Solvable model of a generic trapped mixture of interacting bosons: reduced density matrices and proof of Bose–Einstein condensation

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Received 7 March 2017, revised 6 June 2017
Accepted for publication 12 June 2017
Published 29 June 2017

Abstract

A mixture of two kinds of identical bosons, species 1 with $N_1$ bosons of mass $m_1$ and species 2 with $N_2$ bosons of mass $m_2$, held in a harmonic potential of frequency $\omega$ and interacting by harmonic intra-species and inter-species particle-particle interactions of strengths $\lambda_1$, $\lambda_2$, and $\lambda_{12}$ is discussed. This is an exactly-solvable model of a generic mixture of trapped interacting bosons which allows one to investigate and determine analytically properties of interest. To start, closed form expressions for the frequencies, ground-state energy, and wave-function of the mixture are obtained and briefly analyzed as a function of the masses, numbers of particles, and strengths and signs of interactions. To prove Bose–Einstein condensation of the mixture three steps are needed. First, we integrate the all-particle density matrix, employing a four-parameter matrix-recurrence relations, down to the lowest-order intra-species and inter-species reduced density matrices of the mixture. Second, the coupled Gross–Pitaevskii (mean-field) equations of the mixture are solved analytically. Third, we analyze the mixture’s reduced density matrices in the limit of an infinite number of particles of both species 1 and 2 (when the interaction parameters, i.e. the products of the number of particles times the intra-species and inter-species interaction strengths, are held fixed) and prove that: (i) both species 1 and 2 are 100% condensed; (ii) the inter-species reduced density matrix per particle is separable and given by the product of the intra-species reduced density matrices per particle; and (iii) the mixture’s energy per particle, and reduced density matrices and densities per particle all coincide with the Gross–Pitaevskii quantities. Finally, when the infinite-particle limit is taken with respect to, say, species 1 only (with interaction parameters held fixed) we prove that: (iv) only species 1 is 100% condensed and its reduced density matrix and density per particle, as well as the
mixture’s energy per particle, coincide with the Gross–Pitaevskii quantities of species 1 alone; and (v) the inter-species reduced density matrix per particle is nonetheless separable and given by the product of the intra-species reduced density matrices per particle. The results are compared and discussed with respect to the recent work by Bouvrie et al (2014 Eur. Phys. J. D 68 346) who found for attractive mixtures vanishing bipartite entanglement between the two species and between a single particle (of either kind) and the remaining particles in the mixture. Implications are briefly discussed.

Keywords: Bose–Einstein condensation, solvable model, reduced density matrices, Bosonic mixtures

1. Introduction

Mixtures of Bose–Einstein condensates made of ultra-cold quantum gases and their physical properties have attracted much attention in the past twenty years, see for example [1–26]. The ground state of trapped mixtures has been studied both at the mean-field level (within Gross–Pitaevskii theory) and by different many-body theoretical and numerical tools.

For Bose–Einstein condensates made of a single species, there have been rigorous results connecting in the infinite-particle limit the many-body and mean-field expressions for the energy per particle and density per particle [27], and providing proof of 100% Bose–Einstein condensation [28] in the ground state. The underlying physics behind this proof is as follows. Consider a trapped many-boson system interacting by a two-body interaction, whose scattering length (or, for a large number of particles, strength) inversely depends on the number of particles in the system. The proof of 100% Bose–Einstein condensation stems from the ability to show that the reduced one-particle density matrix per particle of the trapped many-boson system factorizes in the limit of an infinite number of particles, when the interaction parameter (the product of the number of particles times the scattering length of the two-particle interaction) is held fixed, to a simple product. The emerging natural orbital coincides with the orbital solving the corresponding Gross–Pitaevskii equation, i.e. with the non-linear term being (proportional to) the many-boson fixed interaction parameter. Unlike their older (single-species) sibling, there are to the best of our knowledge no such results for trapped mixtures.

To address this topic, we present an exactly-solvable model of a generic mixture of trapped interacting bosons which allows one, for a start, to compute analytically the energy and wavefunction of the mixture for any number of particles. From there, and with some effort as we shall see below, intra-species and inter-species reduced density matrices are computed and analyzed. This allows us to get concrete results in the infinite-particle limit (when the products of the number of particles times the scattering length of the two-particle interaction strengths are held fixed) on the energy per particle, intra-species and inter-species reduced density matrices per particle, and to prove Bose–Einstein condensate of each of the species. By solving analytically for the ground state at the mean-field level (within Gross–Pitaevskii theory), we are also able to compare in the infinite-particle limit the many-body and mean-field results. For a mixture there is a nice twist on the infinite-particle limit, which may be taken with respect to both species or with respect to one of them. The conclusions from both infinite-particle-limit procedures are compared and contrasted.

The model we present for the mixture is that of two species of indistinguishable bosons, species 1 with $N_1$ bosons of mass $m_1$ and species 2 with $N_2$ bosons of mass $m_2$, held in a harmonic potential of frequency $\omega$ and interacting by harmonic intra-species and inter-species
particle-particle interactions of strengths $\lambda_1$, $\lambda_2$, and $\lambda_{12}$, respectively. This is the harmonic-interaction model for trapped bosonic mixtures. The harmonic-interaction model for identical particles has been widely used for single-species bosons [29–36], fermions [34–39], and un-trapped (i.e. translationally-invariant) bosonic mixtures [40–42]. In [43], a model for topologically disjoint systems has been proposed which in a particular limit boils down to the Hamiltonian we present below.

The model we discuss below has recently been studied by Bouvrie et al [44]. Therein, the bipartite entanglement in the ground state between the two species in the mixture and between a single particle (of either kind) and the remaining particles was computed analytically for attractive mixtures as a function of the number of particles. In particular, the authors found that for $N_1 \gg N_2$ the entanglement between particles of different species vanishes and for $N_1 \to \infty$ and (or) $N_2 \to \infty$ the single-particle entanglement vanishes.

In our work we would like to bring the bosonic character of the ground state of the model up front, and exploit it. In the spirit of the proof of Bose–Einstein condensation for single-species systems, we keep the interaction parameters (i.e. the interaction strengths multiplied by the number of particles), rather than the interaction strengths, fixed in the infinite-particle limit. This will not only allow us to prove 100% Bose–Einstein condensation in the ground state, but to treat both attractive and repulsive mixtures.

The original theorem and proof [28] for single-species bosons employ more realistic inter-atomic interactions than harmonic, and require them to have a finite scattering length. Although the harmonic inter-particle interaction does not fall into this category, comparing the many-body and Gross–Pitaevskii analytical solutions of the single-species harmonic-interaction model [29], also see [45], proves that the latter is 100% condensed. In the present work we prove for the harmonic-interaction model for mixtures that it is 100% condensed and strongly believe, correspondingly and inversely, that this would hold true for the ground state of trapped mixtures with more realistic inter-particle interactions.

Most recently, we were able to solve a specific case of the harmonic-interaction model for trapped mixtures, a trapped symmetric mixture for which $N_1 = N_2$, $m_1 = m_2$, and $\lambda_1 = \lambda_2$, and showed that the energy per particle and densities per particle (i.e. the diagonal of reduced density matrices per particle) converge in the infinite-particle limit to their mean-field analogs [46]. To treat the general mixture with unequal numbers of particles, masses, and interaction strengths, and especially to derive its reduced density matrices and prove Bose–Einstein condensation, it is needed to generalize the analytical techniques developed by Cohen and Lee [29] for single-species bosons and extended in [46] for the symmetric mixture substantially further, which is done below.

The structure of the paper is as follows. In section 2 we present the harmonic-interaction model for a generic trapped mixture of bosons and discuss its ground-state energy and wavefunction. In section 3 we construct explicitly the lowest-order intra-species and inter-species reduced density matrices of the mixture, solve analytically the two-coupled Gross–Pitaevskii equations, perform the infinite-particle limit in which the many-body and mean-field results are compared, and prove Bose–Einstein condensation. Concluding remarks are provided in section 4. Further details of the derivations are collected in the appendices.

2. The harmonic-interaction model for trapped Bosonic mixtures

Consider a mixture of two distinguishable types of identical bosons which we label 1 and 2. The bosons are trapped in a three-dimensional isotropic harmonic potential of frequency $\omega$ and interact via harmonic particle-particle interactions. In the present work we only deal with
the ground state of the trapped mixture. We treat the case of a generic mixture. Namely, a mixture consisting of \( N_1 \) bosons of type 1 and mass \( m_1 \) and \( N_2 \) bosons of type 2 and mass \( m_2 \). The total number of particles is denoted by \( N = N_1 + N_2 \). Furthermore, the two intra-species interaction strengths are denoted by \( \lambda_1 \) and \( \lambda_2 \), and the inter-species interaction strength by \( \lambda_{12} \). Positive values of \( \lambda_1 \), \( \lambda_2 \), and \( \lambda_{12} \) mean attractive particle-particle interactions whereas negative values imply repulsive interactions\(^1\).

The Hamiltonian of the mixture is then given by (\( \hbar = 1 \))

\[
\hat{H}(x_1, \ldots, x_N, y_1, \ldots, y_N) = \sum_{j=1}^{N_1} \left( -\frac{1}{2m_1} \frac{\partial^2}{\partial x_j^2} + \frac{1}{2} m_1 \omega^2 x_j^2 \right) + \sum_{j=1}^{N_2} \left( -\frac{1}{2m_2} \frac{\partial^2}{\partial y_j^2} + \frac{1}{2} m_2 \omega^2 y_j^2 \right) + \lambda_1 \sum_{1 \leq j < k \leq N} (x_j - x_k)^2 + \lambda_2 \sum_{1 \leq j < k \leq N} (y_j - y_k)^2 + \lambda_{12} \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} (x_j - y_k)^2.
\]

(1)

Here, the coordinates \( x_j \) denote bosons of type 1 and \( y_k \) bosons of type 2. We work in Cartesian coordinates where the vector \( x = (x_1, x_2, x_3) \) denotes the position of a boson of type 1 in three dimensions, and \( \frac{1}{i} \frac{\partial}{\partial x} = \frac{1}{i} \left( \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3} \right) \) its momentum. To avoid cumbersome notation, we denote \( x^2 \equiv x_1^2 + x_2^2 + x_3^2 \) and \( \frac{\partial^2 x}{\partial x^2} \equiv \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \). Analogous notation is employed for the vector \( y \) of a boson of type 2.

To diagonalize the Hamiltonian (1) we transform to the Jacoby coordinates \([42]\)

\[
Q_k = \frac{1}{\sqrt{k(k+1)}} \sum_{j=1}^{k} (x_{k+1} - x_j), \quad 1 \leq k \leq N_1 - 1,
\]

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

\[
Q_{N-1} = \sqrt{N_2 \over N_1} \sum_{j=1}^{N_1} x_j - \sqrt{N_1 \over N_2} \sum_{j=1}^{N_2} y_j,
\]

\[
Q_N = \frac{m_1}{M} \sum_{j=1}^{N_1} x_j + \frac{m_2}{M} \sum_{j=1}^{N_2} y_j.
\]

(2)

The meaning of (2) is as follows: The first group of \( N_1 - 1 \) coordinates are relative coordinates of the bosons of species 1; the second group of \( N_2 - 1 \) coordinates are relative coordinates of the bosons of species 2; \( Q_{N-1} \) can be seen as a relative coordinate between the center-of-mass of the species 1 and the center-of-mass of the species 2 bosons; and, finally, \( Q_N \) is the center-of-mass coordinate of all particles in the mixture.

