Variance of a Trapped Bose-Einstein Condensate

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Abstract. The ground state of a Bose-Einstein condensate in a two-dimensional trap potential is analyzed numerically at the infinite-particle limit. It is shown that the anisotropy of the many-particle position variance along the $x$ and $y$ axes can be opposite when computed at the many-body and mean-field levels of theory. This is despite the system being 100\% condensed, and the respective energies per particle and densities per particle to coincide.

1. Introduction

We consider the ground state of $N$ interacting bosons in a two-dimensional trap. It has been shown under quite general conditions [1, 2, 3] that the many-body energy per particle and density per particle coincide at the infinite-particle limit with the Gross-Pitaevskii mean-field results,

$$\lim_{N \to \infty} \frac{\rho(r)}{N} = |\phi_{GP}(r)|^2, \quad \lim_{N \to \infty} E_N = \varepsilon_{GP}. \quad (1)$$

Here, the density is the diagonal of the reduced one-particle density matrix [4, 5], $\rho(r) \equiv \rho^{(1)}(r,r)$, $E$ is the ground-state energy, $\phi_{GP}(r)$ and $\varepsilon_{GP}$ are the Gross-Pitaevskii orbital and energy, respectively, and $r = (x, y)$. Furthermore, the bosons are 100\% condensed, at the levels of the reduced one-particle and two-particle (and any finite-order [6]) density matrices,

$$\lim_{N \to \infty} \frac{\rho^{(1)}(r_1, r_1')}{N} = \phi_{GP}(r_1)\phi_{GP}^*(r_1'),$$
$$\lim_{N \to \infty} \frac{\rho^{(2)}(r_1, r_2, r_1', r_2')}{N(N-1)} = \phi_{GP}(r_1)\phi_{GP}(r_2)\phi_{GP}^*(r_1')\phi_{GP}^*(r_2'). \quad (2)$$

The infinite-particle limit implies that the interaction parameter, i.e., the product of the number of particles times the interaction strength, is kept fixed when $N \to \infty$. The question then arises, which differences are there, at the infinite-particle limit, between the many-body and mean-field descriptions of trapped bosons in their ground state.

To research this topic, it has been pointed out recently that the variance of many-particle operators can have substantial differences when computed at the many-body and mean-field levels of theory, even when the bosons are 100\% condensed [7]. In particular, the variance of the many-particle position operator, $\hat{X} = \sum_{j=1}^{N} \hat{x}_j$,

$$\frac{1}{N} \Delta_{\hat{X}}^2 = \int dr \frac{\rho(r)}{N} x^2 - N \left[ \int dr \frac{\rho(r)}{N} x \right]^2 + \int dr_1 dr_2 \frac{\rho^{(2)}(r_1, r_2, r_1, r_2)}{N} x_1 x_2, \quad (3)$$
Figure 1. Density per particle of the ground state of $N = 1,000,000$ bosons in two-dimensional double-well traps for four barrier heights $V_0$. Top row, panels (a)-(d): Many-body computations with $M = 2$ self-consistent orbitals. Bottom row, panels (e)-(h): Mean-field computations with $M = 1$ self-consistent orbitals, i.e., Gross-Pitaevskii results. The respective densities per particle are indistinguishable. On the other hand, the anisotropies of the many-body and mean-field position variances along the $x$ and $y$ directions become opposite with increasing barrier height. See Fig. 4 and the text for further details. The quantities shown are dimensionless.

picks up tiny fluctuations that are completely washed out in the above-mentioned properties at the infinite-particle limit. This is because the two-particle reduced density matrix in the last term of (3) is divided only by $N$ and not by $N(N-1)$ as in (2). Another property of interest is the overlap between the many-body and mean-field wavefunctions, which is always less than and can become much smaller than 1 [3, 8].

