Solvable Model of a Generic Trapped Mixture of Interacting Bosons: Many-Body and Mean-Field Properties at the Infinite-Particle Limit

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Abstract. A solvable model of a generic trapped bosonic mixture, \(N_1\) bosons of mass \(m_1\) and \(N_2\) bosons of mass \(m_2\) trapped in an harmonic potential of frequency \(\omega\) and interacting by harmonic inter-particle interactions of strengths \(\lambda_1, \lambda_2,\) and \(\lambda_{12},\) is discussed. It has recently been shown for the ground state [J. Phys. A \textbf{50}, 295002 (2017)] that in the infinite-particle limit, when the interaction parameters \(\lambda_1 (N_1 - 1), \lambda_2 (N_2 - 1), \lambda_{12} N_1, \lambda_{12} N_2\) are held fixed, each of the species is 100\% condensed and its density per particle as well as the total energy per particle are given by the solution of the coupled Gross-Pitaevskii equations of the mixture. In the present work we investigate properties of the trapped generic mixture at the infinite-particle limit, and find differences between the many-body and mean-field descriptions of the mixture, despite each species being 100\%. We compute analytically and analyze, both for the mixture and for each species, the center-of-mass position and momentum variances, their uncertainty product, the angular-momentum variance, as well as the overlap of the exact and Gross-Pitaevskii wavefunctions of the mixture. The results obtained in this work can be considered as a step forward in characterizing how important are many-body effects in a fully condensed trapped bosonic mixture at the infinite-particle limit.

1. Introduction

Ever since the first experimental demonstration of trapped Bose-Einstein condensates (BECs) in ultra-cold quantum gases [1-3], the connection between the microscopic many-particle Hamiltonian and the macroscopic Gross-Pitaevskii, mean-field theory has drawn much attention [4-14]. Whereas properties like the energy and density per particle, and being 100\% condensed, are exactly reproduced in the infinite-particle limit by the Gross-Pitaevskii theory [5-8], other properties, like the variance of many-particle operators and, ultimately, the many-particle wavefunction itself generally are not reproduced by the mean-field theory [10-14].

Mixtures of BECs have also attracted a lot of interest in their static, thermal, and out-of-equilibrium properties [15-37], yet the connection between their microscopic many-body Hamiltonian and the mean-field solution for mixtures has only recently received attention [38-43]. In particular, that each of the species in the ground state of a generic trapped mixture is, in the infinite-particle limit, 100\% condensed has been recently shown within the exactly-solvable harmonic-interaction model for trapped mixtures [40]. The harmonic-interaction model has
widely been studied for indistinguishable bosons [44-52], fermions [50-55], and bosonic mixtures [56-60]. The purpose of the present work is to compute and compare many-body and mean-field properties of the 100% condensed generic mixture [40] at the infinite-particle limit. The ground-state wavefunction can be prescribed analytically at the exact and mean-field levels, which facilitates a transparent study of properties of the mixture at both levels of theory. We extend and broaden previous results obtained in the specific case of a symmetric mixture [39]. We concentrate on the center-of-mass position an momentum variance, their uncertainty product, and angular-momentum variance of the whole mixture as well as of each species in the mixture. Generally, in comparison with the textbook single-particle case [61] the variances and uncertainty product of many-particle operators are more involved [10, 11, 13], see in this context also [62, 63]. Finally, motivated by recent results in the single-species case [12, 14], we evaluate explicitly the overlap of the exact and Gross-Piatesvkii wavefunctions of the generic mixture. A common line of our investigation is how intra-species and inter-species interaction parameters (in combination with the masses) influence the respective properties of the mixture at the infinite-particle limit.

2. The harmonic-interaction model for a generic trapped mixture
We start from the many-particle Hamiltonian ($\hbar = 1$)

$$H(x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2}) =$$

$$= \sum_{i=1}^{N_1} \left(-\frac{1}{2m_1} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m_1 \omega^2 x_i^2 \right) + \sum_{j=1}^{N_2} \left(-\frac{1}{2m_2} \frac{\partial^2}{\partial y_j^2} + \frac{1}{2} m_2 \omega^2 y_j^2 \right) +$$

$$+ \lambda_1 \sum_{1 \leq i < l} (x_i - x_l)^2 + \lambda_2 \sum_{1 \leq j < m} (y_j - y_m)^2 + \lambda_{12} \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} (x_i - y_j)^2$$

which describes a generic trapped mixture of $N_1$ bosons of mass $m_1$ (species 1) and $N_2$ bosons of mass $m_2$ (species 2) trapped in an harmonic potential of frequency $\omega$ and interacting by harmonic intra-species and inter-species interactions of strengths $\lambda_1$, $\lambda_2$, and $\lambda_{12}$. Positive values of $\lambda_1$, $\lambda_2$, and $\lambda_{12}$ mean attraction, and negative values repulsion. Of course, a combination of repulsive and attractive intra-species and inter-species interactions is possible [40]. The Hamiltonian (1) can be diagonalized by moving from the laboratory frame (i.e., transforming the Cartesian coordinates) to a set of Jacobi coordinates

$$Q_s = \frac{1}{\sqrt{s(s + 1)}} \sum_{i=1}^{s} (x_{s+1} - x_i), \quad 1 \leq s \leq N_1 - 1,$$

$$Q_{N_1-1+s} = \frac{1}{\sqrt{s(s + 1)}} \sum_{j=1}^{s} (y_{s+1} - y_j), \quad 1 \leq s \leq N_2 - 1,$$

$$Q_{N-1} = \sqrt{\frac{N_1}{N_2}} \sum_{i=1}^{N_1} x_i - \sqrt{\frac{N_1}{N_2}} \sum_{j=1}^{N_2} y_j, \quad Q_N = \frac{m_1}{M} \sum_{i=1}^{N_1} x_i + \frac{m_2}{M} \sum_{j=1}^{N_2} y_j.$$  (2)

Note that the Jacobian of the transformation satisfies $|\frac{\partial (Q_1, \ldots, Q_N)}{\partial (x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2})}| = 1$.