Using (2) and (A.2)–(A.4) in appendix A, the Hamiltonian (1) transforms to the diagonal form

\(^1\)There are eight different combinations for which the particle-particle interactions \( \lambda_1, \lambda_2, \) and \( \lambda_{12} \) are either positive (corresponds to attraction) or negative (corresponds to repulsion). Note that the trap potential enables four more combinations compared to the mixture in free space [42], since it allows for repulsion between the two species while the system is still bound.
\[ \hat{H}(Q_1, \ldots, Q_N) = \sum_{k=1}^{N-1} \left( -\frac{1}{2m_1} \frac{\partial^2}{\partial Q_k^2} \right) + \frac{1}{2} m_1 \Omega_1^2 Q_k^2 + \sum_{k=N_1}^{N-2} \left( -\frac{1}{2m_2} \frac{\partial^2}{\partial Q_k^2} \right) + \frac{1}{2} m_2 \Omega_2^2 Q_k^2 + \left( -\frac{1}{2M} \frac{\partial^2}{\partial Q_{N-1}^2} \right) + \frac{1}{2} M \Omega_{N-1}^2 Q_{N-1}^2 + \left( -\frac{1}{2M} \frac{\partial^2}{\partial Q_{N}^2} \right) + \frac{1}{2} M \omega^2 Q_N^2, \right] \]

The transformed Hamiltonian of the mixture (3) is that of \( N \) uncoupled harmonic oscillators having the four masses \( m_1, m_2, M_{12} \) (relative mass of the mixture), and \( M \) (total mass of the mixture), and \( m \), frequencies hold independently of the numbers of bosons

\[ \Omega_1 = \sqrt{\omega^2 + \frac{2}{m_1} (N_1 \lambda_1 + N_2 \lambda_{12})}, \quad \Omega_2 = \sqrt{\omega^2 + \frac{2}{m_2} (N_2 \lambda_2 + N_1 \lambda_{12})}, \]
\[ \Omega_{12} = \sqrt{\omega^2 + 2 \left( \frac{N_1}{m_1} \lambda_1 + \frac{N_2}{m_2} \lambda_{12} \right)}, \quad \omega = \frac{\sqrt{\omega^2 + \frac{2 \lambda_{12}}{M_{12}}}}{M_{12}}. \]

The multiplicity of the frequencies is \( N_1 - 1, N_2 - 1, 1, \) and 1, respectively, corresponding to the types and numbers of Jacobi coordinates.

In some specific cases frequencies can become degenerate and their multiplicity changes. For instance, when the masses and interactions are inter-connected by the relations

\[ m_1 \lambda_1 = m_2 \lambda_2, \]
\[ m_1 \lambda_{12} = m_2 \lambda_{12}, \]
\[ \lambda_1 = \sqrt{\lambda_1 \lambda_2}, \lambda_{12} = \sqrt{\lambda_1 \lambda_2}, \]
\[ \lambda_1 > -\frac{M_{12} \omega^2}{2}, \]
\[ \lambda_2 > -\frac{m_1 \omega^2}{2 N_1}, \]
\[ \lambda_2 > -\frac{m_2 \omega^2}{2 N_2}. \]

one finds that \( \Omega_1 = \Omega_2 = \Omega_{12} \), i.e. all relative coordinates have the same frequency. This degeneracy of the frequencies holds independently of the numbers of bosons \( N_1 \) and \( N_2 \). The ground-state energy reads

\[ E = \frac{1}{2} \left( N - 1 \right) \sqrt{\omega^2 + \frac{2 \lambda_{12}}{M_{12}} + \omega} \]

expressed as a function of the inter-species interaction only. Another example is when the numbers of particles and interactions are inter-connected by the relations

\[ N_1 \lambda_1 + N_2 \lambda_{12} = 0, N_2 \lambda_2 + N_1 \lambda_{12} = 0 \]

one gets that \( \Omega_1 = \Omega_2 = \omega \), i.e. the intra-species relative coordinates have the same frequency as the center-of-mass coordinate. This degeneracy of the frequencies holds independently of the masses of the bosons \( m_1 \) and \( m_2 \). The energy now reads

\[ E = \frac{1}{2} \left( N - 1 \right) \omega + \sqrt{\omega^2 + \frac{2 \lambda_{12}}{m_1}} \]

again expressed as a function of the inter-species interaction only.
The meaning of these bounds are as follows: The inter-species interaction \( \lambda_{12} \) is bounded from below by the frequency of the trap and the relative mass, irrespective of the intra-species interactions \( \lambda_1 \) and \( \lambda_2 \), otherwise the mixture cannot be trapped in the harmonic potential. On the other hand, the intra-species interaction \( \lambda_1 \) is limited by the chosen inter-species interaction \( \lambda_{12} \), the numbers of particles, and the mass \( m_1 \), and analogously \( \lambda_2 \).

We can now proceed and prescribe the normalized ground-state wave-function

\[
\Psi(Q_1, \ldots, Q_N) = \left( \frac{m_1 \Omega_1}{\pi} \right)^{\frac{N_1}{2}} \left( \frac{m_2 \Omega_2}{\pi} \right)^{\frac{N_2}{2}} \left( \frac{M \omega}{\pi} \right)^{\frac{N}{2}} \times \left( \frac{M \omega}{\pi} \right)^{\frac{N}{2}} 
\]

\[
x^{-\frac{1}{2}} \left( m_1 \Omega_1 \sum_{i=1}^{N_1} Q_i^2 + \frac{m_1 \omega}{M} \sum_{i=1}^{N_1} Q_i + M_1 \Omega_1 \right) ,
\]

along with the ground-state energy

\[
E = \frac{3}{2} \left( (N_1 - 1) \Omega_1 + (N_2 - 1) \Omega_2 + \Omega_{12} + \omega \right)
\]

\[
= \frac{3}{2} \left( N_1 \Omega_1 + N_2 \Omega_2 + \frac{2 \lambda_{12}}{M} + \omega \right)
\]

of the trapped mixture\(^3\). Using the bounds for \( \lambda_1, \lambda_2, \) and \( \lambda_{12} \) in (5), we obtain that the ground-state energy of the mixture is bound from below by \( E > \frac{3}{2} \omega \), which is obtained for \( \Omega_1 \rightarrow 0^+, \Omega_2 \rightarrow 0^+, \) and \( \Omega_{12} \rightarrow 0^+ \). This means that all relative degrees of freedom are marginally bound, and essentially only the center-of-mass degree of freedom is bound in the harmonic trap. The system is then predominantly repulsive. At the other end, when the mixture is predominantly attractive, the energy is unbound from above.

To express the wave-function with respect to the original spatial coordinates we use relations (A.5) and find

\[
\Psi(x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2}) = \left( \frac{m_1 \Omega_1}{\pi} \right)^{\frac{N_1}{2}} \left( \frac{m_2 \Omega_2}{\pi} \right)^{\frac{N_2}{2}} \left( \frac{M \omega}{\pi} \right)^{\frac{N}{2}} \times \left( \frac{M \omega}{\pi} \right)^{\frac{N}{2}} 
\]

\[
x^{-\frac{1}{2}} \sum_{i=1}^{N_1} x_i \sum_{i=1}^{N_1} x_i \times e^{-\frac{1}{4} \lambda_2 \sum_{i=1}^{N_2} y_i^2} \times e^{-\frac{1}{4} \lambda_1 \sum_{i=1}^{N_1} x_i^2} \times e^{-\frac{1}{4} \lambda_{12} \sum_{i=1}^{N_1} x_i y_i} ,
\]

where the parameters are

\[
\alpha_1 = m_1 \left[ \Omega_1 \left( 1 - \frac{1}{N_1} \right) + \frac{m_2 N_2 \Omega_{12} + M N_1 \omega}{M N_1} \right] = m_1 \Omega_1 + \beta_1 ,
\]

\[
\beta_1 = m_1 \left[ \Omega_1 \left( 1 - \frac{1}{N_1} \right) + \frac{m_2 N_2 \Omega_{12} + M N_1 \omega}{M N_1} \right] ,
\]

\[
\alpha_2 = m_2 \left[ \Omega_2 \left( 1 - \frac{1}{N_2} \right) + \frac{m_1 N_1 \Omega_{12} + M N_2 \omega}{M N_2} \right] = m_2 \Omega_2 + \beta_2 ,
\]

\[
\beta_2 = m_2 \left[ \Omega_2 \left( 1 - \frac{1}{N_2} \right) + \frac{m_1 N_1 \Omega_{12} + M N_2 \omega}{M N_2} \right] ,
\]

\[
\gamma = \frac{m_1 m_2}{M} \left( \Omega_{12} - \omega \right) = M_1 (\Omega_{12} - \omega) .
\]

\(^3\) In the limit of vanishing trapping frequency, \( \omega \rightarrow 0 \), the relative-motion part of \( \Psi \), which is built from all relative Jacobi coordinates of the mixture \( Q_1, \ldots, Q_{N-1} \) and the energy \( E \) boil down to those of the mixture in free space [42].
The ground-state wave-function of the mixture (8) is seen to be comprised of a product of a type 1 boson part, a type 2 boson part, and a coupling 1–2 part. As required by indistinguishability of identical bosons, \( \Psi \) is symmetric to permutation of the coordinates \( x_j \) and \( x_k \) of any two type 1 bosons, and likewise symmetric to permutation of the coordinates \( y_j \) and \( y_k \) of any two type 2 bosons, but is not symmetric to permutation of the distinguishable 1 and 2 type bosons.

The harmonic-interaction model for a generic trapped mixture of interacting bosons presented above admits a wealth of properties that can all be studied in principle analytically. After all, the ground-state wave-function and energy are given as explicit simple functions of all parameters—masses \( m_1 \) and \( m_2 \), numbers of particles \( N_1 \) and \( N_2 \), interactions strengths \( \lambda_1 \), \( \lambda_2 \) and \( \lambda_{12} \), and trapping frequency \( \omega \). All quantum properties of the mixture can be computed from its wave-function, although, as we shall see in the next section, not necessarily without some effort.

3. Reduced density matrices and proof of Bose–Einstein condensation

To show that the individual species are Bose–Einstein condensed three steps are required. The first, the computation of the intra-species reduced one-particle density matrices. To discuss the complementary question of separability requires the inter-species reduced two-body density matrix. These are calculated analytically in section 3.1 as a function of the masses, interaction strengths, and numbers of particles. The second step is to solve, again analytically, the system at the mean-field level. This means finding the solution to the two-species coupled Gross–Pitaevskii equations. This is performed in section 3.2. The third and final step is to perform the infinite-particle limit and to compare and contrast the exact and mean-field solutions in this limit, which is carried out in section 3.3. In a mixture one can perform the infinite-particle limit with respect to the two species or with respect to one of the species. We will discuss and compare both infinite-particle-limit procedures below.

3.1. The intra-species and inter-species reduced density matrices

We start from the full \( N \)-particle density matrix of the mixture,

\[
\Psi(x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2})\Psi^*(x'_1, \ldots, x'_{N_1}, y'_1, \ldots, y'_{N_2}) = \left( \frac{m_1 \Omega_1}{\pi} \right)^{\frac{N_1(N_1-1)}{2}} \left( \frac{m_2 \Omega_2}{\pi} \right)^{\frac{N_2(N_2-1)}{2}} \left( \frac{M_{12} \Omega_{12}}{\pi} \right)^\frac{N_1 N_2}{2} \int \frac{d\omega}{\pi} \int d\gamma \ e^{\frac{i}{\hbar} \sum_{j=1}^{N_1} (x_j^2 + x'^2_j) - \frac{\hbar}{\pi} \sum_{k=1}^{N_2} (y_k^2 + y'^2_k) - \frac{\hbar}{\pi} \sum_{k=1}^{N_2} (y_k y_k')}
\]

which for convenience is here normalized to one, \( \int dx_1 \cdots dx_{N_1} dy_1 \cdots dy_{N_2} |\Psi|^2 = 1 \). The intra-species reduced one-body density matrices of the mixture,

\[
\rho_1(x, x') = N_1 \int dx_2 \cdots dx_{N_1} dy_1 \cdots dy_{N_2} \Psi(x, x_2, \ldots, x_{N_1}, y_1, y_2, \ldots, y_{N_2}) \Psi^*(x', x_2, \ldots, x_{N_1}, y_1, y_2, \ldots, y_{N_2}),
\]

\[
\rho_2(y, y') = N_2 \int dx_1 \cdots dx_{N_1} dy_2 \cdots dy_{N_2} \Psi(x_1, x_2, \ldots, x_{N_1}, y, y_2, \ldots, y_{N_2}) \Psi^*(x_1, x_2, \ldots, x_{N_1}, y', y_2, \ldots, y_{N_2}),
\]

(11)
are given by integrating over $N-1$ coordinates, and the inter-species reduced two-body density matrix

$$\rho_{12}(x, x', y, y') = N_1 N_2 \int dx_2 \cdots dx_N \, dy_2 \cdots dy_N \Psi(x, x_2, \ldots, x_N, y, y_2, \ldots, y_N) \times \Psi^+(x', x_2, \ldots, x_N, y', y_2, \ldots, y_N),$$

which is the lowest-order inter-species reduced density matrix of the mixture, is obtained by integrating over $N-2$ coordinates.

