annihilation operators are associated with the time-dependent natural orbitals $\alpha_j(\mathbf{r};t)$.

To express the variance and uncertainty product of operators we begin simply with the operator

$$\hat{A} = \sum_{j=1}^{N} \hat{a}(\mathbf{r}_j) \tag{5}$$

of the many-particle system, where $\hat{a}(\mathbf{r})$ is a Hermitian operator. A straightforward calculation gives the average per particle of $\hat{A}$ in the state $|\Psi(t)\rangle$,

$$\frac{1}{N}\langle\Psi(t)|\hat{A}|\Psi(t)\rangle = \int d\mathbf{r}\frac{\rho(\mathbf{r};t)}{N}a(\mathbf{r}), \tag{6}$$

which is directly expressed in terms of the system's density per particle in case of a local operator in coordinate space $\mathbf{r}$. In the case of a local operator in momentum space $\mathbf{p}$ we can write $\frac{1}{N}\langle\Psi(t)|\hat{A}|\Psi(t)\rangle = \int d\mathbf{p}\frac{\rho(\mathbf{p};t)}{N}a(\mathbf{p})$.

To proceed we also need the expectation value of the square of $\hat{A}$,

$$\hat{A}^2 = \sum_{j=1}^{N}\hat{a}^2(\mathbf{r}_j) + \sum_{j<k}2\hat{a}(\mathbf{r}_j)\hat{a}(\mathbf{r}_k), \tag{7}$$

which is comprised of one-body *and* two-body operators. Expressed in terms of the density per particle and natural orbitals, the time-dependent variance per particle of the operator $\hat{A}$ can be written as a sum of two terms

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

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

$$\Delta_{\hat{a},MB}^2(t) = \frac{\rho_{1111}(t)}{N}\left[\int d\mathbf{r}|\alpha_1(\mathbf{r};t)|^2 a(\mathbf{r})\right]^2 - (N-1)\left[\int d\mathbf{r}\frac{\rho(\mathbf{r};t)}{N}a(\mathbf{r})\right]^2 +$$

$$+ \sum_{jpkq\neq 1111}\frac{\rho_{jpkq}(t)}{N}\left[\int d\mathbf{r}\alpha_j^*(\mathbf{r};t)\alpha_k(\mathbf{r};t)a(\mathbf{r})\right]\left[\int d\mathbf{r}\alpha_p^*(\mathbf{r};t)\alpha_q(\mathbf{r};t)a(\mathbf{r})\right]. \tag{8}$$

The first term, which is denoted by $\Delta_{\hat{a},density}^2(t)$, describes the variance of $\hat{a}(\mathbf{r})$ resulting *solely* from the density per particle $\frac{\rho(\mathbf{r};t)}{N}$. The second term, which is denoted by $\Delta_{\hat{a},MB}^2(t)$, collects all other contributions to the many-particle variance and is identically zero within Gross-Pitaevskii theory. $\Delta_{\hat{a},MB}^2(t)$ is generally non-zero within a many-body theory.

Finally, taking two many-particle operators,

$$\hat{A} = \sum_{j=1}^{N}\hat{a}(\mathbf{r}_j), \qquad \hat{B} = \sum_{j=1}^{N}\hat{b}(\mathbf{r}_j), \tag{9}$$

and their respective time-dependent variances per particle, $\frac{1}{N}\Delta_{\hat{A}}^2(t)$ and $\frac{1}{N}\Delta_{\hat{B}}^2(t)$, their uncertainty product satisfies the inequality

$$\frac{1}{N}\Delta_{\hat{A}}^2(t)\frac{1}{N}\Delta_{\hat{B}}^2(t) \equiv \Delta_{\frac{\hat{A}}{N}}^2(t)\Delta_{\hat{B}}^2(t) \geq \frac{1}{4}\left|\int d\mathbf{r}\frac{\rho(\mathbf{r};t)}{N}[\hat{a}(\mathbf{r}),\hat{b}(\mathbf{r})]\right|^2, \tag{10}$$

where $[\hat{a}(\mathbf{r}),\hat{b}(\mathbf{r})]$ is the commutator of the two Hermitian operators $\hat{a}(\mathbf{r})$ and $\hat{b}(\mathbf{r})$.