The transformed many-particle Hamiltonian is separable and reads

$$\hat{H}(Q_1, \ldots, Q_N) = \sum_{s=1}^{N_1-1} \left(-\frac{1}{2m_1} \frac{\partial^2}{\partial Q_s^2} + \frac{1}{2} m_1 \Omega_1^2 Q_s^2 \right) + \sum_{s=1}^{N_2-1} \left(-\frac{1}{2m_2} \frac{\partial^2}{\partial Q_s^2} + \frac{1}{2} m_2 \Omega_2^2 Q_s^2 \right) +$$

$$+ \left(\frac{1}{2m_1} \frac{\partial^2}{\partial Q_{N-1}^2} + \frac{1}{2} m_1 \Omega_1^2 Q_{N-1}^2 \right) + \left(\frac{1}{2m_2} \frac{\partial^2}{\partial Q_N^2} + \frac{1}{2} m_2 \Omega_2^2 Q_N^2 \right),$$  (3)
where \( M_{12} = \frac{m_1 m_2}{m} \) and \( M = N_1 m_1 + N_2 m_2 \) are the reduced and total mass, respectively, and

\[
\Omega_1 = \sqrt{\omega^2 + \frac{2}{m_1} \left( \Lambda_1 \frac{N_1}{N_1 - 1} + \Lambda_{21} \right)}, \quad \Omega_2 = \sqrt{\omega^2 + \frac{2}{m_2} \left( \Lambda_2 \frac{N_2}{N_2 - 1} + \Lambda_{12} \right)},
\]

\[
\Omega_{12} = \sqrt{\omega^2 + 2 \left( \frac{\Lambda_{12}}{m_2} + \frac{\Lambda_{21}}{m_1} \right)}, \quad \omega
\]

are the eigen-frequencies of the decoupled oscillators. \( \Omega_1 \) and \( \Omega_2 \) are associated with the intra-species relative coordinates, \( \Omega_{12} \) with the inter-species relative coordinate (between the center-of-mass of species 1 and the center-of-mass of species 2), and the eigen-frequency of the center-of-mass coordinate of the whole mixture is equal to the trapping potential \( \omega \). Herein, the so called mean-field interaction parameters are defined, \( \Lambda_1 = \lambda_1 (N_1 - 1) \), \( \Lambda_2 = \lambda_1 (N_2 - 1) \), \( \Lambda_{12} = \lambda_{12} N_1 \), and \( \Lambda_{21} = \lambda_{12} N_2 \), and shall have an important role below.

The ground-state wavefunction of the mixture is thus

\[
\Psi(Q_1, \ldots, Q_N) = \left( \frac{m_1 \Omega_1}{\pi} \right)^{3(N_1-1)/4} \left( \frac{m_2 \Omega_2}{\pi} \right)^{3(N_2-1)/4} \left( \frac{M \Omega_{12}}{\pi} \right)^{3/4} \left( \frac{M \omega}{\pi} \right)^{3/4} \times
\]

\[
x e^{-\frac{1}{2} \left( m_1 \Omega_1 \sum_{i=1}^{N_1} x_i^2 + m_2 \Omega_2 \sum_{j=1}^{N_2} y_j^2 + M \Omega_{12} \sum_{i=1}^{N_1} x_i + M \Omega_{12} \sum_{j=1}^{N_2} y_j + M \omega \sum_{i=1}^{N_1} x_i \sum_{j=1}^{N_2} y_j \right)}
\]

and

\[
E = \frac{3}{2} \left( (N_1 - 1) \sqrt{\omega^2 + \frac{2}{m_1} \left( \Lambda_1 \frac{N_1}{N_1 - 1} + \Lambda_{21} \right)} + \right.
\]

\[
+ (N_2 - 1) \sqrt{\omega^2 + \frac{2}{m_2} \left( \Lambda_2 \frac{N_2}{N_2 - 1} + \Lambda_{12} \right)} + \sqrt{\omega^2 + 2 \left( \frac{\Lambda_{12}}{m_2} + \frac{\Lambda_{21}}{m_1} \right)} + \omega \tag{5}
\]

is the ground-state energy which can be seen as a functional of the numbers and masses of the particles and the interaction parameters.