To obtain the lowest-order reduced density matrices (11) and (12) we need to perform multiple integrations of the $N$-particle density matrix of the mixture (10). Moreover, the latter contains a coupling 1–2 part because of the inter-species interaction. Thus, without an appropriate construction, the task becomes quickly impractical with increasing $N_1$ and $N_2$. Below, to perform the integration, we derive a four-parameter matrix-recurrence relations, thus generalizing the one-parameter and two-parameter vector-recurrence relations put forward, respectively, in the cases of the single-species [29] and symmetric-mixture [46] harmonic-interaction models.

To integrate the $N$-particle density matrix we begin by introducing the auxiliary function

$$F_{N_1,N_2}(x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2}, x'_1, \ldots, x'_{N_1}, y'_1, \ldots, y'_{N_2};$$

$$\alpha_1, \beta_1, \alpha_2, \beta_2, C_{N_1,N_2}, C'_{N_1,N_2}, D_{N_1,N_2}, D'_{N_1,N_2})$$

$$= e^{-\alpha_2 \sum_{j=1}^{N_1} (x_j^2 + x'_j^2) - \beta_1 \sum_{i,j \leq l < k} (x_i - x_j + x'_i - x'_j)^2} e^{-\alpha_2 \sum_{j=1}^{N_1} (y_j^2 + y'_j^2) - \beta_2 \sum_{j \leq l < k} (y_j - y'_j + y'_j y'_j)^2}$$

$$\times e^{-\frac{1}{2} C_{N_1,N_2} (x_N + x'_N)^2} e^{-\frac{1}{2} C'_{N_1,N_2} (y_N + y'_N)^2}$$

$$\times e^{\frac{1}{2} D_{N_1,N_2} (x_N - x'_N) (y_N - y'_N)} e^{\frac{1}{2} D'_{N_1,N_2} (x_N - x'_N) (y_N - y'_N)},$$

(13)

where $\alpha_1, \beta_1, \alpha_2$, and $\beta_2$, are given in (9),

$$X_{N_1} = \sum_{j=1}^{N_1} x_j, \quad X'_{N_1} = \sum_{j=1}^{N_1} x'_j, \quad Y_{N_2} = \sum_{j=1}^{N_2} y_j, \quad Y'_{N_2} = \sum_{j=1}^{N_2} y'_j,$$

(14)

are vectors, and $C_{N_1,N_2}, C'_{N_1,N_2}, D_{N_1,N_2},$ and $D'_{N_1,N_2}$ are constants to play a further role below.

We note that if one were to equate the $N$-particle density (10) and the auxiliary function $F_{N_1,N_2}$ then this would imply that

$$C_{N_1,N_2} = 0, \quad C'_{N_1,N_2} = 0, \quad D_{N_1,N_2} = \gamma, \quad D'_{N_1,N_2} = \gamma.$$

(15)

We will perform the integration of the auxiliary function $F_{N_1,N_2}$ in two steps, first by integrating the $y_{N_1}, y'_{N_1} = y_N$ variables and then the $x_{N_1}, x'_{N_1} = x_N$ variables. We shall call the first step the horizontal reduction of the auxiliary function $F_{N_1,N_2}$ and the second step the vertical reduction.

The relations

$$\begin{align*}
(X_{N_1} + X'_{N_1})^2 &= (X_{N_1-1} + X'_{N_1-1})^2 + 2(X_{N_1-1} + X'_{N_1-1})(X_{N_1} + X'_{N_1}) + (X_{N_1} + X'_{N_1})^2, \\
(Y_{N_1} + Y'_{N_1})^2 &= (Y_{N_1-1} + Y'_{N_1-1})^2 + 2(Y_{N_1-1} + Y'_{N_1-1})(Y_{N_1} + Y'_{N_1}) + (Y_{N_1} + Y'_{N_1})^2, \\
\langle X_{N_1} \pm X'_{N_1} \rangle \langle Y_{N_1} \pm Y'_{N_1} \rangle &= \langle X_{N_1-1} \pm X'_{N_1-1} \rangle \langle Y_{N_1} \pm Y'_{N_1} \rangle + \langle X_{N_1} \pm X'_{N_1} \rangle \langle Y_{N_1} \pm Y'_{N_1} \rangle \\
&= \langle X_{N_1} \pm X'_{N_1} \rangle \langle Y_{N_1-1} \pm Y'_{N_1-1} \rangle + \langle X_{N_1} \pm X'_{N_1} \rangle \langle Y_{N_1} \pm Y'_{N_1} \rangle
\end{align*}$$

between the vectors introduced in (14) and the variables of the degrees of freedom to be integrated $x_{N_1}, x'_{N_1}, y_N$, and $y'_{N_1}$ hold.
reduction. The sequences of integrations to be performed below may be written symbolically as

\[
\begin{align*}
F_{N_1,N_2} & \quad \Rightarrow \quad F_{N_1,1} \quad \Rightarrow \quad F_{N_1,0} \\
F_{1,N_2} & \quad \Rightarrow \quad F_{1,1} \quad \Rightarrow \quad F_{1,0} \\
F_{0,N_2} & \quad \Rightarrow \quad F_{0,1}
\end{align*}
\]

(16)

The end terms of these integrations, \(F_{1,1}\) and \(F_{1,0}, F_{0,1}\), will be connected with the reduced density matrices (12) and (11), respectively.

Thus, to perform the multiple integration steps in the horizontal reduction (16), we seek for a recurrence relation and write

\[
\int \mathcal{D} y_N F_{N_1,N_2}
\]

\[
\begin{align*}
&= e^{-\frac{\alpha_1}{2} \sum_{i=1}^{N_1} (x_i^2 + x_i'^2) - \beta_1 \sum_{i < j} (x_i x_j + x_i' x_j')} e^{-\frac{\alpha_2}{2} \sum_{i=1}^{N_2} (y_i^2 + y_i'^2) - \beta_2 \sum_{i < j} (y_i y_j + y_i' y_j')} \\
&\times e^{-\frac{1}{2} C_{N_1,N_2}(x_{N_1} + x_{N_1}')^2} e^{-\frac{1}{2} C_{N_1,N_2}(y_{N_2} + y_{N_2}')^2} \\
&\times e^{\frac{1}{2} D_{N_2,N_1}(x_{N_1} + x_{N_1}') (y_{N_2} + y_{N_2}') - \frac{1}{2} D_{N_2,N_1} (x_{N_1} - x_{N_1}') (y_{N_2} - y_{N_2}')} \\
&\times \int \mathcal{D} y_N e^{-((\alpha_1 + C_{N_1,N_2}) y_{N_2})^2 - (\beta_2 + C_{N_1,N_2}) (y_{N_2} - y_{N_2}')^2 - D_{N_2,N_1} (x_{N_1} + x_{N_1}')} y_N \\
&= \left(\frac{\pi}{\alpha_2 + C_{N_1,N_2}}\right)^{\frac{N_2}{2}} F_{N_1,N_2-1} (x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2-1}; x_1', \ldots, x_{N_1}', y_1', \ldots, y_{N_2-1}'; \\
&\quad \alpha_1, \beta_1, \alpha_2, \beta_2, C_{N_1,N_2-1}, C_{N_1,N_2-1}', D_{N_2,N_1-1}, D_{N_2,N_1-1}')
\end{align*}
\]

(17)

where the Gaussian integral \(\int \mathcal{D} y_N e^{-\frac{1}{2} x^2} = (\frac{\pi}{2})^{\frac{N}{2}} e^{\frac{\alpha}{2}}\) is used and \(\int \mathcal{D} y_N F_{N_1,N_2} \ldots\) implicitly implies that \(y_{N_2} = y_{N_2}'\) is used in the integrand. The equality (17) relates the auxiliary function \(F_{N_1,N_2}\) with \(N_1 + N_2\) coordinates and constants \(C_{N_1,N_2}, C_{N_1,N_2}', D_{N_1,N_2}, D_{N_1,N_2}'\), to the auxiliary function \(F_{N_1,N_2-1}\) of the same functional form, with \(N_1 + (N_2 - 1)\) coordinates and corresponding constants \(C_{N_1,N_2-1}, C_{N_1,N_2-1}', D_{N_1,N_2-1}, D_{N_1,N_2-1}'\) which depend on all constants appearing in \(F_{N_1,N_2}\); and read

\[
\begin{align*}
C_{N_1,N_2-1} &= C_{N_1,N_2} - \frac{D_{N_1,N_2}}{\alpha_2 + C_{N_1,N_2}}, \\
C_{N_1,N_2-1}' &= C_{N_1,N_2}' - \frac{(\beta_2 + C_{N_1,N_2})^2}{\alpha_2 + C_{N_1,N_2}'}, \\
D_{N_1,N_2-1} &= D_{N_1,N_2} - \frac{\beta_2 + C_{N_1,N_2} D_{N_1,N_2}}{\alpha_2 + C_{N_1,N_2}}, \\
D_{N_1,N_2-1}' &= D_{N_1,N_2}'.
\end{align*}
\]

(18)

Recall that the initial values of \(C_{N_1,N_2}, C_{N_1,N_2}', D_{N_1,N_2}, D_{N_1,N_2}'\) are given by (15) and obtained when we equate the auxiliary function \(F_{N_1,N_2}\) and the \(N\)-body density (10).

According to (16), the horizontal reduction makes a ‘stopover’ at the auxiliary function
$F_{N,1}(x_1, \ldots, x_N, y_1; x'_1, \ldots, x'_N, y'_1; \alpha_1, \beta_1, \alpha_2, \beta_2, C_{N,1}, C'_{N,1}, D_{N,1}, D'_{N,1})$

$= e^{-\frac{\alpha_1}{2} \sum_{i=1}^{N-1} (x_i^2 + x'_i) - \beta_1 \sum_{i<j} (x_i x_j + x'_i x'_j)} e^{-\frac{\beta_1}{2} (y_i^2 + y'_i)}$

$\times e^{-\frac{\alpha_2}{2} \sum_{i=1}^{N-1} (x_i + x'_i)} e^{-\frac{\alpha_2}{2} (y_i + y'_i)} e^\frac{1}{2} D_{N,1}(x_N + x'_N)(y_N + y'_N) e^\frac{1}{2} D'_{N,1}(x_N - x'_N)(y_N - y'_N)$.

(19)

Its respective constants, $C_{N,1}$, $C'_{N,1}$, $D_{N,1}$, and $D'_{N,1}$, are required as initial conditions for the vertical reduction in route to evaluate the inter-species reduced density matrix of the mixture (12). Note that the dependence of $F_{N,1}$ on $\beta_2$ is now implicit, representing the situation that all but the last boson of type 2 are integrated out. The final result for the constants is

$C_{N,1} = -\gamma^2 \frac{N_2 - 1}{(\alpha_2 - \beta_2) + (N_2 - 1)\beta_2}$,  

$C'_{N,1} = -\beta_2 \frac{N_2 - 1}{(\alpha_2 - \beta_2) + (N_2 - 1)\beta_2}$,  

$D_{N,1} = \gamma \frac{\alpha_2 - \beta_2}{(\alpha_2 - \beta_2) + (N_2 - 1)\beta_2}$,  

$D'_{N,1} = \gamma$.