Generally, for repulsive interactions the many-body position variance is smaller than the mean-field variance, and vice versa for attractive interactions. This result is transparent to see analytically when considering bosons in an harmonic trap, and requires accurate numerics to arrive at for anharmonic traps [7, 9]. In two spatial dimensions, one is drawn to look for properties and phenomena that cannot take place in one dimension. The anisotropy of the position and momentum variance along the $x$ and $y$ directions was investigated in [10] and the variance of the many-particle angular-momentum operator in [11]. So far, it has not been shown that the ground state can exhibit opposite anisotropy of the variance at the infinite-particle limit, i.e., that the many-body and mean-field anisotropies of 100% condensed bosons are different. This is the main finding of the present work, i.e., that trapped Bose-Einstein condensates at the infinite-particle limit can be classified according to whether the anisotropies of their many-body and mean-field position variances are alike or opposite.
Figure 2. Difference between the mean-field and many-body energies per particle for $N = 10^2, \ldots, 10^6$ bosons as a function of the barrier height. The interaction parameter is $\Lambda = \lambda_0(N - 1) = 0.1$. The difference decreases with increasing number of particles $N$ for a given barrier height $V_0$. See the text for further details. Actual data is marked by symbols, the continuous curves are to guide the eye only. The quantities shown are dimensionless.

2. System and results
We consider $N$ repulsively interacting bosons in a two-dimensional double-well potential. The height of the barrier is varied and we follow the changes in the system. The interaction parameter $\Lambda = \lambda_0(N - 1)$ is held fixed and the number of bosons is increased towards the infinite-particle limit. We see saturation of the quantities under investigation with $N$ for a given barrier height, thereby providing strong numerical support of the conclusions to be made at the infinite-particle limit.

The many-particle Hamiltonian whose ground state we are to investigate is $\hat{H}(r_1, \ldots, r_N) = \sum_{j=1}^N \hat{h}(r_j) + \lambda_0 \hat{W}(r_j - r_k)$. The one-particle Hamiltonian is $\hat{h}(r) = -\frac{1}{2} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) + \frac{1}{4}x^2 + \frac{1}{4}y^2 + V_0 e^{-x^2}$. Note that the harmonic part of the confining potential is anisotropic, and wider along the $y$ direction than along the $x$ direction. The inter-particle interaction is Gaussian, $\lambda_0 \hat{W}(r) = \frac{\lambda_0}{2\pi\sigma} e^{-x^2+y^2} / (2\pi\sigma^2)$, with width of $\sigma = 0.25$. Throughout this work $\Lambda = 0.1$.

The ground-state of the trapped bosons is computed within the multiconfigurational time-dependent Hartree for bosons (MCTDHB) method [12, 13]. We use the numerical implementation in [14, 15]. The method is well documented, used, benchmarked, and extended in the literature [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32], and a brief account suffices here. In the MCTDHB method, the self-consistent ground state [33] is obtained by imaginary-time propagation and determined according to the variational principle. The wavefunction is expanded by all time-dependent permanents, where $N$ bosons are distributed over $M$ optimized orthonormal one-particle functions, with time-dependent coefficients, such
that the energy of the ground state is minimized. For \( M = 1 \) orbitals MCTDHB boils down to Gross-Pitaevskii theory.

The Hamiltonian is represented by an equidistant grid of 128 \( \times \) 128 points in a box of size \([-10, 10) \times [-10, 10)\) with periodic boundary conditions. Convergence with respect to the grid size has been verified using a 256 \( \times \) 256 points for the highest barrier, \( V_0 \), and largest number of self-consistent orbitals, \( M \), employed.

Fig. 1 displays the densities per particle of \( N = 1,000,000 \) bosons computed at the \( M = 2 \) many-body and \( M = 1 \) mean-field levels of theory. The respective densities per particle cannot be distinguished from each other, in accordance with the left-hand-side of (1). The accuracy and adequacy of the \( M = 2 \) computations for the two-dimensional trap and various barrier heights considered here are verified against \( M = 4 \) computations, see below.