It is possible to solve the Hamiltonian (1) at the mean-field level [40]. The Gross-Pitaevskii (mean-field) wavefunction is

\[
\phi^{GP}(x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2}) =
\]

\[
= \left( \frac{m_1 \Omega_1^{GP}}{\pi} \right)^{3N_1/4} \left( \frac{m_2 \Omega_2^{GP}}{\pi} \right)^{3N_2/4} e^{-\frac{1}{2} \left( m_1 \Omega_1^{GP} \sum_{i=1}^{N_1} x_i^2 + m_2 \Omega_2^{GP} \sum_{j=1}^{N_2} y_j^2 \right)},
\]

\[
\Omega_1^{GP} = \sqrt{\omega^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21})}, \quad \Omega_2^{GP} = \sqrt{\omega^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12})}. \tag{6}
\]

It is a double-product wavefunction made of the (interaction-dressed) Gross-Pitaevskii orbitals

\[
\phi_1^{GP}(x) = \left( \frac{m_1 \Omega_1^{GP}}{\pi} \right)^{3/4} e^{-\frac{1}{2} m_1 \Omega_1^{GP} x^2}, \quad \phi_2^{GP}(y) = \left( \frac{m_2 \Omega_2^{GP}}{\pi} \right)^{3/4} e^{-\frac{1}{2} m_2 \Omega_2^{GP} y^2}. \tag{8}
\]

\( \Omega_1^{GP} \) and \( \Omega_2^{GP} \) are the Gross-Pitaevskii frequencies. For \( N_1 \gg 1 \) and \( N_2 \gg 1 \) they coincide with the respective many-body eigen-frequencies \( \Omega_1 \) and \( \Omega_2 \) (4).

The mean-field energy per particle is given by

\[
\varepsilon^{GP} = \frac{E^{GP}}{N} = \frac{3}{2(\Lambda_1 + \Lambda_{21})} \left[ \Lambda_{12} \sqrt{\omega^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21})} + \Lambda_{21} \sqrt{\omega^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12})} \right] \tag{9}
\]

and expressed solely via the masses of the bosons and the interaction parameters for any number of particles (\( N_1 \) and \( N_2 \) and therefore) \( N \). A connection between masses and interaction parameters will further serve below.
3. Properties at the infinite-particle limit

In the two-species infinite-particle limit, i.e., when \( N_1 \to \infty \) and \( N_2 \to \infty \) such that the interaction parameters \( \Lambda_1, \Lambda_2, \Lambda_{12}, \) and \( \Lambda_{21} \) (and therefore \( \frac{N_1}{N_2} = \frac{\Lambda_{12}}{\Lambda_{21}} \)) are held fixed (hereafter briefly, the infinite-particle limit) we have \([40]\) for the frequencies \( \lim_{N \to \infty} \Omega_1 = \Omega_1^{GP} \) and \( \lim_{N \to \infty} \Omega_2 = \Omega_2^{GP} \), for the energy per particle

\[
\lim_{N \to \infty} \frac{E}{N} = \varepsilon^{GP},
\]

and for the reduced density matrices \([64, 65]\) per particle

\[
\frac{\rho_1(x, x')}{N_1} = \rho_1^{GP}(x, x'), \quad \frac{\rho_2(y, y')}{N_2} = \rho_2^{GP}(y, y'),
\]

and

\[
\frac{\rho_{12}(x, x', y, y')}{N_1 N_2} = \rho_1^{GP}(x, x') \rho_2^{GP}(y, y').
\]

The reduced one-particle density matrices at the Gross-Pitaevskii level are given by \( \rho_1^{GP}(x, x') = \phi_1^{GP}(x) \left\{ \phi_1^{GP}(x') \right\}^* \) and \( \rho_2^{GP}(y, y') = \phi_2^{GP}(y) \left\{ \phi_2^{GP}(y') \right\}^* \). The question we would like to address in this work is in what capacity (i.e., for which quantities and by how much) the many-body and mean-field solutions are different, even when each of the species in the mixture is 100% condensed \([Eq. (11)]\)?

To proceed we need to express the Gross-Pitaevskii wavefunction (7) via the Jacobi coordinates (2). Using (A.1) and (A.2) we have

\[
\Phi^{GP}(Q_1, \ldots, Q_N) = \left( \frac{m_1 \Omega_1^{GP}}{\pi} \right)^{\frac{3 N_1}{2}} \left( \frac{m_2 \Omega_2^{GP}}{\pi} \right)^{\frac{3 N_2}{2}} \times
\]

\[
e^{-\frac{m_1 \Omega_1^{GP}}{2} \sum_{s=1}^{N_1} Q_s^2 + \left( \sum_{s=1}^{N_1} Q_s + \sqrt{N_1} Q_N \right)^2} e^{-\frac{m_2 \Omega_2^{GP}}{2} \sum_{s=1}^{N_2} Q_s^2 + \left( \sum_{s=1}^{N_2} Q_s + \sqrt{N_2} Q_N \right)^2} =
\]

\[
= \left( \frac{m_1 \Omega_1^{GP}}{\pi} \right)^{\frac{3 N_1}{2}} \left( \frac{m_2 \Omega_2^{GP}}{\pi} \right)^{\frac{3 N_2}{2}} e^{-\frac{m_1 \Omega_1^{GP}}{2} \sum_{s=1}^{N_1} Q_s^2} e^{-\frac{m_2 \Omega_2^{GP}}{2} \sum_{s=1}^{N_2} Q_s^2} \times
\]

\[
e^{-\frac{M}{2} \left[ \frac{m_1 N_1}{M} \Omega_1^{GP} + \frac{m_2 N_2}{M} \Omega_2^{GP} \right]} Q_{N-1}^2 e^{-\frac{M}{2} \left[ \frac{m_1 N_1}{M} \Omega_1^{GP} + \frac{m_2 N_2}{M} \Omega_2^{GP} \right]} Q_N^2 e^{-M_{12} \sqrt{N_1 N_2} \left[ \Omega_1^{GP} - \Omega_2^{GP} \right]} Q_{N-1} Q_N.
\]