(20)

where the initial conditions (15) have been used, see appendix B for further details.

We can now perform the vertical reduction of $F_{N,1}$ where (20) serve as the initial conditions for the constants to be computed. Thus we seek for a recurrence relation

$\int dx_N F_{N,1}$

$= e^{-\frac{\alpha_1}{2} \sum_{i=1}^{N-1} (x_i^2 + x'_i) - \beta_1 \sum_{i<j} (x_i x_j + x'_i x'_j)} e^{-\frac{\beta_1}{2} (y_i^2 + y'_i)}$

$\times e^{-\frac{\alpha_2}{2} \sum_{i=1}^{N-1} (x_i + x'_i)} e^{-\frac{\alpha_2}{2} (y_i + y'_i)} e^\frac{1}{2} D_{N,1}(x_N + x'_N)(y_N + y'_N) e^\frac{1}{2} D'_{N,1}(x_N - x'_N)(y_N - y'_N) x_N$

$= \left(\frac{\pi}{\alpha_1 + C_{N,1}}\right)^\frac{1}{2} F_{N-1,1}(x_1, \ldots, x_{N-1}, y_1; x'_1, \ldots, x'_{N-1}, y'_1; \alpha_1, \beta_1, \alpha_2, \beta_2, C_{N-1,1}, C'_{N-1,1}, D_{N-1,1}, D'_{N-1,1})$.

(21)

where

$C_{N-1,1} = C_{N,1} - \frac{(\beta_1 + C_{N,1})^2}{\alpha_1 + C_{N,1}}$,  

$C'_{N-1,1} = C'_{N,1} - \frac{D_{N,1}^2}{\alpha_1 + C_{N,1}}$,  

$D_{N-1,1} = D_{N,1} - \frac{\beta_1 + C_{N,1}}{\alpha_1 + C_{N,1}} D_{N,1}$,  

$D'_{N-1,1} = D'_{N,1}$.

(22)

The relations between the constants in the vertical reduction (22) are seen to be analogous to the relations between the constants in the horizontal reduction (18), see appendix B for further details.

Thus, combining and interchanging the order of both horizontal and vertical reductions, the integration of $F_{N,N_2}$ (16) ends with the auxiliary functions
\[ F_{1,1} = e^{-\frac{1}{2}(x_1^2 + x_1^2)} e^{-\frac{1}{2}(y_1^2 + y_1^2)} e^{-\frac{1}{2}C_{1,1}(x_1 + x_1)^2} e^{-\frac{1}{2}C_{1,1}(y_1 + y_1)^2} \times e^{\frac{1}{2}D_{1,1}(x_1 + x_1)^2(y_1 + y_1) + \frac{1}{4}D_{1,1}(x_1 - x_1)(y_1 - y_1)} . \]

\[ F_{1,0} = e^{-\frac{1}{2}(x_1^2 + x_1^2)} e^{-\frac{1}{2}C_{1,0}(x_1 + x_1)^2}, \]

\[ F_{0,1} = e^{-\frac{1}{2}(y_1 + y_1)^2} e^{-\frac{1}{2}C_{0,1}(y_1 + y_1)^2}. \]

(23)

Because \( F_{N,1} \) with the initial conditions (15) is proportional to the \( N \)-particle density matrix (10), \( F_{1,1} \) is proportional to the inter-species reduced density matrix (12), and similarly \( F_{1,0} \) and \( F_{0,1} \) to the intra-species ones (11). The final expressions for the constants in \( F_{1,1} \) are

\[ C_{1,1} = \frac{(\alpha_1 - \beta_1)C_{N,1} - (N_1 + 1)(C_{1,1} + \beta_1)\beta_1}{(\alpha_1 - \beta_1) + (N_1 + 1)(C_{1,1} + \beta_1)}, \]

\[ C'_{1,1} = \frac{(\alpha_2 - \beta_2)C'_{N,1} - (N_2 + 1)(C'_{1,1} + \beta_2)\beta_2}{(\alpha_2 - \beta_2) + (N_2 + 1)(C'_{1,1} + \beta_2)}, \]

\[ D_{1,1} = \gamma \frac{[(\alpha_1 - \beta_1) + (N_1 + 1)\beta_1][(\alpha_2 - \beta_2) + (N_2 + 1)\beta_2] - \gamma^2(N_1 - 1)(N_2 - 1)}{(\alpha_1 - \beta_1)(\alpha_2 - \beta_2)} \]

(24)

and for the constants in \( F_{1,0} \) and \( F_{0,1} \) are

\[ C_{1,0} = \frac{(\alpha_1 - \beta_1)C_{N,0} - (N_1 + 1)(C_{0,1} + \beta_1)\beta_1}{(\alpha_1 - \beta_1) + (N_1 + 1)(C_{0,1} + \beta_1)}, \]

\[ C'_{0,1} = \frac{(\alpha_2 - \beta_2)C'_{0,N} - (N_2 + 1)(C'_{0,1} + \beta_2)\beta_2}{(\alpha_2 - \beta_2) + (N_2 + 1)(C'_{0,1} + \beta_2)}. \]

(25)

The explicit dependence of the bottommost constants (24) and (25) on \( C_{N,1} \) in (20) and

\[ C_{N,0} = -\gamma^2 \frac{N_2}{(\alpha_2 - \beta_2) + N_2\beta_2}, \]

\[ C'_{0,N} = -\gamma^2 \frac{N_1}{(\alpha_1 - \beta_1) + N_1\beta_1} \]

(26)

is to remind us that both horizontal and vertical reductions have been combined to evaluate the former, see appendix B for further details. All in all, the inter-species (12) and intra-species (11) reduced density matrices read

\[ \rho_{12}(x, x', y, y') = N_1 N_2 \left[ (\alpha_1 + C_{1,1})(\alpha_2 + C'_{1,1} - D_{1,1}^2) \right]^{\frac{1}{2}} e^{-\frac{1}{2}(x_1^2 + x_1^2)} e^{-\frac{1}{2}(y_1^2 + y_1^2)} \times e^{-\frac{1}{2}C_{1,1}(x_1 + x_1)^2} e^{-\frac{1}{2}C'_{1,1}(y_1 + y_1)^2} e^{\frac{1}{2}D_{1,1}(x_1 - x_1)(y_1 - y_1)} \]

(27)

and

\[ \rho_1(x, x') = N_1 \left( \frac{\alpha_1 + C_{1,0}}{\pi} \right)^{\frac{1}{2}} e^{-\frac{1}{2}(x_1^2 + x_1^2)} e^{-\frac{1}{2}C_{1,0}(x_1 + x_1)^2}, \]

\[ \rho_2(y, y') = N_2 \left( \frac{\alpha_2 + C'_{0,1}}{\pi} \right)^{\frac{1}{2}} e^{-\frac{1}{2}(y_1^2 + y_1^2)} e^{-\frac{1}{2}C_{0,1}(y_1 + y_1)^2}. \]

(28)
For completeness, we paste below their diagonal parts, i.e. the two-body
\[
\rho_{12}(x, y) = N_1 N_2 \left[ \frac{(\alpha_1 + C_{1,1})(\alpha_2 + C_{1,1}) - D_{1,1}^2}{\pi^2} \right] \frac{1}{e^{-(\alpha_1+C_{1,1})x^2}e^{-(\alpha_2+C_{1,1})y^2}e^{+2\alpha_{1,1}x\cdot y}}
\]
and one-body
\[
\rho_1(x) = N_1 \left( \frac{\alpha_1 + C_{1,0}}{\pi} \right) \frac{1}{e^{-(\alpha_1+C_{1,0})x^2}}, \quad \rho_2(y) = N_2 \left( \frac{\alpha_2 + C_{0,1}'}{\pi} \right) \frac{1}{e^{-(\alpha_2+C_{0,1}')y^2}}.
\]

3.2. Solution of the harmonic-interaction model for trapped mixtures at the mean-field level

At the other end of the exact, many-body treatment of the harmonic-interaction model for trapped mixtures lies the Gross–Pitaevskii, mean-field solution. In the mean-field theory the many-particle wave-function is approximated as a product state, where all the bosons of species 1 lie in one orbital \(\phi_1(x)\) and all the bosons of species 2 lie in another orbital \(\phi_2(y)\). Thus, the mean-field ansatz for the mixture is the product wave-function
\[
\Phi^{\text{GP}}(x_1, \ldots, x_N, y_1, \ldots, y_N) = \prod_{j=1}^{N_1} \phi_1(x_j) \prod_{k=1}^{N_2} \phi_2(y_k).
\]

The Gross–Pitaevskii energy functional of the mixture reads
\[
E^{\text{GP}} = N_1 \left[ \int dx \phi_1^*(x) \left( -\frac{1}{2m_1} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m_1 \omega^2 x^2 \right) \phi_1(x) \right]
\]
\[
+ \frac{\Lambda_1}{2} \int dx dx' |\phi_1(x)|^2 |\phi_1(x')|^2 (x - x')^2 + \frac{\Lambda_{21}}{2} \int dx dy |\phi_1(x)|^2 |\phi_2(y)|^2 (x - y)^2 \right]
\]
\[
+ N_2 \left[ \int dy \phi_2^*(y) \left( -\frac{1}{2m_2} \frac{\partial^2}{\partial y^2} + \frac{1}{2} m_2 \omega^2 y^2 \right) \phi_2(y) \right]
\]
\[
+ \frac{\Lambda_2}{2} \int dy dy' |\phi_2(y)|^2 |\phi_2(y')|^2 (y - y')^2 + \frac{\Lambda_{12}}{2} \int dx dy |\phi_1(x)|^2 |\phi_2(y)|^2 (x - y)^2 \right],
\]

where the mean-field interaction parameters are given by \(\Lambda_1 = \lambda_1(N_1 - 1)\), \(\Lambda_2 = \lambda_2(N_2 - 1)\), \(\Lambda_{12} = \lambda_{12}N_1\), and \(\Lambda_{21} = \lambda_{12}N_2\) and satisfy \(N_1 \Lambda_{21} = N_2 \Lambda_{12}\). We denote hereafter \(e^{\text{GP}} = \frac{E^{\text{GP}}}{N}\) as the total mean-field energy of the mixture divided by the total number of particles \(N = N_1 + N_2\). Minimizing the energy functional (32) with respect to the shapes of the orbitals \(\phi_1(x)\) and \(\phi_2(y)\), the two-coupled Gross–Pitaevskii equations of the mixture are derived
\[
\left\{ -\frac{1}{2m_1} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m_1 \omega^2 x^2 + \int dx' [\Lambda_1 |\phi_1(x')|^2 + \Lambda_{21} |\phi_2(x')|^2] (x - x')^2 \right\} \phi_1(x) = \mu_1 \phi_1(x),
\]
\[
\left\{ -\frac{1}{2m_2} \frac{\partial^2}{\partial y^2} + \frac{1}{2} m_2 \omega^2 y^2 + \int dy' [\Lambda_2 |\phi_2(y')|^2 + \Lambda_{12} |\phi_1(y')|^2] (y - y')^2 \right\} \phi_2(y) = \mu_2 \phi_2(y).
\]
where \( \mu_1 \) and \( \mu_2 \) are the chemical potentials of the species, see appendix C.