3. Applications

As mentioned above we would like to go beyond [17, 18] in the investigation of the variance and uncertainty product of trapped BECs. To this end, we here study trapped bosons with a long-range interaction and when the system is no longer condensed. We treat structureless bosons with harmonic inter-particle interaction trapped in a single-well anharmonic potential. The time-dependent Schrödinger equation of the trapped BEC has no analytical solution in the present study, see in this respect [23, 29], nor even the variance and uncertainty product can be computed analytically, thus a numerical solution of the out-of-equilibrium dynamics is a must. This will lead to interesting results.

We need a suitable and proved many-body tool to make the calculations. Such a many-body tool is the multiconfigurational time-dependent Hartree for bosons (MCTDHB) method, which has been well documented [30-35], benchmarked [36], and extensively used [37-55] in the literature.

3.1. Breathing dynamics

We consider $N = 100$ and separately $N = 100,000$ trapped bosons in one spatial dimension. The one-body Hamiltonian is $-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{x^4}{4}$ and the inter-particle interaction is harmonic, $\lambda_0 \hat{W}(x_1 - x_2) = -\lambda_0(x_1 - x_2)^2, \lambda_0 > 0$. The system is prepared in the ground state of the trap for the interaction parameter $\Lambda = \lambda_0(N-1) = 0.19$. At $t = 0$ the interaction parameter is suddenly quenched to $\Lambda = 0.38$ and we inquire what the out-of-equilibrium dynamics of the system would be like. Fig. 1 collects the results.

Fig. 1a depicts snapshots of the density per particle, $\frac{\rho(x;t)}{N}$, as a function of time. The Gross-Pitaevskii and many-body results are seen to match very well. The density is seen to perform breathing dynamics [56-58]. Since the interaction is repulsive and at $t = 0$ quenched up, the density first expands at short times. In Fig. 1b the total number of depleted particles outside the condensed mode [$\alpha_1(x; t)$ natural orbital] are shown as a function of time. The systems are essentially fully condensed with only a fraction of a particle depleted. In Fig. 1c the time-dependent many-particle position variance per particle, $\frac{1}{N}\Delta^2_{\hat{X}}(t)$, momentum variance, $\frac{1}{N}\Delta^2_{\hat{P}}(t)$, and uncertainty product, $\frac{1}{N}\Delta^2_{\hat{X}}(t)\frac{1}{N}\Delta^2_{\hat{P}}(t) \equiv \Delta^2_{\hat{X}_{CM}}(t)\Delta^2_{\hat{P}_{CM}}(t)$ are shown. Note the opposite behavior of the variance at short times when computed at the many-body and Gross-Pitaevskii level. Despite the expansion of the cloud (at short times), the time-dependent position variance increases and momentum variance decreases, implying that $\Delta^2_{\hat{x},MB}(t)$ and $\Delta^2_{\hat{p},MB}(t)$ are opposite in sign with respect to and dominate $\Delta^2_{\hat{x},density}(t)$ and $\Delta^2_{\hat{p},density}(t)$. This is an interesting time-dependent many-body effect.