We see that the Gross-Pitaevskii wavefunction is ‘nearly’ separable in terms of the Jacobi coordinates, except of the last term which couples \( Q_{N-1} \) and \( Q_N \). Interestingly, along the sector in parameter space in which the mean-field frequencies \([see (7)]\) are equal,

\[
\sqrt{\omega^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21})} = \sqrt{\omega^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12})} \iff m_2 (\Lambda_1 + \Lambda_{21}) = m_1 (\Lambda_2 + \Lambda_{12}),
\]

the Gross-Pitaevskii wavefunction is separable in terms of the Jacobi coordinates, as does the exact wavefunction. Relation (14) defines an interaction–mass balance condition between the two species for the separability of the center-of-mass coordinate of the mixture at the mean-field level. Surprisingly, this condition for separability is required even in the case the interspecies interaction is zero. In other words, the center-of-mass coordinate \( Q_M \) of two (harmonic-interacting) trapped BECs is not separable at the Gross-Pitaevskii level, even if the two species do not interact with each other, unless \( m_2 \Lambda_1 = m_1 \Lambda_2 \). We note that condition (14) obviously holds for the symmetric mixture \([39]\). On the other hand, the Gross-Pitaevskii wavefunction
is separable in terms of the center-of-mass coordinates of the individual species (see below), whereas the exact wavefunction is not.

We now express the position and momentum center-of-mass operators of the mixture and of each of the species in terms of the Jacobi coordinates. Thus we have

\[ \hat{R}_{CM} = Q_N, \quad \hat{P}_{CM} = \frac{1}{i} \frac{\partial}{i \partial Q_N}, \quad [\hat{R}_{CM}, \hat{P}_{CM}] = i \quad \forall N \]  \hspace{1cm} (15)

for the mixture (\( i \) and similarly 1 below are shorthand symbols for i and 1 in each of the three Cartesian components) and

\[ [\hat{X}_{CM}, \hat{P}_{XCM}] = i, \quad \forall N, \]
\[ \hat{Y}_{CM} = -\sqrt{\frac{M}{N_1}} Q_{N-1} + Q_N, \quad \hat{P}_{YCM} = \frac{1}{i} \frac{\partial}{i \partial Y_{CM}} = -\sqrt{\frac{N_1N_2}{N_2}} \frac{\partial}{\partial Q_{N-1}} + \frac{N_1m_1}{M} \frac{\partial}{\partial Q_N}, \]
\[ [\hat{Y}_{CM}, \hat{P}_{YCM}] = i, \quad \forall N, \]  \hspace{1cm} (16)

for each of the species. The center-of-mass operators of the species and mixture are related by the relations

\[ \frac{m_1N_1X_{CM} + m_2N_2Y_{CM}}{M} = \hat{R}_{CM}, \quad \hat{P}_{XCM} + \hat{P}_{YCM} = \hat{P}_{CM} \]  \hspace{1cm} (17)

which are to be used in the computation of the variances at the mean-field level.

In what follows we use a compact notation to denote the variance (of the three Cartesian components) of an operator \( \hat{O} = (\hat{O}_1, \hat{O}_2, \hat{O}_3) \) with respect to the exact and Gross-Pitaevskii wavefunctions,

\[ \Delta^2_O = \langle \Psi | \hat{O}^2 | \Psi \rangle - \langle \Psi | \hat{O} | \Psi \rangle^2, \quad \Delta^2_{O,GP} = \langle \Phi^{GP} | \hat{O}^2 | \Phi^{GP} \rangle - \langle \Phi^{GP} | \hat{O} | \Phi^{GP} \rangle^2, \]  \hspace{1cm} (18)

where \( \hat{O}^2 = (\hat{O}_1^2, \hat{O}_2^2, \hat{O}_3^2) \).

The variances of the center-of-mass position and momentum operators of the mixture, at the exact many-body level, are given by

\[ \Delta^2_{R_{CM}} = \frac{1}{M} \frac{1}{2\omega} 1, \quad \Delta^2_{P_{CM}} = M \frac{\omega}{2} 1, \quad \forall N. \]  \hspace{1cm} (19)

The position variance decreases with the mass of the mixture, whereas the momentum variance increases with the mass. Otherwise, they do not depend on other parameters of the mixture, like the interaction parameters for instance. Consequently, their uncertainty product

\[ \Delta^2_{R_{CM}} \Delta^2_{P_{CM}} = \frac{1}{4} 1, \quad \forall N \]  \hspace{1cm} (20)

holds for any number of particles. The uncertainty product is minimal, reflecting the separability of the center-of-mass of the mixture in the harmonic trap.