The solution of (33) follows a similar strategy as for the single-species [29] and symmetric-mixture [46] harmonic-interaction models. Expanding the interaction terms in (33) we find

\[
\begin{align*}
- \frac{1}{2m_1} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m_1 \left[ \omega_1^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21}) \right] x^2 \phi_1(x) \\
= \left\{ \mu_1 - \int dx' [\Lambda_1 |\phi_1(x')|^2 + \Lambda_{21} |\phi_2(x')|^2] x^2 \right\} \phi_1(x),
\end{align*}
\]

and

\[
\begin{align*}
- \frac{1}{2m_2} \frac{\partial^2}{\partial y^2} + \frac{1}{2} m_2 \left[ \omega_2^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12}) \right] y^2 \phi_2(y) \\
= \left\{ \mu_2 - \int dy' [\Lambda_2 |\phi_2(y')|^2 + \Lambda_{12} |\phi_1(y')|^2] y^2 \right\} \phi_2(y),
\end{align*}
\]

where, since \( \phi_1(x) \) and \( \phi_2(y) \) are even functions (see below), there are no linear in \( x, y \) terms in (34). A particular solution of (34) are the following (interaction-dressed) Gaussian functions:

\[
\phi_1(x) = \left( \frac{m_1}{\pi} \right)^{\frac{1}{4}} \left( \frac{\omega_1^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21})}{\sqrt{\Omega_1^2 - \frac{2 \Lambda_1}{m_1}}} \right)^{\frac{3}{4}} e^{-\frac{\omega_1^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21})}{2 \sqrt{\Omega_1^2 - \frac{2 \Lambda_1}{m_1}}} x^2},
\]

\[
\phi_2(y) = \left( \frac{m_2}{\pi} \right)^{\frac{1}{4}} \left( \frac{\omega_2^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12})}{\sqrt{\Omega_2^2 - \frac{2 \Lambda_2}{m_2}}} \right)^{\frac{3}{4}} e^{-\frac{\omega_2^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12})}{2 \sqrt{\Omega_2^2 - \frac{2 \Lambda_2}{m_2}}} y^2}. \tag{35}
\]

We can now compute the mean-field energy per particle \( \varepsilon_{\text{GP}} \) which reads

\[
\varepsilon_{\text{GP}} = \frac{E_{\text{GP}}}{N} = \frac{3}{2} \left[ \frac{N_1}{N} \sqrt{\omega_1^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21})} + \frac{N_2}{N} \sqrt{\omega_2^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12})} \right]
\]

\[
= \frac{3}{2(\Lambda_{12} + \Lambda_{21})} \left[ \Lambda_{12} \sqrt{\omega_1^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21})} + \Lambda_{21} \sqrt{\omega_2^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12})} \right], \tag{36}
\]

where \( \frac{N_1}{N} = \frac{\Lambda_{12}}{\Lambda_{21}} \) is used. Of course, the many-body energy (7) is always lower than the mean-field energy because of the variational principle.

---

\[5\] We follow [29] and [46] in demonstrating that (interaction-dressed) Gaussian functions solve the corresponding Gross–Pitaevskii equations. We exclude the possibility of demixing (symmetry preserving or symmetry broken) in the mean-field solution for the ground state of the trapped mixture. To recall, the many-body solution does not exhibit demixing, see the densities (30). While we do not provide a mathematically-rigorous proof that other than Gaussian-shaped (symmetry preserving or symmetry broken) solutions may occur as the ground-state solution of the two-coupled Gross–Pitaevskii equations of the harmonic-interaction model for trapped mixtures, this is not necessary for the proof of Bose–Einstein condensation of the many-body solution. Furthermore, the fact that the energy per particle and reduced density matrices per particle of the exact many-body ground state and of the Gaussian-shaped mean-field solution coincide in the infinite-particle limit constitutes in our opinion a rather solid support that the Gaussian-shaped orbitals (35) are indeed the Gross–Pitaevskii ground state.
We now discuss the reduced density matrices at the mean-field level. The Gross–Pitaevskii wave-function reads

\[
\Phi^{GP}(x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2}) = \left( \frac{m_1}{\pi} \right)^{\frac{N_1}{2}} e^{-\frac{m_1}{\pi} \sqrt{\omega^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21})} \sum_{i=1}^{N_1} x_i^2} \\
\times \left( \frac{m_2}{\pi} \right)^{\frac{N_2}{2}} e^{-\frac{m_2}{\pi} \sqrt{\omega^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12})} \sum_{i=1}^{N_2} y_i^2}. \tag{37}
\]

From (37) we have

\[
\rho_1^{MF}(x, x') = N_1 \rho_1^{GP}(x, x') = N_1 \phi_1^{GP}(x) \phi_1^{GP}(x')^*, \tag{38}
\]

\[
= N_1 \left( \frac{m_1}{\pi} \right)^{\frac{1}{2}} e^{-\frac{m_1}{2 \pi} \sqrt{\omega^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21})}(x^2 + x'^2)},
\]

\[
\rho_2^{MF}(y, y') = N_2 \rho_2^{GP}(y, y') = N_2 \phi_2^{GP}(y) \phi_2^{GP}(y')^*, \tag{39}
\]

\[
= N_2 \left( \frac{m_2}{\pi} \right)^{\frac{1}{2}} e^{-\frac{m_2}{2 \pi} \sqrt{\omega^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12})}(y^2 + y'^2)},
\]

for the reduced one-body density matrices and

\[
\rho_{12}^{MF}(x, x', y, y') = N_1 N_2 \phi_1^{GP}(x) \phi_2^{GP}(y) \phi_1^{GP}(x') \phi_2^{GP}(y')^*, \tag{38}
\]

\[
= N_1 N_2 \left( \frac{m_1}{\pi} \right)^{\frac{1}{2}} \left( \frac{m_2}{\pi} \right)^{\frac{1}{2}} e^{-\frac{m_1}{2 \pi} \sqrt{\omega^2 + \frac{2}{m_1} (\Lambda_1 + \Lambda_{21})}(x^2 + x'^2)} e^{-\frac{m_2}{2 \pi} \sqrt{\omega^2 + \frac{2}{m_2} (\Lambda_2 + \Lambda_{12})}(y^2 + y'^2)},
\]

\[
= N_1 N_2 \left( \frac{m_1}{\pi} \right)^{\frac{1}{2}} \left( \frac{m_2}{\pi} \right)^{\frac{1}{2}} e^{-\frac{m_1}{2 \pi} \sqrt{\Omega_1^2 - \frac{2\Lambda_1}{m_1}}(x^2 + x'^2)} e^{-\frac{m_2}{2 \pi} \sqrt{\Omega_2^2 - \frac{2\Lambda_2}{m_2}}(y^2 + y'^2)},
\]

\[
= N_1 N_2 \phi_1^{GP}(x, x') \phi_2^{GP}(y, y'). \tag{39}
\]

for the inter-species reduced density matrix. Quite generally and as might have been expected, for mixtures with a finite number of particles, the mean-field reduced density matrices (38) and (39) differ from their many-body counterparts (28) and (27). The intra-species reduced density matrices are factorized to products of Gross–Pitaevskii orbitals, and the inter-species reduced density matrix is factorized to product of Gross–Pitaevskii intra-species reduced density matrices. This concludes our derivation of the mean-field solution of the harmonic-interaction model for trapped mixtures.
3.3. The infinite-particle limit

We are now in the position to put together the above two sections, and investigate the energy and reduced density matrices per particle of the mixture at the infinite-particle limit, and how these quantities are connected in this limit with the Gross–Pitaevskii solution of the mixture. Interestingly, for a mixture we can discuss separately two such limits, hereafter referred to as the two-species infinite-particle limit and the one-species infinite-particle limit. In the first, the numbers of particles of both species are taken to infinity whereas in the second the number of particles of one of the species is taken to infinity and the number of particles of the second species remains fixed and finite (in both limits interaction parameters are held fixed, the precise way is discussed below). This is unlike the case of the single-species and symmetric-mixture harmonic-interaction models. We compare and contrast the properties of the mixture in the two limits. We start with the two-species infinite-particle limit.

3.3.1. The two-species infinite-particle limit.

In the two-species infinite-particle limit, namely for \( N_1 \to \infty \) and \( N_2 \to \infty \) and holding the interaction parameters \( \Lambda_{11}, \Lambda_{22}, \Lambda_{12}, \) and \( \Lambda_{21} \) fixed, we find from (7) that

\[
\lim_{N \to \infty} E_N = \frac{3}{2(\Lambda_{12} + \Lambda_{21})} \left[ \Lambda_{12} \sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})} + \Lambda_{21} \sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})} \right] = \epsilon_{GP},
\]

which establishes the connection between the exact energy per particle and mean-field (Gross–Pitaevskii) energy per particle in this limit for the generic mixture. Like the literature cases of single-species bosons and the symmetric-mixture harmonic-interaction model, the many-body and mean-field solutions coincide in the limit of an infinite number of particles as far as the energy per particle in examined. Note that the two-species limit of an infinite number of particles \( N \to \infty \) implies that \( N_1 \to \infty \) and \( N_2 \to \infty \) such the the ratio \( \frac{N_1}{N_2} = \frac{\Lambda_{12}}{\Lambda_{21}} \).

To discuss the two-species infinite-particle limit for the reduced density matrices we first have to evaluate the limit of relevant quantities. Thus we find for the frequencies (4)

\[
\lim_{N \to \infty} \Omega_1 = \sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})}, \quad \lim_{N \to \infty} \Omega_2 = \sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})},
\]

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

for the parameters (9) of the wave-function

\[
\lim_{N \to \infty} \alpha_1 = m_1 \sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})}, \quad \lim_{N \to \infty} \alpha_2 = m_2 \sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})},
\]

\[
\lim_{N \to \infty} \beta_1 = 0, \quad \lim_{N \to \infty} \beta_2 = 0, \quad \lim_{N \to \infty} \gamma = 0,
\]

and therefore for the constants (24) and (25) of the reduced density matrices

\[
\lim_{N \to \infty} C_{11} = 0, \quad \lim_{N \to \infty} C_{11}' = 0, \quad \lim_{N \to \infty} D_{11} = 0, \quad \lim_{N \to \infty} D_{11}' = 0,
\]

\[
\lim_{N \to \infty} C_{10} = 0, \quad \lim_{N \to \infty} C_{01} = 0.
\]
In particular, that \( \lim_{N \to \infty} D_{11} = \lim_{N \to \infty} D'_{11} = 0 \) stems from \( \lim_{N \to \infty} \gamma = 0 \) and implies that there is no coupling at the level of the inter-species reduced density matrix, see (27), between the species 1 and 2 in the two-species infinite-particle limit. Combining the above we find

\[
\lim_{N \to \infty} \rho_1(x, x') = \frac{m_1}{\pi} \left( \sqrt{\omega^2 + \frac{m_1}{2} (\Lambda_1 + \Lambda_{21})} \right) \frac{1}{2} e^{-\frac{\pi}{2} \sqrt{m_1} (\Lambda_1 + \Lambda_{21})(x^2 + x'^2)}
\]

\[
= \rho_{1GP}(x, x'),
\]

\[
\lim_{N \to \infty} \rho_2(y, y') = \frac{m_2}{\pi} \left( \sqrt{\omega^2 + \frac{m_2}{2} (\Lambda_2 + \Lambda_{12})} \right) \frac{1}{2} e^{-\frac{\pi}{2} \sqrt{m_2} (\Lambda_2 + \Lambda_{12})(y^2 + y'^2)}
\]

\[
= \rho_{2GP}(y, y')
\]

(44)

for the reduced one-body density matrices per particle and

\[
\lim_{N \to \infty} \rho_{12}(x, x', y, y') = \frac{m_1}{\pi N_1 N_2} \left( \sqrt{\omega^2 + \frac{m_1}{2} (\Lambda_1 + \Lambda_{21})} \right) \left( \sqrt{\omega^2 + \frac{m_2}{2} (\Lambda_2 + \Lambda_{12})} \right) \frac{1}{2} e^{-\frac{\pi}{2} \sqrt{m_1} (\Lambda_1 + \Lambda_{21})(x^2 + x'^2)} e^{-\frac{\pi}{2} \sqrt{m_2} (\Lambda_2 + \Lambda_{12})(y^2 + y'^2)}
\]

\[
= \lim_{N \to \infty} \rho_1(x, x') \frac{m_1}{N_1} \lim_{N \to \infty} \rho_2(y, y') \frac{m_2}{N_2}
\]

\[
= \rho_{1GP}(x, x') \rho_{2GP}(y, y')
\]

(45)

for the inter-species reduced density matrix per particle. With this, we have established the 100\% condensation of each species in the generic mixture, in the two-species infinite-particle limit. Furthermore, the inter-species reduced density matrix per particle is separable in this limit and given as a product of the intra-species reduced density matrices per particle. Each condensate is described by the Gross–Pitaevskii quantities. In the spirit of [44], the results (44) and (45) are in agreement with vanishing of the single-particle bipartite entanglement, here, however, for repulsive and attractive mixtures in the two-species infinite-particle (mean-field) limit. This constitutes a generalization for generic mixtures of interacting bosons, at least within the exactly-solvable harmonic-interaction model for trapped mixtures, of what is known in the literature for single-species trapped Bose–Einstein condensates [27, 28].