3.2. Pathway from condensation to fragmentation

We next study the pathway from condensation to fragmentation of the ground state [59-63]. Fragmentation of BECs has drawn much attention, see, e.g., [64-71]. 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, 72-75]. Fig. 2 depicts the results for $N = 20$ bosons. The one-body Hamiltonian is again $-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{x^4}{4}$ and the inter-particle interaction is harmonic, $\lambda_0 \hat{W}(x_1 - x_2) = -\lambda_0(x_1 - x_2)^2, \lambda_0 > 0$. Fig. 2a shows snapshots of the density per particle, $\frac{\rho(x;t)}{N}$, as a function of the interaction strength λ_0. As the interaction is increased the density broadens and splits into two parts; Side by side, the ground state fragments [58, 72-75], see Fig. 2b. The ground state essentially evolves from 100% condensed to 50%–50% fragmented. Finally, Fig. 2c displays the many-particle position variance per particle, $\frac{1}{N}\Delta^2_{\hat{X}}$, momentum variance, $\frac{1}{N}\Delta^2_{\hat{P}}$, and uncertainty product, $\frac{1}{N}\Delta^2_{\hat{X}}\frac{1}{N}\Delta^2_{\hat{P}} \equiv \Delta^2_{\hat{X}_{CM}}\Delta^2_{\hat{P}_{CM}}$ of the ground state as a function of the interaction strength. We find
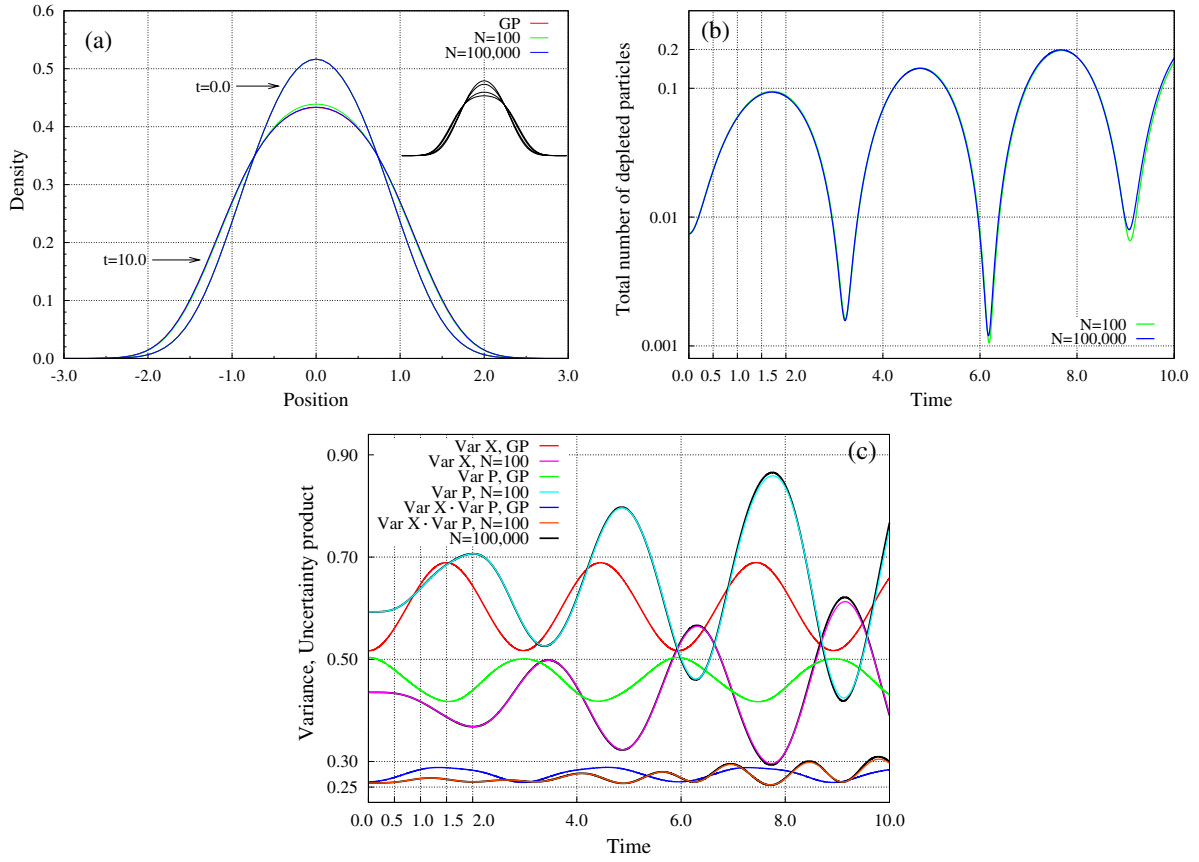