On the other hand, at the Gross-Pitaevskii level we find

\[ \Delta^2_{R_{CM,GP}} = \frac{1}{M} \left[ \frac{m_1N_1}{M} \sqrt{1 + \frac{2}{m_1 \omega^2} (\Lambda_1 + \Lambda_{21})} + \frac{m_2N_2}{M} \sqrt{1 + \frac{2}{m_2 \omega^2} (\Lambda_2 + \Lambda_{12})} \right] \frac{1}{2\omega} 1, \]  \hspace{1cm} (21)
\[ \Delta^2_{P_{CM,GP}} = M \left[ \frac{m_1N_1}{M} \sqrt{1 + \frac{2}{m_1 \omega^2} (\Lambda_1 + \Lambda_{21})} + \frac{m_2N_2}{M} \sqrt{1 + \frac{2}{m_2 \omega^2} (\Lambda_2 + \Lambda_{12})} \right] \frac{\omega}{2} 1, \quad \forall N. \]
The center-of-mass momentum (position) variance again scales with the (inverse) mass of the system, but depends explicitly on the products of the relative mass of each species times the corresponding (inverse) Gross-Pitaevskii frequency. The variances depend explicitly on all parameters of the mixture, in particular on the interaction parameters. This is entirely different than the many-body dependence (19), and reflects the dressing of the frequency (and inseparability) of the center-of-mass coordinate at the mean-field level. Consequently, the uncertainty product

$$\Delta^2 \hat{R}_{CM,GP} \Delta^2 \hat{P}_{CM,GP} = \left\{ \begin{array}{l}
\frac{1}{4} \left[ \frac{1}{4} \right] \left[ \frac{1}{4} \right], \forall N (22)
\end{array} \right.$$  

is larger than the minimal, except when the interaction–mass balance condition (14) holds and the Gross-Pitaevskii wavefunction (13) becomes separable with respect to the center-of-mass coordinate. For instance, increasing either of the intra-species interaction parameters $\Lambda_1$ or $\Lambda_2$ leads to an increase of the uncertainty product. The above described discrepancy between the mean-field and exact results can be used as a characterization and measure of the many-body contribution to the physics of a given 100%-condensed trapped mixture.

We now move to the properties of the center-of-mass operators of the species. Using relations (16) in terms of the Jacobi coordinates we find

$$\Delta^2 \hat{R}_{CM,GP} \Delta^2 \hat{P}_{CM,GP} = \left\{ \begin{array}{l}
\frac{1}{4} \left[ \frac{1}{4} \right] \left[ \frac{1}{4} \right], \forall N (22)
\end{array} \right.$$  

The center-of-mass position and momentum variances of each species depend only on the inter-species interaction parameters $\Lambda_{12}$ and $\Lambda_{21}$, and not on the intra-species parameters $\Lambda_1$ and $\Lambda_2$. Increasing the inter-species interaction, such that the species attract each other more, decreases (increases) the position (momentum) variance, and vice versa. Generally, the variances of species 1 are different than those of species 2 because of the mass–particle imbalance (i.e.,
product state. It hence satisfies at the level of a single particle \( \hat{x} \) (Cartesian coordinates). The mean-field wavefunction (7) is a 'spherically symmetric' double-

\[ \Delta_{X_{CM}}^2 \Delta_{P_{X_{CM}}}^2 = \Delta_{Y_{CM}}^2 \Delta_{P_{Y_{CM}}}^2 = \left\{ 1 + \frac{m_1 m_2 \Lambda_{12}}{(m_1 \Lambda_{12} + m_2 \Lambda_{21})^2} \frac{1}{\sqrt{1 + \frac{2}{\omega^2} \left( \frac{\Lambda_{12}}{m_2} + \frac{\Lambda_{21}}{m_1} \right)}} + \frac{\Delta_{Y_{CM}}^2}{\Delta_{P_{Y_{CM}}}^2} \right\} \frac{1}{4} \frac{1}{4} \frac{1}{4} , \quad \forall \Lambda \).

The uncertainty products of the individual species are always larger than (the minimal uncertainty product) \( \frac{1}{4} \), unless the inter-species interaction is zero, and we have two decoupled systems. The dependence on the mass–particle imbalance is then absorbed. In the specific case of a symmetric mixture, these expressions boil down to those given in [39].

At the mean-field level, the Gross-Pitaevskii wavefunction (7,13) is separable in terms of the center-of-mass coordinates of each species and we thus have

\[ \Delta_{X_{CM,GP}}^2 = \frac{1}{m_1 N_1} \frac{1}{2 \omega} \sqrt{1 + \frac{2}{m_1 \omega^2} (\Lambda_1 + \Lambda_{21})}, \]

\[ \Delta_{P_{X_{CM,GP}}}^2 = \frac{m_1 N_1}{2} \frac{\omega}{\sqrt{1 + \frac{2}{m_1 \omega^2} (\Lambda_1 + \Lambda_{21})}}, \quad \forall \Lambda, \]

\[ \Delta_{Y_{CM,GP}}^2 = \frac{1}{m_2 N_2} \frac{1}{2 \omega} \sqrt{1 + \frac{2}{m_2 \omega^2} (\Lambda_2 + \Lambda_{21})}, \]

\[ \Delta_{P_{Y_{CM,GP}}}^2 = \frac{m_2 N_2}{2} \frac{\omega}{\sqrt{1 + \frac{2}{m_2 \omega^2} (\Lambda_2 + \Lambda_{21})}}, \quad \forall \Lambda. \]

Again, the center-of-mass position and momentum variances of species 1 are generally different than those of species 2. However, at the mean-field level they depend on both the intra-species and inter-species interaction parameters, rather than only on the inter-species interaction parameters. Furthermore, the (non-trivial) dependence on the mass–particle imbalance is absent. The two uncertainty products are again equal,

\[ \Delta_{X_{CM,GP}}^2 \Delta_{P_{X_{CM,GP}}}^2 = \Delta_{Y_{CM,GP}}^2 \Delta_{P_{Y_{CM,GP}}}^2 = \frac{1}{4} \frac{1}{4} \frac{1}{4} , \quad \forall \Lambda, \]

but, in contrast to the exact relation (24), are actually minimal. This is because of the (artificial) separation of the center-of-mass coordinates of the individual species in the Gross-Pitaevskii wavefunction. This result adds to our above conclusion, i.e., that in addition to the uncertainty product of the whole mixture also the uncertainty products of the individual species can be used for characterizing and defining the many-body contributions to the physics of a 100%-condensed trapped mixture.