3.3.2. The one-species infinite-particle limit. Let us discuss what happens in (and how to define) the limit of an infinite number of particles of one of the species, say, species 1. For \( N_1 \to \infty \) the interaction parameters \( \Lambda_1 = \Lambda_1(N_1 - 1) \) and \( \Lambda_{12} = \Lambda_{12}N_1 \) are held fixed by diminishing the interaction strengths \( \lambda_1 \) and \( \lambda_{12} \) accordingly. Since the number of particles of the second species \( N_2 \) is finite (and fixed) the interaction parameter \( \Lambda_2 = \Lambda_2(N_2 - 1) \) is fixed for constant \( \lambda_2 \). However, \( \Lambda_{21} = \Lambda_{12}N_2 \to 0 \). Thus, we get for the energy per particle in the one-species infinite-particle limit

\[
\lim_{N_1 \to \infty} E = \frac{3}{2} \sqrt{\omega^2 + \frac{2 \Lambda_1}{m_1}} = \epsilon_{GP}.
\]

(46)

When only species 1 is taken to the infinite-particle limit it naturally becomes dominant over species 2. The energy per particle is that of species 1 only, with apparently no contribution or
influence from species 2, and is given by the Gross–Pitaevskii energy per particle of species 1 alone. What happens then with the reduced density matrices?

To discuss the one-species infinite-particle limit for the reduced density matrices we first have to evaluate with some care the limit of the relevant quantities. Now we find for the frequencies (4)

$$\lim_{N_1 \to \infty} \Omega_1 = \sqrt{\omega^2 + \frac{2\Lambda_1}{m_1}}, \quad \lim_{N_1 \to \infty} \Omega_2 = \sqrt{\omega^2 + \frac{2}{m_2} (\Lambda_2 + \lambda_2 + \Lambda_{12})},$$

$$\lim_{N_1 \to \infty} \Omega_{12} = \sqrt{\omega^2 + \frac{2\Lambda_{12}}{m_2}},$$

for the parameters (9) of the wave-function

$$\lim_{N_1 \to \infty} \alpha_1 = m_1 \sqrt{\omega^2 + \frac{2\Lambda_1}{m_1}}, \quad \lim_{N_1 \to \infty} \beta_1 = 0, \quad \lim_{N_1 \to \infty} \gamma = 0,$$

$$\lim_{N_1 \to \infty} \alpha_2 = m_2 \left(1 - \frac{2\Lambda_1}{N_2 \omega} \right) \sqrt{\omega^2 + \frac{2}{m_2} (\Lambda_2 + \lambda_2 + \Lambda_{12})} + \frac{1}{N_2} \sqrt{\omega^2 + \frac{2\Lambda_{12}}{m_2}} \equiv \tilde{\alpha}_2,$$

$$\lim_{N_1 \to \infty} \beta_2 = \frac{m_2}{N_2} \left(\sqrt{\omega^2 + \frac{2\Lambda_{12}}{m_2}} - \sqrt{\omega^2 + \frac{2}{m_2} (\Lambda_2 + \lambda_2 + \Lambda_{12})}\right),$$

and consequently for the constants (24) and (25) of the reduced density matrices

$$\lim_{N_1 \to \infty} C_{1,1} = 0, \quad \lim_{N_1 \to \infty} C_{1,0} = 0, \quad \lim_{N_1 \to \infty} D_{1,1} = 0, \quad \lim_{N_1 \to \infty} D_{1,1}' = 0,$$

$$\lim_{N_1 \to \infty} C_{1,1}' = -\frac{m_2(N_2 - 1)}{N_2} \frac{\left[\sqrt{\omega^2 + \frac{2\Lambda_1}{m_1} (\Lambda_2 + \lambda_2 + \Lambda_{12})} - \sqrt{\omega^2 + \frac{2\Lambda_{12}}{m_2}}\right]^2}{\sqrt{\omega^2 + \frac{2\Lambda_{12}}{m_2}} + (N_2 - 1) \sqrt{\omega^2 + \frac{2\Lambda_{12}}{m_2}}} \equiv C_{1,1}'$$

$$\lim_{N_1 \to \infty} C_{0,1}' \equiv \tilde{C}_{0,1}' = \tilde{C}_{1,1},$$

where the last equality stems from \(\lim_{N_1 \to \infty} C_{1,N_1} = \lim_{N_1 \to \infty} C_{0,N_1} = 0\) and is instrumental in what follows. In particular, that \(\lim_{N_1 \to \infty} D_{1,1} = \lim_{N_1 \to \infty} D_{1,1}' = 0\) stems from \(\lim_{N_1 \to \infty} \gamma = 0\) and implies that there is no coupling at the level of the inter-species reduced density matrix, see (27), between the species 1 and 2 also in the one-species infinite-particle limit. Note that the corresponding quantities associated with species 2 do not vanish in the one-species infinite-particle limit, compare (47)–(49) with (41)–(43). Now we can prescribe in the one-species infinite-particle limit the single-particle reduced density matrices per particle,

$$\lim_{N_1 \to \infty} \rho_1(\mathbf{x}, \mathbf{x}') = \frac{m_1}{\pi} \left[\frac{\omega^2}{\sqrt{\omega^2 + \frac{2\Lambda_1}{m_1}}} \right]^\frac{1}{2} e^{-\frac{\omega^2}{2} \sqrt{\omega^2 + \frac{2\Lambda_1}{m_1}} (\mathbf{x}^2 + \mathbf{x}'^2)} \equiv \rho_1^G(\mathbf{x}, \mathbf{x}'),$$

$$\lim_{N_1 \to \infty} \rho_2(\mathbf{y}, \mathbf{y}') = \frac{\tilde{\alpha}_2 + \tilde{C}_{0,1}'}{\pi} \frac{1}{\sqrt{\omega^2 + \frac{2\Lambda_{12}}{m_2}}} e^{\frac{\omega^2}{2} \sqrt{\omega^2 + \frac{2\Lambda_{12}}{m_2}} (\mathbf{y}_1 + \mathbf{y}'_1)} e^{-\frac{\omega^2}{2} \sqrt{\omega^2 + \frac{2\Lambda_{12}}{m_2}} (\mathbf{y}_2 + \mathbf{y}'_2)} \equiv \frac{\tilde{\rho}_2(\mathbf{y}, \mathbf{y}')}{N_2} \equiv \rho_2^G(\mathbf{y}, \mathbf{y}'),$$

and the inter-species reduced density matrix per particle,
\[ \lim_{N_1 \to \infty} \frac{\rho_{12}(x, x', y, y')}{N_1 N_2} = \left( \frac{m_1}{\pi} \sqrt{\omega^2 + \frac{2 \Lambda_1}{m_1}} \right)^2 e^{-\frac{m_1}{2} \sqrt{\omega^2 + \frac{2 \Lambda_1}{m_1}}} (x^2 + x')^2 \times \left( \frac{1}{\pi} \right)^2 e^{-\frac{m_1}{2} \left( y_1^2 + y_1'^2 \right)} e^{-\frac{m_1}{2} \left( y_2^2 + y_2'^2 \right)} e^{-\frac{m_1}{2} \left( y_3^2 + y_3'^2 \right)} \]

\[ = \lim_{N_1 \to \infty} \frac{\rho_1(x, x')}{N_1} \lim_{N_2 \to \infty} \frac{\rho_2(y, y')}{N_2} = \frac{\rho_{1\text{GP}}(x, x')}{N_1} \frac{\rho_{2\text{GP}}(y, y')}{N_2} \neq \rho_1^{\text{GP}}(x, x') \rho_2^{\text{GP}}(y, y'). \] (51)

We find that species 1 is described in this limit by the Gross–Pitaevskii quantity whereas species 2, as might have been expected, is not, implying that species 2 remains correlated. Interestingly, the inter-species reduced density matrix per particle is separable in this limit, and precisely given by the product of the Gross–Pitaevskii quantity for species 1 and the correlated quantity for species 2, see (50). This is on the account of the last equality in (49). In the spirit of [44], the result (51) is in agreement with vanishing of the entanglement between particles of different species, here, however, for repulsive and attractive mixtures in the one-species infinite-particle limit. This concludes our studies of the reduced density matrices of a generic mixture within the harmonic-interaction model for trapped mixtures in the one-species infinite-particle limit.

4. Concluding remarks

Are the different species in the ground state of a trapped bosonic mixture 100% condensed? Are the many-body and mean-field energies per particle of a trapped bosonic mixture equal at the infinite-particle limit? In the present work we answered these and more questions by treating an exactly-solvable model— the harmonic-interaction model for trapped bosonic mixtures.

From the ground-state wave-function of the mixture we have computed the lowest-order intra-species and inter-species reduced density matrices, by generalizing Cohen and Lee [29] recurrence relations for the single-species harmonic-interaction model to a generic mixture. We have also obtained analytically the Gross–Pitaevskii solution for the ground state of the mixture. Thereafter, by taking the infinite-particle limit with respect to the two species, we were able to show that each of the species is indeed 100% condensed, and that the many-body and Gross–Pitaevskii quantities for the energy per particle and reduced density matrices per particle coincide in this limit. When the infinite-particle limit is taken with respect to one of the species, only this species becomes 100% condensed, whereas the other species remains correlated. Interestingly, in either of the infinite-particle-limit procedures the inter-species density matrix per particle becomes exactly the product of the intra-species reduced density matrices per particle.

It would be interesting to investigate other properties of the harmonic-interaction model for mixtures presented in the present work, e.g. quantities whose many-body and mean-field descriptions may not coincide in the infinite-particle limit [45, 47]. For finite systems, the model may prove deductive as well, for instance to investigate properties of an impurity made of a few interacting particles embedded inside a larger Bose–Einstein condensate, and to benchmark numerical tools.
Acknowledgments

I thank Shachar Klaiman, Alexej Streltsov, and Lorenz Cederbaum for fruitful discussions. This research was supported by the Israel Science Foundation (Grant No. 600/15).