We now examine other quantities and their values as the infinite-particle limit is taken. Fig. 2 depicts the difference between the mean-field and many-body ground-state energies per particle as a function of the barrier height \( V_0 = 7, \ldots, 16 \) and the number of particles \( N = 10^2, \ldots, 10^6 \), all at a constant interaction parameter \( \Lambda \). The difference is found to increase with \( V_0 \) for a given \( N \) and to decrease with \( N \) for a given \( V_0 \). The latter is in accordance with the right-hand-side of (1). To verify that \( M = 2 \) self-consistent orbitals accurately describe the energy in the two-dimensional double well for the various barrier heights, we have performed calculations using \( M = 4 \) and \( N = 100 \) bosons, which are seen to fall on top of the \( M = 2 \) and \( N = 100 \) bosons results, see Fig. 2. Since the interaction parameter is kept fixed, this implies the accuracy of the \( M = 2 \) and \( N > 100 \) results as well.

Fig. 3 presents the depletion per particle, \( 1 - \frac{n_1}{N} \) for \( N = 10^2, \ldots, 10^6 \) bosons as a function of the barrier height. The interaction parameter is \( \Lambda = \lambda_0 (N - 1) = 0.1 \). The depletion per particle decreases with increasing number of particles \( N \) for a given barrier height \( V_0 \). See the text for further details. Actual data is marked by symbols, the continuous curves are to guide the eye only. The quantities shown are dimensionless.

**Figure 3.** Depletion per particle \( 1 - \frac{n_1}{N} \) for \( N = 10^2, \ldots, 10^6 \) bosons as a function of the barrier height. The interaction parameter is \( \Lambda = \lambda_0 (N - 1) = 0.1 \). The depletion per particle decreases with increasing number of particles \( N \) for a given barrier height \( V_0 \). See the text for further details. Actual data is marked by symbols, the continuous curves are to guide the eye only. The quantities shown are dimensionless.
Figure 4. Many-particle position variances per particle along the $x$ and $y$ directions, $\frac{1}{N}\Delta^2_X$ and $\frac{1}{N}\Delta^2_Y$, for $N = 10^2, \ldots, 10^6$ bosons as a function of the barrier height. The interaction parameter is $\Lambda = \lambda_0(N - 1) = 0.1$. The anisotropies of the many-particle position variances at the many-body and mean-field levels of theory become opposite to each other at a barrier height just above $V_0 = 14$. See the text for further details. Actual data is marked by symbols, the continuous curves are to guide the eye only. The quantities shown are dimensionless.

number obtained from diagonalization of the reduced one-particle density matrix $\rho^{(1)}(r, r')$. Equivalently, the sum of all other occupation numbers, $\sum_{j>1} n_j$, is the total number of depleted particles. We see that the total number of depleted particles increases with the barrier height $V_0$. There are around 20 bosons outside the condensed mode for $V_0 = 16$. Whereas the total number of depleted particles saturates for increasing $N$ and a given barrier height, the depletion per particle decreases. This is in accordance with the first relation in (2). To verify that $M = 2$ self-consistent orbitals accurately describe the depletion in the two-dimensional double well for all $V_0$, we have performed calculations using $M = 4$ and $N = 100$ bosons, which are seen to lie on top of the $M = 2$ and $N = 100$ bosons results, see Fig. 3. Since the interaction parameter is held fixed, this implies the accuracy of the $M = 2$ and $N > 100$ results as well. Furthermore, we have found for $N = 100$ bosons that the system becomes two-fold fragmented with increasing barrier height $[33, 34, 35, 36]$, with $n_3/N, n_4/N < 10^{-7}$ for all $V_0$. The two macroscopically-occupied natural orbitals are gerade and ungerade along the $x$ direction and gerade along the $y$ direction. The next two marginally-occupied natural orbitals are (for $V_0 \geq 8$) ungerade along the $y$ direction and gerade and ungerade along the $x$ direction. As the number of bosons is enlarged for a given barrier height and the fixed interaction strength, Fig. 3 shows that the fragmentation disappears $[35]$ until 100% condensation is obtained at the infinite-particle limit $[2]$.