We now move to discuss the variance of the angular momentum in the mixture at both the exact and mean-field levels. To identify the contribution to the angular momentum at the level of a single particle, individual species, and the whole mixture,

\[ \mathbf{l}_{1,i} = \frac{1}{i} \mathbf{x}_i \times \frac{\partial}{\partial \mathbf{x}_i}, \quad \mathbf{l}_{2,j} = \frac{1}{i} \mathbf{y}_j \times \frac{\partial}{\partial \mathbf{y}_j}, \quad \mathbf{L}_1 = \sum_{i=1}^{N_1} \mathbf{l}_{1,i}, \quad \mathbf{L}_2 = \sum_{j=1}^{N_2} \mathbf{l}_{2,j}, \quad \mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2, \]

it is instrumental to exploit the representation of the wavefunctions in the laboratory frame (Cartesian coordinates). The mean-field wavefunction (7) is a 'spherically symmetric' double-product state. It hence satisfies at the level of a single particle \( \mathbf{L}_{1,i} \Phi_{GP} = 0 \Phi_{GP} \) and
\[ \hat{L}_{1,2} \Phi^{GP} = 0 \Phi^{GP}. \]

Consequently,

\[ \Delta_{L_{1,2},GP}^2 = \Delta_{L_{2},GP}^2 = \Delta_{L,GP}^2 = 0, \quad \forall N. \quad (28) \]

For the exact wavefunction we recall its structure in the laboratory frame [40]

\[ \Psi(x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2}) = \left( \frac{m_1 \Omega_1}{\pi} \right)^{\frac{3(N_1-1)}{4}} \left( \frac{m_2 \Omega_2}{\pi} \right)^{\frac{3(N_2-1)}{4}} \left( \frac{M_1 \Omega_{12}}{\pi} \right)^{\frac{2}{3}} \left( \frac{M \omega}{\pi} \right)^{\frac{2}{3}} \times \]

\[ \times e^{-\frac{i}{2} \sum_{j=1}^{N_1} x_j^2 - \frac{i}{2} \sum_{1<j<k} x_j x_k} e^{-\frac{i}{2} \sum_{j=1}^{N_2} y_j^2 - \frac{i}{2} \sum_{1<j<k} y_j y_k} e^{i \gamma \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} x_j y_k}, \quad (29) \]

where the inter-species coupling constant is

\[ \gamma = M_{12} (\Omega_{12} - \omega) = \frac{\omega}{N_1 m_2 + N_2 m_1} \left( \sqrt{1 + \frac{2}{\omega^2} \left( \frac{\Lambda_{12}}{m_2} + \frac{\Lambda_{21}}{m_1} \right)} - 1 \right). \quad (30) \]

The other constants \( \alpha_1, \beta_1, \alpha_2, \) and \( \beta_2 \) appearing in (29) are not needed for the computation of the angular momentum and given in [40]. Examining the structure of (29) we see that the \( \alpha_1, \alpha_2 \) terms alone are eigenfunctions of \( \hat{L}_1 \) and \( \hat{L}_2 \), respectively, the \( \beta_1, \beta_2 \) terms alone are eigenfunctions of \( \hat{L}_1 \) and \( \hat{L}_2 \), respectively, and the \( \gamma \) term is an eigenfunction of \( \hat{L} \). All in all, whereas \( \hat{L} \Psi = 0 \Psi \), only \( \langle \Psi | \hat{L}_1 | \Psi \rangle = 0 \) and \( \langle \Psi | \hat{L}_2 | \Psi \rangle = 0 \) hold for the exact ground state. This is unlike the structure and above properties of the Gross-Pitaevskii wavefunction (7). Of course,

\[ \Delta_{L}^2 = 0, \quad \forall N. \quad (31) \]

Since \( \Psi \) is not an eigenfunction of either \( \hat{L}_1 \) or \( \hat{L}_2 \) (unless the inter-species interaction is zero and the species decoupled), fluctuations are expected. Making use of the structure of (29) we have

\[ \hat{L}_1 \Psi = -\hat{L}_2 \Psi = \frac{1}{i} \gamma N_1 N_2 (\hat{X}_{CM} \times \hat{Y}_{CM}) \Psi = \]

\[ = \frac{1}{i} \gamma N_1 N_2 \left( \sqrt{\frac{N_2 m_2}{N_1 M}} Q_{N-1} + Q_N \right) \times \left( -\sqrt{\frac{N_1 m_1}{N_2 M}} Q_{N-1} + Q_N \right) \Psi = \]

\[ = \frac{1}{i} \gamma \sqrt{N_1 N_2} (Q_{N-1} \times Q_N) \Psi. \quad (32) \]