Appendix A. Further details of Diagonalizing the Hamiltonian of the mixture

Opening the braces of the particle-particle interaction terms in (1) and collecting the diagonal contributions together we have

$$\hat{H} = \sum_{j=1}^{N_1} \left\{ -\frac{1}{2m_1} \frac{\partial^2}{\partial x_j^2} + \frac{1}{2} \left[ m_1 \omega^2 + 2(N_1 - 1) \lambda_1 + 2N_2 \lambda_{12} \right] x_j^2 \right\}$$

$$+ \sum_{j=1}^{N_2} \left\{ -\frac{1}{2m_2} \frac{\partial^2}{\partial y_j^2} + \frac{1}{2} \left[ m_2 \omega^2 + 2(N_2 - 1) \lambda_2 + 2N_1 \lambda_{12} \right] y_j^2 \right\}$$

$$- 2\lambda_1 \sum_{1 \leq j < k} x_j \cdot x_k - 2\lambda_2 \sum_{1 \leq j < k} y_j \cdot y_k - 2\lambda_{12} \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} x_j \cdot y_k. \quad (A.1)$$

With the Jacobi-coordinate transformation (2) the harmonic trapping and kinetic energy remain diagonal, since from

$$\sum_{j=1}^{N_1} x_j^2 = \sum_{k=1}^{N_1 - 1} \mathcal{Q}_k^2 + \left( \frac{\sqrt{N_2 m_2}}{M} \mathcal{Q}_{N-1} + \sqrt{N_1} \mathcal{Q}_N \right)^2$$

$$= \sum_{k=1}^{N_1 - 1} \mathcal{Q}_k^2 + \frac{N_2 m_2}{M^2} \mathcal{Q}_{N-1}^2 + N_1 \mathcal{Q}_N^2 + \frac{2\sqrt{N_1 N_2 m_2}}{M} \mathcal{Q}_{N-1} \mathcal{Q}_N,$$

$$\sum_{j=1}^{N_2} y_j^2 = \sum_{k=N_1}^{N_2 - 1} \mathcal{Q}_k^2 + \left( -\frac{\sqrt{N_1 m_1}}{M} \mathcal{Q}_{N-1} + \sqrt{N_2} \mathcal{Q}_N \right)^2$$

$$= \sum_{k=N_1}^{N_2 - 1} \mathcal{Q}_k^2 + \frac{N_1 m_1}{M^2} \mathcal{Q}_{N-1}^2 + N_2 \mathcal{Q}_N^2 - \frac{2\sqrt{N_1 N_2 m_1}}{M} \mathcal{Q}_{N-1} \mathcal{Q}_N \quad (A.2)$$

and

$$\sum_{j=1}^{N_1} \frac{\partial^2}{\partial x_j^2} = \sum_{k=1}^{N_1 - 1} \frac{\partial^2}{\partial \mathcal{Q}_k^2} + \left( \sqrt{N_2} \frac{\partial}{\partial \mathcal{Q}_{N-1}} + \frac{\sqrt{N_1 m_1}}{M} \frac{\partial}{\partial \mathcal{Q}_N} \right)^2$$

$$= \sum_{k=1}^{N_1 - 1} \frac{\partial^2}{\partial \mathcal{Q}_k^2} + \frac{N_2}{M^2} \frac{\partial^2}{\partial \mathcal{Q}_{N-1}^2} + \frac{N_1 m_1}{M^2} \frac{\partial^2}{\partial \mathcal{Q}_N^2} + \frac{2\sqrt{N_1 N_2 m_1}}{M} \frac{\partial}{\partial \mathcal{Q}_{N-1}} \frac{\partial}{\partial \mathcal{Q}_N},$$

$$\sum_{j=1}^{N_2} \frac{\partial^2}{\partial y_j^2} = \sum_{k=N_1}^{N_2 - 1} \frac{\partial^2}{\partial \mathcal{Q}_k^2} + \left( -\sqrt{N_1} \frac{\partial}{\partial \mathcal{Q}_{N-1}} + \sqrt{N_2 m_2} \frac{\partial}{\partial \mathcal{Q}_N} \right)^2$$

$$= \sum_{k=N_1}^{N_2 - 1} \frac{\partial^2}{\partial \mathcal{Q}_k^2} + \frac{N_1}{M^2} \frac{\partial^2}{\partial \mathcal{Q}_{N-1}^2} + \frac{N_2 m_2}{M^2} \frac{\partial^2}{\partial \mathcal{Q}_N^2} - \frac{2\sqrt{N_1 N_2 m_2}}{M} \frac{\partial}{\partial \mathcal{Q}_{N-1}} \frac{\partial}{\partial \mathcal{Q}_N}. \quad (A.3)
we have
\[
\begin{align*}
m_1 \sum_{j=1}^{N_1} x_j^2 + m_2 \sum_{j=1}^{N_2} y_j^2 &= m_1 \sum_{k=1}^{N_1-1} Q_k^2 + m_2 \sum_{k=N_1}^{N_2-2} Q_k^2 + M_{12} Q_{N_2-1}^2 + M Q_N^2, \\
\frac{1}{m_1} \sum_{j=1}^{N_1} \frac{\partial^2}{\partial x_j^2} + \frac{1}{m_2} \sum_{j=1}^{N_2} \frac{\partial^2}{\partial y_j^2} &= \sum_{k=1}^{N_1} \frac{1}{m_1} \frac{\partial^2}{\partial Q_k^2} + \sum_{k=N_1}^{N_2-2} \frac{1}{m_2} \frac{\partial^2}{\partial Q_k^2} + \frac{1}{M_{12}} \frac{\partial^2}{\partial Q_{N_2-1}^2} + \frac{1}{M} \frac{\partial^2}{\partial Q_N^2}.
\end{align*}
\]
\[
M_{12} = \frac{1}{m_1} + \frac{N_1}{m_2} = \frac{m_1 m_2}{M}, \quad M = N_1 m_1 + N_2 m_2.
\]

Finally, using the quadratic relations
\[
\begin{align*}
\sum_{k=1}^{N_1-1} Q_k^2 &= \left(1 - \frac{1}{N_1} \right) \sum_{j=1}^{N_1} x_j^2 - \frac{2}{N_1} \sum_{1 \leq j < k} x_j \cdot x_k, \\
\sum_{k=N_1}^{N_2-1} Q_k^2 &= \left(1 - \frac{1}{N_2} \right) \sum_{j=1}^{N_2} y_j^2 - \frac{2}{N_2} \sum_{1 \leq j < k} y_j \cdot y_k, \\
Q_{N_1-1}^2 &= \frac{N_1}{N_1} \sum_{j=1}^{N_1} x_j^2 + \frac{N_2}{N_2} \sum_{j=1}^{N_2} y_j^2 + 2 \left[ \frac{N_1}{N_1} \sum_{1 \leq j < k} x_j \cdot x_k + \frac{N_2}{N_2} \sum_{1 \leq j < k} y_j \cdot y_k - \sum_{j=1}^{N_1} \sum_{j=1}^{N_2} x_j \cdot y_k \right], \\
Q_N^2 &= \frac{m_1^2}{M^2} \sum_{j=1}^{N_1} x_j^2 + \frac{m_2^2}{M^2} \sum_{j=1}^{N_2} y_j^2 + 2 \left[ \frac{m_1^2}{M^2} \sum_{1 \leq j < k} x_j \cdot x_k + \frac{m_2^2}{M^2} \sum_{1 \leq j < k} y_j \cdot y_k + \frac{m_1 m_2}{M^2} \sum_{j=1}^{N_1} \sum_{j=1}^{N_2} x_j \cdot y_k \right].
\end{align*}
\]

the coupling terms in the Hamiltonian (A.1) are diagonalized too, and the ground-state wave-function transforms from the Jacobi-coordinate to the lab-frame representation, see (6) and (8).

**Appendix B. Further details of the solution of the coupled recurrence relations**

Within the horizontal reduction of \(F_{N_1 N_2}\), see (16)–(18), the recurrence relations between the corresponding constants are
\[
\begin{align*}
C_{N_1,j-1}' &= C_{N_1,j} - \frac{(\beta_2 + C_{N_1,j})^2}{\alpha_2 + C_{N_1,j}'}, \\
D_{N_1,j-1}' &= D_{N_1,j} - \frac{\beta_2 + C_{N_1,j}}{\alpha_2 + C_{N_1,j}'} D_{N_1,j} = \frac{\alpha_2 - \beta_2}{\alpha_2 + C_{N_1,j}'} D_{N_1,j}, \\
C_{N_1,j-1} &= C_{N_1,j} - \frac{D_{N_1,j}'}{\alpha_2 + C_{N_1,j}'} = C_{N_1,j} - \frac{D_{N_1,j} D_{N_1,j-1}}{\alpha_2 - \beta_2}, \\
D_{N_1,j-1}' &= D_{N_1,j}'.
\end{align*}
\]
The recurrence relations (B.1) consist of one non-linear relation (for $C_{Ni,j}$) and the linear relations for $D_{Ni,j}$, $C_{Ni,j}$, and $D'_{Ni,j}$. We see from (B.1) that first the relation for $C'_{Ni,j}$ needs to be solved, then for the $D_{Ni,j}$, and then for the $C_{Ni,j}$. The linear relation for $D'_{Ni,j}$ is trivial and does not depend on the other constants.

The recurrence relation for $C_{Ni,j}$ has exactly the same structure as the recurrence relation emerging in the integration of the single-species harmonic-interaction model [29]. Making use of this observation and substituting the result into $D_{Ni,j}$ and then together into $C_{Ni,j}$ relations (B.1) are solved. The final result reads

$$
C_{Ni,j} = -\alpha_2 + \frac{(\alpha_2 - \beta_2)(1 + j\eta_2)}{1 + (j + 1)\eta_2}, \quad \eta_2 = -\frac{\beta_2}{\alpha_2 + N_2\beta_2},
$$

$$
D_{Ni,j} = \gamma + \frac{(N_2 + 1)\eta_2}{1 + (j + 1)\eta_2},
$$

$$
C_{Ni,j} = -\frac{1}{\alpha_2 - \beta_2} \sum_{k=N_2}^{j+1} D_{Ni,k}D_{Ni,k-1} = -\frac{\gamma^2[1 + (N_2 + 1)\eta_2]}{\alpha_2 - \beta_2} \frac{(N_2 - j)}{1 + (j + 1)\eta_2},
$$

$$
D'_{Ni,j} = \gamma,
$$

where the initial conditions for $C_{Ni,Ni}$, $D_{Ni,Ni}$, $C_{Ni,Ni}$, and $D'_{Ni,Ni}$ in (15) have been used. From (B.2) we obtain the constants $C_{Ni,1}$, $D_{Ni,1}$, $C_{Ni,1}$, and $D'_{Ni,1}$ in (20) entering the auxiliary function $F_{Ni,1}$, and $C_{Ni,0}$ in (26) entering the auxiliary function $F_{Ni,0}$.

Proceeding now to the vertical reduction of $F_{Ni,1}$ to $F_{1,1}$, see (16), (21) and (22), we write

$$
C_{j-1,1} = C_{j,1} - \frac{(\beta_1 + C_{j,1})^2}{\alpha_1 + C_{j,1}},
$$

$$
D_{j-1,1} = D_{j,1} - \frac{\beta_1 + C_{j,1}}{\alpha_1 + C_{j,1}} D_{j,1},
$$

$$
C'_{j-1,1} = C'_{j,1} - \frac{D'_{j,1}}{\alpha_1 + C'_{j,1}},
$$

$$
D'_{j-1,1} = D'_{j,1},
$$

The vertical recursion relations (B.3) consist again one non-linear relation (for $C_{1,1}$), and the linear relations for $C'_{1,1}$, $D_{1,1}$, and $D'_{1,1}$. The linear relation for $D'_{1,1}$ is again trivial. Note the interchange of roles of the $C$ and $C'$ constants when moving from horizontal to vertical reductions. We can hence interchange the order of horizontal and vertical reductions in order to prescribe $C_{1,1}$ based on the solution for $C_{1,1}$. Then, $C'_{1,Ni}$ in (26) obtained from the vertical reduction is used as an initial condition for the recurrence relation. Combining all the above we find for the constants of the auxiliary function $F_{1,1}$

$$
C_{1,1} = -\alpha_1 + \frac{(\alpha_1 - \beta_1)(1 + \eta_1)}{1 + 2\eta_1}, \quad \eta_1 = \frac{(\alpha_1 - \beta_1) - (\alpha_1 + C_{1,1})}{(N_1 + 1)(\alpha_1 + C_{1,1}) - N_1(\alpha_1 - \beta_1)},
$$

$$
D_{1,1} = D_{N_1,1} + \frac{(N_1 + 1)\eta_1}{1 + 2\eta_1},
$$

$$
C'_{1,1} = -\alpha_2 + \frac{(\alpha_2 - \beta_2)(1 + \eta'_1)}{1 + 2\eta'_1}, \quad \eta'_1 = \frac{(\alpha_2 - \beta_2) - (\alpha_2 + C'_{1,Ni})}{(N_2 + 1)(\alpha_2 + C'_{1,Ni}) - N_2(\alpha_2 - \beta_2)},
$$

$$
D'_{1,1} = D'_{N_1,1}.
$$

(B.4)
Upon substitution we arrive at the final result (24).