Figure 1. Breathing dynamics following an interaction quench. Shown and compared are many-body results for $N = 100$ (using $M = 4$ time-adaptive orbitals) and $N = 100,000$ (using $M = 2$ time-adaptive orbitals) bosons, and the mean-field results (equivalent to $M = 1$ time-adaptive orbitals). The one-body Hamiltonian is $-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{x^4}{4}$ and the inter-particle interaction is harmonic, $\lambda_0 \hat{W}(x_1 - x_2) = -\lambda_0(x_1 - x_2)^2, \lambda_0 > 0$. (a) Snapshots of the density per particle, $\frac{\rho(x;t)}{N}$, as a function of time following a sudden increase of the interaction parameter from $\Lambda = \lambda_0(N - 1) = 0.19$ to 0.38 at $t = 0$. The inset shows the density per particle at instances, from top to bottom, $t = 0.0, 0.5, 1.0$, and 1.5 for $N = 100$ bosons. (b) Total number of depleted particles outside the condensed mode as a function of time. Note the values on the y axis. (c) Time-dependent many-particle position variance per particle, $\frac{1}{N}\Delta_{\hat{X}}^2(t)$, momentum variance, $\frac{1}{N}\Delta_{\hat{P}}^2(t)$, and uncertainty product, $\frac{1}{N}\Delta_{\hat{X}}^2(t)\frac{1}{N}\Delta_{\hat{P}}^2(t) \equiv \Delta_{\hat{X}_{CM}}^2(t)\Delta_{\hat{P}_{CM}}^2(t)$. Note the opposite behavior of the variance at short times when computed at the many-body and mean-field level. See the text for more details. The quantities shown are dimensionless.