Thus, for the variance of the intra-species angular momentum operators \( \hat{L}_1 \) and \( \hat{L}_2 \) we find

\[ \Delta_{L_1}^2 = \Delta_{L_2}^2 = \gamma^2 N_1 N_2 \langle (Q_{N-1} \times Q_N)^2 \rangle = \]

\[ = \frac{1}{2} \left( \frac{\Lambda_{12}}{m_2} + \frac{\Lambda_{21}}{m_1} \right)^2 \sqrt{1 + \frac{2}{\omega^2} \left( \frac{\Lambda_{12}}{m_2} + \frac{\Lambda_{21}}{m_1} \right)} - 1 \right]^2, \quad \forall N, \quad (33) \]

where we have used the separability of \( \Psi \) in terms of the Jacobi coordinates and the spherical symmetry of the problem. The variance is independent of the number of particles and is always non-zero for non-zero inter-species interaction. On the other hand, if we examine the variances of the intra-species angular-momentum operators per particle, \( \hat{L}_1 \frac{N_1}{N} \) and \( \hat{L}_2 \frac{N_2}{N} \), we find from
\[ \Delta_{Li}^2 = \frac{1}{N_i} \Delta_{Li}^2, \quad \Delta_{N_i}^2 = \frac{1}{N} \Delta_{N_i}^2 \] 

that they vanish in the infinite-particle limit. In other words, at the single-particle level the angular-momentum each boson carries in the infinite-particle limit vanishes, just like the mean-field behavior. It would be instructive to study then the variance of the appropriate conjugate angular-momentum (angle) variable \[66\] in the mixture, which is left for further investigations.

The exact and Gross-Pitaevskii wavefunctions are given analytically above for any number \(N_1, N_2\) of particles in the mixture, and are obviously different from each other even in the limit \(N \to \infty\). Motivated by recent results in the single-species case \[12, 14\], we would like to study the overlap between the Gross-Pitaevskii and exact wavefunctions which, by virtue of their difference, must be smaller than 1.

For the final result of the overlap we find

\[
S_{12}(N_1, N_2, \Lambda_1, \Lambda_2, \Lambda_{12}, \Lambda_{21}) = \langle \Phi^{GP} | \Psi \rangle =
\]

\[
= 2^{\frac{3}{2}} \frac{\Omega_{12}^{(N_1 - 1)}}{\Omega_{1}^{(N_1 - 1)}} \frac{\Omega_{2}^{(N_2 - 1)}}{\Omega_{2}^{(N_2 - 1)}} \frac{\Omega_{GP}^{(N_2 - 1)}}{\Omega_{GP}^{(N_2 - 1)}} \times \]

\[
\times \left[ \Omega_{12} + \frac{m_2 N_2 \Omega_{GP}}{M} + \frac{m_1 N_1 \Omega_{GP}}{M} \right] \left( \omega + \frac{m_1 N_1 \Omega_{GP}}{M} + \frac{m_2 N_2 \Omega_{GP}}{M} \right) - \frac{m_1 N_1 m_2 N_2}{(m_1 + m_2) \omega^2} \left( \Omega_{GP}^2 - \Omega_{12}^2 \right) \right]^{\frac{1}{2}}. \tag{34}
\]

The overlap depends on all interaction parameters in the mixture and explicitly on the number of particles in each species. We can now perform the infinite-particle limit. The final result reads

\[
\lim_{N \to \infty} S_{12}(N_1, N_2, \Lambda_1, \Lambda_2, \Lambda_{12}, \Lambda_{21}) =
\]

\[
= 2^{\frac{3}{2}} \left[ 1 + \frac{2}{m_1 \omega} (\Lambda_1 + \Lambda_{21}) \right]^{\frac{3}{2}} \left[ 1 + \frac{2}{m_2 \omega} (\Lambda_2 + \Lambda_{12}) \right]^{\frac{3}{2}} \left[ 1 + \frac{2}{\omega^2} \left( \frac{\Lambda_1}{m_2} + \frac{\Lambda_2}{m_1} \right) \right] \frac{1}{|AB - C^2|^\frac{1}{2}}. \tag{35}
\]

with

\[
A = \left[ 1 + \frac{2}{\omega^2} \left( \frac{\Lambda_1}{m_2} + \frac{\Lambda_2}{m_1} \right) \right] + \frac{m_2 \Lambda_{21}}{m_1 \Lambda_{12} + m_2 \Lambda_{21}} \left[ 1 + \frac{2}{m_1 \omega^2} (\Lambda_1 + \Lambda_{21}) \right] + \frac{m_1 \Lambda_{12}}{m_1 \Lambda_{12} + m_2 \Lambda_{21}} \left[ 1 + \frac{2}{m_2 \omega^2} (\Lambda_2 + \Lambda_{12}) \right],
\]

\[
B = 1 + \frac{m_1 \Lambda_{12}}{m_1 \Lambda_{12} + m_2 \Lambda_{21}} \left[ 1 + \frac{2}{m_1 \omega^2} (\Lambda_1 + \Lambda_{21}) \right] + \frac{m_2 \Lambda_{21}}{m_1 \Lambda_{12} + m_2 \Lambda_{21}} \left[ 1 + \frac{2}{m_2 \omega^2} (\Lambda_2 + \Lambda_{12}) \right],
\]

\[
C = \sqrt{m_1 m_2 \Lambda_{21} \Lambda_{12}} \left[ \left( 1 + \frac{2}{m_1 \omega^2} (\Lambda_1 + \Lambda_{21}) \right) - \left( 1 + \frac{2}{m_2 \omega^2} (\Lambda_2 + \Lambda_{12}) \right) \right]. \tag{36}
\]