Last are the constants of $F_{1,0}$ and $F_{0,1}$. From the recurrence relation

$$C_{j-1,0} = C_{j,0} - \frac{(\beta_1 + C_{j,0})^2}{\alpha_1 + C_{j,0}}$$

we find

$$C_{1,0} = -\alpha_1 + \frac{(\alpha_1 - \beta_1)(1 + \eta_0)}{1 + 2\eta_0}, \quad \eta_0 = \frac{(\alpha_1 - \beta_1) - (\alpha_1 + C_{N_1,0})}{(N_1 + 1)(\alpha_1 + C_{N_1,0}) - N_1(\alpha_1 - \beta_1)},$$

$$C_{0,1} = -\alpha_2 + \frac{(\alpha_2 - \beta_2)(1 + \eta_0)}{1 + 2\eta_0}, \quad \eta_0 = \frac{(\alpha_2 - \beta_2) - (\alpha_2 + C_{0,0})}{(N_2 + 1)(\alpha_2 + C_{0,0}) - N_2(\alpha_2 - \beta_2)},$$

where the initial conditions $C_{N_1,0}$ and $C_{0,0}$ are given in (26), and where interchanging the order of the vertical and horizontal reductions allows one to obtain $C_{0,1}$ analogously to $C_{1,0}$. Substituting all quantities we arrive at the final expressions for the constants (25).

**Appendix C. Further details of the mean-field solution of the mixture**

Given the orbitals $\phi_1(x)$ and $\phi_2(y)$ (35), we can now evaluate the integrals

$$\int dx' |\phi_1(x')|^2 x'^2 = \frac{3}{2\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_2)}}$$

and

$$\int dy' |\phi_2(y')|^2 y'^2 = \frac{3}{2\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_1)}}$$

in (34) and determine the chemical potentials

$$\mu_1 = \frac{3}{2} \sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_2)} + \frac{3}{2} \left( \frac{\Lambda_1}{\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_2)}} + \frac{\Lambda_2}{\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_1)}} \right),$$

$$\mu_2 = \frac{3}{2} \sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_1)} + \frac{3}{2} \left( \frac{\Lambda_2}{\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_1)}} + \frac{\Lambda_1}{\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_2)}} \right).$$

With this, the mean-field energy is given by

$$E_{\text{MF}} = N_1 \mu_1 + N_2 \mu_2$$

$$- \frac{N_1}{2} \left[ \Lambda_1 \int dx' dx |\phi_1(x')|^2 |\phi_1(x')|^2 (x' - x)^2 + \Lambda_2 \int dx' dx |\phi_1(x')|^2 |\phi_2(y')|^2 (x - y)^2 \right]$$

$$- \frac{N_2}{2} \left[ \Lambda_2 \int dy' dy |\phi_2(y')|^2 |\phi_2(y')|^2 (y' - y)^2 + \Lambda_1 \int dx' dx |\phi_1(x')|^2 |\phi_2(y')|^2 (x - y)^2 \right]$$

$$= \frac{3}{2} \left[ N_1 \sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_2)} + N_2 \sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_1)} \right]$$

$$= \frac{3}{2} \left[ N_1 \Omega_1^2 + \frac{2\lambda_1}{m_1} + N_2 \Omega_2^2 + \frac{2\lambda_2}{m_2} \right].$$

(C.2)
where \( \int \mathrm{d}x \mathrm{d}x' |\phi_1(x)|^2 |\phi_1(x')|^2 (x - x')^2 = \frac{2}{\sqrt{\omega^2 + \frac{1}{\Lambda_1 + \Lambda_{12}}} \omega^2 + \frac{1}{\Lambda_1 + \Lambda_{12}}} \int \mathrm{d}y \mathrm{d}y' |\phi_2(y)|^2 |\phi_2(y')|^2 (y - y')^2 = \frac{2}{\sqrt{\omega^2 + \frac{1}{\Lambda_1 + \Lambda_{12}}} \omega^2 + \frac{1}{\Lambda_1 + \Lambda_{12}}} + \)

\( (y - y')^2 = \frac{1}{\sqrt{\omega^2 + \frac{1}{\Lambda_1 + \Lambda_{12}}} \omega^2 + \frac{1}{\Lambda_1 + \Lambda_{12}}} \) are used.

References

[1] Myatt C J, Burt E A, Ghrist R W, Cornell E A and Wieman C E 1997 Production of two overlapping Bose–Einstein condensates by sympathetic cooling Phys. Rev. Lett. 78 586
[2] Stamper-Kurn D M, Andrews M R, Chikkatur A P, Inouye S, Miesner H-J, Stenger J and Ketterle W 1998 Optical confinement of a Bose–Einstein condensate Phys. Rev. Lett. 80 2027
[3] Ho T-L and Shenoy V B 1996 Binary mixtures of Bose condensates of Alkali atoms Phys. Rev. Lett. 77 3276
[4] Esry B D, Greene C H, Burke J P Jr and Bohn J L 1997 Hartree–Fock theory for double condensates Phys. Rev. Lett. 78 3594
[5] Pu H and Bigelow N P 1998 Properties of two-species Bose condensates Phys. Rev. Lett. 80 1130
[6] Timmermans E 1998 Phase separation of Bose–Einstein condensates Phys. Rev. Lett. 81 5718
[7] Altman E, Hofstetter W, Demler E and Lukin M D 2003 Phase diagram of two-component bosons on an optical lattice New J. Phys. 5 113
[8] Koklov A B and Svistunov B V 2003 Counterflow superfluidity of two-species ultracold atoms in a commensurate optical lattice Phys. Rev. Lett. 90 100401
[9] Eckardt A, Weiss C and Holthaus M 2004 Ground-state energy and depletions for a dilute binary Bose gas Phys. Rev. A 70 043615
[10] Alon O E, Streltsov A I and Cederbaum L S 2006 Demixing of bosonic mixtures in optical lattices from macroscopic to microscopic Phys. Rev. Lett. 97 230403
[11] Alon O E, Streltsov A I and Cederbaum L S 2007 Multiconfigurational time-dependent Hartree method for mixtures consisting of two types of identical particles Phys. Rev. A 76 062501
[12] Sakhei A R, DuBois J L and Glyde H R 2008 Condensate depletion in two-species Bose gases: A variational quantum Monte Carlo study Phys. Rev. A 77 043627
[13] Oleś B and Sacha K 2008 N-conserving Bogoliubov vacuum of a two-component Bose–Einstein condensate: density fluctuations close to a phase-separation condition J. Phys. A: Math. Gen. 41 145005
[14] Hao Y and Chen S 2009 Density-functional theory of two-component Bose gases in one-dimensional harmonic traps Phys. Rev. A 80 043608
[15] Girardeau M D 2009 Pairing, off-diagonal long-range order, and quantum phase transition in strongly attracting ultracold Bose gas mixtures in tight waveguides Phys. Rev. Lett. 102 245303
[16] Smyrakas J, Bargi S, Kavoulakis G M, Kärkkäinen K and Reimann S 2009 Mixtures of Bose gases confined in a ring potential Phys. Rev. Lett. 103 100404
[17] Girardeau M D and Aastrakarchik G E 2010 Ground state of a mixture of two bosonic Calogero–Sutherland gases with strong odd-wave interspecies attraction Phys. Rev. A 81 043601
[18] Gautam S and Angom D 2010 Ground state geometry of binary condensates in axisymmetric traps J. Phys. B: At. Mol. Opt. Phys. 43 095302
[19] Kronske S, Cao L, Vendrell O and Schmelcher P 2013 Non-equilibrium quantum dynamics of ultracold atomic mixtures: the multi-layer multi-configuration time-dependent Hartree method for bosons New J. Phys. 15 063018
[20] Garcia-March M A and Busch T 2013 Quantum gas mixtures in different correlation regimes Phys. Rev. A 87 063633
[21] Anoshkin K, Wu Z and Zarembo E 2013 Persistent currents in a bosonic mixture in the ring geometry Phys. Rev. A 88 013609
[22] Cao L, Kronske S, Vendrell O and Schmelcher P 2013 The multi-layer multi-configuration time-dependent Hartree method for bosons: theory, implementation, and applications J. Chem. Phys. 139 134103
[23] Peña Ardila L A and Giorgini S 2015 Impurity in a Bose–Einstein condensate: Study of the attractive and repulsive branch using quantum Monte Carlo methods Phys. Rev. A 92 033612
[24] Kröner S, Knörzer J and Schmelcher P 2015 Correlated quantum dynamics of a single atom collisionally coupled to an ultracold finite bosonic ensemble New J. Phys. 17 053001
[25] Petrov D S 2015 Quantum mechanical stabilization of a collapsing Bose–Bose mixture Phys. Rev. Lett. 115 155302
[26] Anapolitanos I, Hott M and Hundertmark D 2017 Derivation of the Hartree equation for compound Bose gases in the mean field limit (arXiv:1702.00827v2 [math-ph])
[27] Lieb E H and Seiringer R 2002 Proof of Bose–Einstein condensation for dilute trapped gases Phys. Rev. Lett. 88 170409
[28] Cohen L and Lee C 1985 Exact reduced density matrices for a model problem J. Math. Phys. 26 3105
[29] Yan J 2003 Harmonic interaction model and its applications in Bose–Einstein condensation J. Stat. Phys. 113 623
[30] Gajda M 2006 Criterion for Bose–Einstein condensation in a harmonic trap in the case with attractive interactions Phys. Rev. A 73 023603
[31] Armstrong J R, Zinner N T, Fedorov D V and Jensen A S 2011 Analytic harmonic approach to the N-body problem J. Phys. B: At. Mol. Opt. Phys. 44 055303
[32] Lode A U J, Sakmann K, Alon O E, Cederbaum L S and Streltsov A I 2012 Numerically exact quantum dynamics of bosons with time-dependent interactions of harmonic type Phys. Rev. A 86 063606
[33] Zaluska-Kotur M A, Gajda M, Orłowski A and Mostowski J 2000 Soluble model of many interacting quantum particles in a trap Phys. Rev. A 61 033613
[34] Schilling C 2013 Natural orbitals and occupation numbers for harmonium: Fermions versus bosons Phys. Rev. A 88 042105
[35] Benavides-Riveros C L, Toranzo I V and Dehesa J S 2014 Entanglement in N-harmonium: bosons and fermions J. Phys. B: At. Mol. Opt. Phys. 47 195503
[36] Armstrong J R, Zinner N T, Fedorov D V and Jensen A S 2012 Virial expansion coefficients in the harmonic approximation Phys. Rev. E 86 021115
[37] Faasshauer E and Lode A U J 2016 Multiconfigurational time-dependent Hartree method for fermions: implementation, exactness, and few-fermion tunneling to open space Phys. Rev. A 93 033635
[38] Hall R L 1979 Some exact solutions to the translation-invariant N-body problem J. Phys. A: Math. Gen. 11 1227
[39] Hall R L 1979 Exact solutions of Schrödinger’s equation for translation-invariant harmonic matter J. Phys. A: Math. Gen. 11 1235
[40] Osachii M S and Muraktanov V V 1991 The system of harmonically interacting particles: an exact solution of the quantum-mechanical problem Int. J. Quantum Chem. 39 173
[41] Armstrong J R, Volosniev A G, Fedorov D V, Jensen A S and Zinner N T 2015 Analytic solutions of topologically disjoint systems J. Phys. A: Math. Gen. 48 085301
[42] Bouvrie P A, Majtey A P, Tichy M C, Dehesa J S and Plastino A R 2014 Entanglement and the Born–Oppenheimer approximation in an exactly solvable quantum many-body system Eur. Phys. J. D 68 346
[43] Kliman S and Cederbaum L S 2014 Overlap of exact and Gross–Pitaevskii wave functions in Bose–Einstein condensates of dilute gases Phys. Rev. A 94 063648
[44] Kliman S, Streltsov A I and Alon O E 2017 Solvable model of a trapped mixture of Bose–Einstein condensates Chem. Phys. 482 362
[45] Kliman S and Alon O E 2015 Variance as a sensitive probe of correlations Phys. Rev. A 91 063613