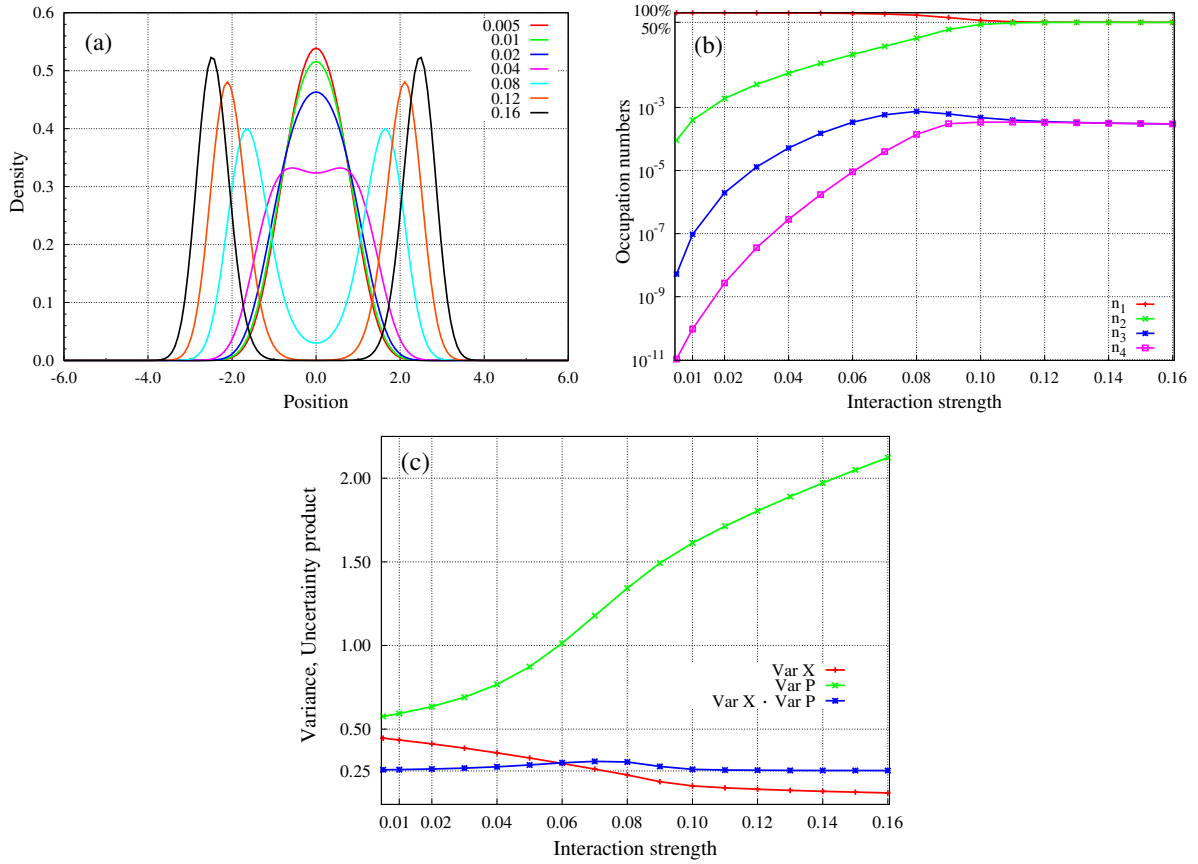
Figure 2. Pathway from condensation to fragmentation of the ground state. Shown are many-body results for $N = 20$ bosons (using $M = 4$ time-adaptive orbitals). The one-body Hamiltonian is $-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{x^4}{4}$ and the inter-particle interaction is harmonic, $\lambda_0 \hat{W}(x_1 - x_2) = -\lambda_0(x_1 - x_2)^2, \lambda_0 > 0$. (a) Snapshots of the density per particle, $\frac{\rho(x;t)}{N}$, as a function of the interaction strength $\lambda_0 = 0.005, \ldots, 0.16$. As the interaction is increased the density broadens and splits into two parts. (b) The four largest occupation numbers as a function of the interaction strength λ_0 (points' symbols are data; smooth curves are to guide the eye). The ground state essentially evolves from 100% condensed to 50%–50% fragmented. (c) Many-particle position variance per particle, $\frac{1}{N}\Delta^2_{\hat{X}}$, momentum variance, $\frac{1}{N}\Delta^2_{\hat{P}}$, and uncertainty product, $\frac{1}{N}\Delta^2_{\hat{X}}\frac{1}{N}\Delta^2_{\hat{P}} \equiv \Delta^2_{\hat{X}_{CM}}\Delta^2_{\hat{P}_{CM}}$. Note that, although the cloud's density broadens while the system's fragments, the position variance actually decreases whereas the momentum variance increases. See the text for more details. The quantities shown are dimensionless.