At the infinite-particle limit, the overlap depends on the interaction parameters only and, as expected, is always smaller than 1 in presence of either intra-species or inter-species interactions. At this limit, the overlap boils down to a product of two single-species overlaps (at the infinite-particle limit) provided there is no inter-species interaction and then only when the interaction–mass balance condition \(14\) holds and the mean-field frequencies are equal. This separability relation between the overlap in the mixture and the overlaps within each of its species, in the infinite-particle limit, reads \(S_{12}(\Lambda_1, \frac{m_2}{m_1} \Lambda_1, 0, 0) = S_1(\Lambda_1) S_2(\frac{m_2}{m_1} \Lambda_1)\), with obvious notation for the quantities. This concludes our study.
4. Summary
We have considered in the present work a generic trapped mixture of Bose-Einstein condensates whose ground-state wavefunction can be prescribed analytically at the exact and mean-field levels. This situation greatly facilitates a transparent and comparative study of properties of the mixture at both levels of theory. We have derived in this work general expressions for any number of particle in the mixture, and have concentrated on the infinite-particle limit in which both wavefunctions admit the same energy per particle and 100% condensation of each of the species.

We have computed and investigated the center-of-mass position and momentum variances, their uncertainty product, and the angular-momentum variance of each of the species in the mixture as well as of the whole mixture. Particular attention has been paid at identifying how differences between the exact and mean-field wavefunctions lead to explicit deviations between the respective quantities. The renormalization of the center-of-mass frequency and that of the relative coordinate between the center-of-mass of each species, as well as the (artificial) coupling between these two Jacobi coordinates and the (artificial) decoupling between the center-of-mass of each species, all in the Gross-Pitaevskii wavefunction, lead to discrepancies between the exact and mean-field properties. At the bottom line, the two different wavefunctions must have a lower than 1 overlap, which has been computed explicitly and analytically as well. The results obtained in this study can be considered as a step forward in characterizing how important are many-body effects in a generic trapped 100%-condensed bosonic mixture.

As a brief outlook, it would be interesting to study more involved uncertainty relations [67, 68] in a generic mixture, to extend the investigations on the relation of the exact and mean-field solutions to excited states, when possible, and to explore the further opportunities hiding in trapped multi-species mixtures.

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Appendix A. Transformation between the quadratic terms in Cartesian coordinates (laboratory frame) and Jacobi coordinates
The position terms are related by

\[
\sum_{i=1}^{N_1} x_i^2 = \sum_{s=1}^{N_1-1} Q_s^2 + \left( \sqrt{\frac{N_2 m_2}{M}} Q_{N-1} + \sqrt{N_1 Q_N} \right)^2 = \\
= \sum_{s=1}^{N_1-1} Q_s^2 + \frac{N_2 m_2}{M^2} Q_{N-1}^2 + N_1 Q_N^2 + \frac{2\sqrt{N_1 N_2 m_2}}{M} Q_{N-1} Q_N,
\]

\[
\sum_{j=1}^{N_2} y_j^2 = \sum_{s=N_1}^{N-2} Q_s^2 + \left( -\frac{\sqrt{N_1 m_1}}{M} Q_{N-1} + \sqrt{N_2 Q_N} \right)^2 = \\
= \sum_{s=N_1}^{N-2} Q_s^2 + \frac{N_1 m_1}{M^2} Q_{N-1}^2 + N_2 Q_N^2 - \frac{2\sqrt{N_1 N_2 m_1}}{M} Q_{N-1} Q_N
\]  
(A.1)
and the momentum terms by

\[
\sum_{i=1}^{N_1} \frac{\partial^2}{\partial Q_i^2} = \sum_{s=1}^{N_1-1} \frac{\partial^2}{\partial Q_{s+1}^2} + \left( \sqrt{N_2} \frac{\partial}{\partial Q_{N-1}} + \frac{\sqrt{N_1} m_1}{M} \frac{\partial}{\partial Q_N} \right)^2 = \\
= \sum_{s=1}^{N_1-1} \frac{\partial^2}{\partial Q_s^2} + N_2 \frac{\partial^2}{\partial Q_{N-1}^2} + \frac{N_1 m_1^2}{M^2} \frac{\partial^2}{\partial Q_N^2} + 2 \sqrt{N_1 N_2 m_1} \frac{\partial}{\partial Q_{N-1}} \frac{\partial}{\partial Q_N},
\]

\[
\sum_{j=1}^{N_2} \frac{\partial^2}{\partial y_j^2} = \sum_{s=N_1}^{N-2} \frac{\partial^2}{\partial Q_s^2} + \left( - \sqrt{N_1} \frac{\partial}{\partial Q_{N-1}} + \frac{\sqrt{N_2} m_2}{M} \frac{\partial}{\partial Q_N} \right)^2 = \\
= \sum_{s=N_1}^{N-2} \frac{\partial^2}{\partial Q_s^2} + N_1 \frac{\partial^2}{\partial Q_{N-1}^2} + \frac{N_2 m_2^2}{M^2} \frac{\partial^2}{\partial Q_N^2} - 2 \sqrt{N_1 N_2 m_2} \frac{\partial}{\partial Q_{N-1}} \frac{\partial}{\partial Q_N}. \tag{A.2}
\]

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