Figs. 1, 2, 3 have demonstrated numerically the literature results on the density per particle, energy per particle, and depletion per particle of a trapped bosonic system in two spatial dimensions with a constant interaction parameter at the infinite-particle limit $[1, 2, 3]$. We
now move to investigate the many-particle position variances in the system. Complementary results on the many-particle momentum variances and the respective uncertainty products are given and briefly discussed in the Appendix. Fig. 4 depicts the results. It is instrumental to analyze them in view of the study of bosons in the one-dimensional double well as a function of the barrier height at the infinite-particle limit in [7]. We begin with the variance per particle along the $x$ direction, $\frac{1}{N} \Delta^2 X$, the direction along which the barrier is ramped up. The variance computed at the mean-field level of theory increases monotonously, signifying the spread of the density seen in Fig. 1. In contrast, the quantity computed and the many-body level reaches a maximum at about $V_0 \approx 9$, then it starts to decrease. There are about 0.04 particles depleted then, see Fig. 3. This is sufficient for the difference between the mean-field and many-body variances to become qualitative. With increasing barrier height, the many-body $\frac{1}{N} \Delta^2 X$ decreases further. The same qualitative difference is found in the one-dimensional double well [7].

The variance per particle along the $y$ direction, $\frac{1}{N} \Delta^2 Y$, behaves completely different, see Fig. 4. First, the variance is practically independent of the height of the barrier. Second, its value is essentially $\frac{1}{\sqrt{2}}$, i.e., half the inverse frequency of the harmonic confinement along the $y$ direction. This implies a very weak coupling between the $x$ and $y$ directions of the interacting bosons in the studied two-dimensional double-well trap for all barrier heights, at least as far as the transverse variance is examined. We emphasize that no assumptions have been made on the shape of the orbitals and many-boson wavefunction which are determined numerically self-consistently according to the variational principle. For the respective essential independence of the momentum variance along the $y$ direction on the barrier height, see the Appendix. Third and finally, the mean-field and many-body variances practically coincide.

We can now combine the results for the position variances along the $x$ and $y$ directions together. At the mean-field level, $\frac{1}{N} \Delta^2 X > \frac{1}{N} \Delta^2 Y$ for all barrier heights. This is in line with Fig. 1, showing that the system’s density is wider along the $x$ direction than along the $y$ direction. At the many-body level, $\frac{1}{N} \Delta^2 X > \frac{1}{N} \Delta^2 Y$ up to barrier height of $V_0 \approx 14$, see Fig. 4. Just above this barrier height the situation reverses, namely, $\frac{1}{N} \Delta^2 X < \frac{1}{N} \Delta^2 Y$. Thus, despite the fact that the density along the $x$ direction is wider than along the $y$ direction, the many-particle position variance is smaller along the $x$ direction than along the $y$ direction. This inverse relation between the density and position variance constitutes an opposite anisotropy of the many-particle position variance. Furthermore, the anisotropy $\frac{1}{N} \Delta^2 X < \frac{1}{N} \Delta^2 Y$ of the ground state saturates when increasing the number of particles while keeping the interaction parameter fixed, see Fig. 4, i.e., it persists in the infinite-particle limit.

The system considered here is a two-dimensional double-well potential with a barrier of height $V_0$. The $x$ and $y$ directions are very weakly coupled, at least at as far as the position variance is examined. Just above $V_0 = 14$, when the position variance becomes anisotropic, the total number of depleted particles is $\sum_{j>1} n_j < 10$. It is intriguing that already less then 10 bosons can have such a sizable effect on a trapped Bose-Einstein condensate at the infinite-particle limit which is 100% condensed. This makes investigating the anisotropy of the position variance in traps of other shapes a fundamental and appealing direction to follow.

3. Summary and outlook

The ground state of a Bose-Einstein condensate in a two-dimensional trap potential is analyzed numerically at the infinite-particle limit. It is demonstrated that the anisotropy of the many-particle position variance can be opposite when computed at the many-body and mean-field levels of theory, despite the system being 100% condensed. It would be interesting to find analogous situations for the momentum variance and, in three spatial dimensions, for the variance of the many-particle angular-momentum operator.
Figure A1. Many-particle momentum variances per particle along the $x$ and $y$ directions, $\frac{1}{N} \Delta^2 P_X$ and $\frac{1}{N} \Delta^2 P_Y$, for $N = 10^2, \ldots, 10^6$ bosons as a function of the barrier height. The interaction parameter is $\Lambda = \Lambda_0 (N - 1) = 0.1$. The many-body and mean-field momentum quantities are essentially the same along both the $x$ and $y$ directions. See the text for further details. Actual data is marked by symbols, the continuous curves are to guide the eye only. The quantities shown are dimensionless.