that, although the cloud's density broadens while the system's fragments, the position variance decreases and the momentum variance increases, unlike from what one would expect by just examining the density. When the variances are combined, the uncertainty product exhibits a maximum along the pathway from condensation to fragmentation. This is an interesting static many-body effect.

4. Summary and Conclusions

We have studied in the present work the variance and uncertainty product of the position and momentum many-particle operators of structureless bosons interacting by a long-range inter-particle interaction and trapped in an anharmonic single-well potential. There is no analytical solution to the many-particle Schrödinger equation of this system, not even to the variance and uncertainty product themselves, which makes a numerical solution of the out-of-equilibrium dynamics a must. In the out-of-equilibrium interaction-quench scenario, we have found that, despite the system being fully condensed, already when a fraction of a particle is depleted differences with respect to the mean-field quantities arise. In the static pathway from condensation to fragmentation scenario, we found out that, although the cloud's density broadens while the system's fragments, the position variance decreases, the momentum variance increases, and the uncertainty product exhibits a maximum. Both scenarios suggest a richness of effects emanating from the many-body term of the variance and uncertainty product in interacting trapped many-boson systems. Such many-body effects need not coincide with the information that can be extracted based on the system's density alone.

Appendix A. Details and convergence of the numerical computations

The multiconfigurational time-dependent Hartree for bosons (MCTDHB) method [30-35] is used in the present work to compute the time-dependent and ground-state properties of trapped bosons interacting by a long-range inter-particle interaction. To obtain the ground state we propagate the MCTDHB equations of motion in imaginary time [36, 63]. For the computations the many-body Hamiltonian is represented by 256 exponential discrete-variable-representation grid points (using a Fast-Fourier Transform routine) in a box of size $[-10, 10]$. We use the numerical implementation in the software packages [76, 77]. Convergence of the variance and uncertainty product with increasing number M of time-adaptive orbitals is demonstrated for $N = 100$ bosons in Fig. A1a for the out-of-equilibrium dynamics [18] and for $N = 20$ bosons in Fig. A1b for the ground state [17], also see in this context [78]. It is found that, respectively, the results with $M = 2$ and $M = 4$ orbitals are converged.

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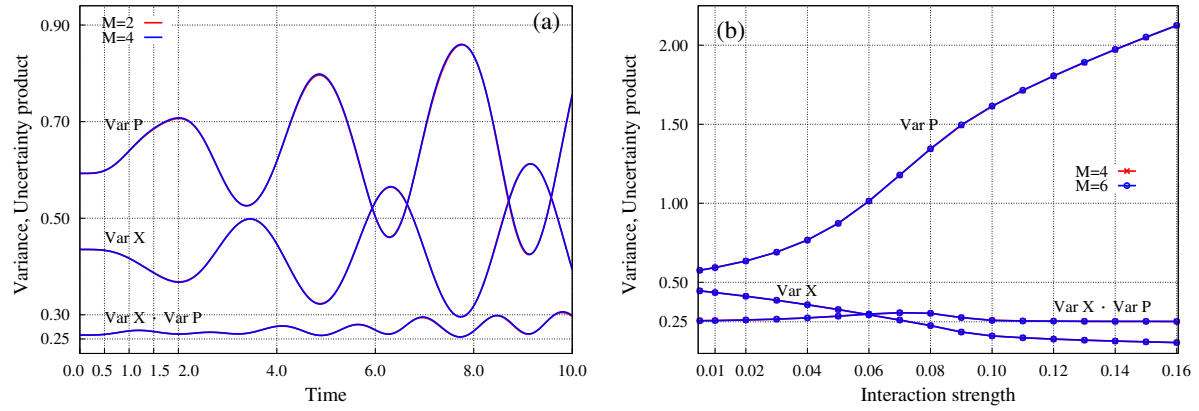**Figure A1.** Convergence of the many-particle position variance per particle, $\frac{1}{N}\Delta^2_{\hat{X}}(t)$, momentum variance, $\frac{1}{N}\Delta^2_{\hat{P}}(t)$, and uncertainty product, $\frac{1}{N}\Delta^2_{\hat{X}}(t)\frac{1}{N}\Delta^2_{\hat{P}}(t) \equiv \Delta^2_{\hat{X}_{CM}}(t)\Delta^2_{\hat{P}_{CM}}(t)$ with the number of time-adaptive orbitals M used in the MCTDHB computations for the systems consisting of $N = 100$ and $N = 20$ bosons discussed in the main text. (a) The out-of-equilibrium interaction-quench breathing dynamics in Sec. 3.1 (propagation of the MCTDHB equations of motion in real time). It is found that the results with $M = 2$ and $M = 4$ orbitals lie atop each other. (b) The pathway from condensation to fragmentation of the ground state in Sec. 3.2 (propagation of the MCTDHB equations of motion in imaginary time). It is found that the results with $M = 4$ and $M = 6$ orbitals lie atop each other. The quantities shown are dimensionless.

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