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Appendix A. Many-particle momentum variance and uncertainty product

The appendix presents complementary results. Fig. A1 presents the many-particle momentum variances per particle $\frac{1}{N} \Delta^2 P_X$ and $\frac{1}{N} \Delta^2 P_Y$ as a function of the barrier height. Unlike the position variance, here the respective many-body and mean-field quantities along the $x$ and the $y$ directions are essentially the same. This means that there is no anisotropy of the momentum variance for the ground state in the double-well potential, let alone at the infinite-particle limit. We remark that anisotropy of the momentum variance has been found in the out-of-equilibrium scenario of [10] at the infinite-particle limit. It would be interesting to find a ground state whose momentum variance exhibits anisotropy at the infinite-particle limit.

The momentum variance along the $x$ direction grows monotonously with $V_0$. This growth of the momentum variance originates from the narrowing of each of the two density peeks in their potential wells with increasing barrier height, despite the overall broadening of the density along the $x$ direction, see Fig. 1. The momentum variance along the $y$ direction is practically independent of the barrier height, its value being essentially $\frac{1}{2 \sqrt{2}}$, i.e., half the frequency of the
Figure A2. Many-particle uncertainty products along the $x$ and $y$ directions, $\frac{1}{N} \Delta^2 X \frac{1}{N} \Delta^2 P_x = \Delta^2 X_{CM} \Delta^2 P_{XCM}$ and $\frac{1}{N} \Delta^2 Y + \Delta^2 P_y = \Delta^2 Y_{CM} \Delta^2 P_{YCM}$, for $N = 10^2, \ldots, 10^6$ bosons as a function of the barrier height. The interaction parameter is $\Lambda = \lambda_0 (N - 1) = 0.1$. The many-body and mean-field uncertainty products differ substantially along the $x$ direction, whereas they are essentially the same along the $y$ direction. See the text for further details. Actual data is marked by symbols, the continuous curves are to guide the eye only. The quantities shown are dimensionless.

harmonic trap along the $y$ direction. This matches the finding for the position variance, see Fig. 4, and corroborates the very weak coupling between the $x$ and $y$ directions found at the level of the many-particle position variance also at the level of the many-particle momentum variance.

Last but not least, we combine the results for the position and momentum variances together. This is most naturally done in terms of their uncertainty products, $\frac{1}{N} \Delta^2 X \frac{1}{N} \Delta^2 P_x = \Delta^2 X_{CM} \Delta^2 P_{XCM}$ and $\frac{1}{N} \Delta^2 Y + \Delta^2 P_y = \Delta^2 Y_{CM} \Delta^2 P_{YCM}$ [7]. Fig. A2 presents the uncertainty products along the $x$ and $y$ directions. Summing up all the above results, we can see for the ground state at the infinite-particle limit that: (i) The many-particle uncertainty product along the $x$ direction computed at the mean-field level of theory increases monotonously with the barrier height $V_0$, whereas that computed at the many-body level increases first and then decreases. (ii) The many-particle uncertainty products computed at the many-body and mean-field levels along the $y$ direction are essentially independent of the barrier height, and are practically minimal, $\frac{1}{4} \Delta^2 Y \frac{1}{4} \Delta^2 P_y = \frac{1}{4} \Delta^2 Y_{CM} \frac{1}{4} \Delta^2 P_{YCM}$, reflecting the very weak coupling of the $x$ and $y$ directions discussed above. (iii) In the ‘competition’ between the many-particle position variance, which exhibits anisotropy, see Fig. 4, and the many-particle momentum variance which does not, see Fig. A1, the latter ‘wins’; $\frac{1}{N} \Delta^2 X \frac{1}{N} \Delta^2 P_x > \frac{1}{N} \Delta^2 Y + \frac{1}{N} \Delta^2 P_y$ for all considered barrier heights $V_0$ at the infinite-particle limit. This is a good place to conclude our investigations.
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