Effects Beyond Center-of-Mass Separability in a Trapped Bosonic Mixture: Exact Results

O E Alon[1,2] **and L S Cederbaum**[3]

[1] Department of Mathematics, University of Haifa, Haifa, Israel

[2] Haifa Research Center for Theoretical Physics and Astrophysics, University of Haifa, Haifa, Israel

[3] Theoretical Chemistry, Physical Chemistry Institute, Heidelberg University, Heidelberg, Germany

E-mail: `ofir@research.haifa.ac.il`

Abstract.   An exactly solvable model mimicking demixing of two Bose-Einstein condensates at the many-body level of theory is devised. Various properties are expressed in closed form along the demixing pathway and investigated. The connection between the center-of-mass coordinate and in particular the relative center-of-mass coordinate and demixing is explained. The model is also exactly solvable at the mean-field level of theory, allowing thereby comparison between many-body and mean-field properties. Applications are briefly discussed.

1. Introduction

Demixing of Bose-Einstein condensates has drawn an extensive attention and usually studied numerically, either at the mean-field level or at the many-body level of theory, see, e.g., [1-29]. Spatial inhomogeneity makes the problem analytically almost intractable. Here we introduce a solvable model which enables one to emulate demixing, or mixing, of two Bose-Einstein condensates at the many-body as well as at mean-field levels of theory. With a solvable model we can investigate analytically various properties along the pathway of demixing, such as the energetics, spatial overlap of the bosonic clouds, and entanglement between the two species to list a few. To this end, we extend the harmonic-interaction model for mixtures [30-32] to treat demixing. Our work builds on and naturally goes beyond [33-35]. The harmonic-interaction model for bosons, fermions, and mixtures has drawn much attention, see, e.g., [36-51].

2. Theory and Properties

Consider two Bose-Einstein condensates which consist of species 1 and species 2 bosons, respectively. Condensate 1 is placed in an harmonic potential localized at the origin and condensate 2 is held in an harmonic potential centered at a distance L from the first. All

particle-particle interactions are harmonic. The many-particle Hamiltonian hence reads

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

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

$$+ \lambda_1 \sum_{1 \le j < k}^{N_1} (x_j - x_k)^2 + \lambda_2 \sum_{1 \le j < k}^{N_2} (y_j - y_k)^2 + \lambda_{12} \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} (x_j - y_k)^2. \tag{1}$$

Throughout this investigation we work in one spatial dimension and take $\hbar = 1$. There are N_1 bosons of type 1 and N_2 bosons of type 2, the corresponding masses are m_1 and m_2, the intra-species interaction strengths are λ_1 and λ_2, and the inter-species interaction strength is λ_{12}. The total number of bosons is denoted by $N = N_1 + N_2$.

Expressed in terms of the Jacoby coordinates of the mixture, $Q_k = \frac{1}{\sqrt{k(k+1)}} \sum_{j=1}^{k} (x_{k+1} - x_j)$, $1 \le k \le N_1 - 1$; $Q_{N_1 - 1 + k} = \frac{1}{\sqrt{k(k+1)}} \sum_{j=1}^{k} (y_{k+1} - y_j)$, $1 \le k \le N_2 - 1$; $Q_{N-1} = \sqrt{N_1 N_2} \left(X_{N_1} - Y_{N_2} \right)$; and $Q_N = \frac{m_1 N_1}{M} X_{N_1} + \frac{m_2 N_2}{M} Y_{N_2}$, where $X_{N_1} = \frac{1}{N_1} \sum_{j=1}^{N_1} x_j$ and $Y_{N_2} = \frac{1}{N_2} \sum_{j=1}^{N_2} y_j$ are the center-of-mass coordinates of the individual species, the Hamiltonian (1) is diagonalized and takes on the form

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

$$+ \left[-\frac{1}{2M_{12}} \frac{\partial^2}{\partial Q_{N-1}^2} + \frac{1}{2} M_{12} \Omega_{12}^2 \left(Q_{N-1} - Q_{N-1}^0 \right)^2 \right] + \left[-\frac{1}{2M} \frac{\partial^2}{\partial Q_N^2} + \frac{1}{2} M \omega^2 \left(Q_N - Q_N^0 \right)^2 \right] +$$

$$+ \frac{1}{2} \frac{m_1 N_1 m_2 N_2}{M} \omega^2 L^2 \left(1 - \frac{\omega^2}{\Omega_{12}^2} \right), \tag{2}$$

where $M_{12} = \frac{m_1 m_2}{M}$ and $M = N_1 m_1 + N_2 m_2$ are the relative center-of-mass and total masses, respectively. The shifts in the relative center-of-mass and center-of-mass coordinates

$$Q_{N-1}^0 = -\sqrt{N_1 N_2} \frac{\omega^2}{\Omega_{12}^2} L, \qquad Q_N^0 = \frac{m_2 N_2}{M} L \tag{3}$$

emerge from completing the squares but actually govern, as we shall discuss below, the demixing of the two condensates. In particular, unless $L \neq 0$, demixing cannot occur in our model. The specific case $L = 0$, which cannot exhibit demixing, has been analyzed in [32]. Finally, the interaction-dressed frequencies are given by

$$\Omega_{12} = \sqrt{\omega^2 + 2 \left(\frac{N_1}{m_2} + \frac{N_2}{m_1} \right) \lambda_{12}},$$

$$\Omega_1 = \sqrt{\omega^2 + \frac{2}{m_1} (N_1 \lambda_1 + N_2 \lambda_{12})}, \quad \Omega_2 = \sqrt{\omega^2 + \frac{2}{m_2} (N_2 \lambda_2 + N_1 \lambda_{12})} \tag{4}$$

and seen to be independent of L. For attractive inter-species interaction $\frac{\Omega_{12}}{\omega} > 1$ and for repulsive interaction $0 < \frac{\Omega_{12}}{\omega} < 1$. Correspondingly, $|Q_{N-1}^0| \to 0$ with increasing inter-species attraction and $|Q_{N-1}^0| \to \infty$ with increasing repulsion. From a different perspective, for an attractive inter-species interaction the last term in the Hamiltonian (2) and hence the total energy, see below,

decrease as $L \to 0$ whereas for repulsive inter-species interaction the total energy decreases as $L \to \infty$, as is expected for attractive and repulsive forces. The center-of-mass of the mixture is localized at Q_{N-1}^0 independently of any interaction.

With diagonalization of the Hamiltonian (1) to (2), the wavefunction and energy of the ground state are readily given by

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

$$\times e^{-\frac{1}{2}\left\{m_1\Omega_1 \sum_{k=1}^{N_1-1} Q_k^2 + m_2\Omega_2 \sum_{k=N_1}^{N-2} Q_k^2 + M_{12}\Omega_{12}\left[Q_{N-1}-Q_{N-1}^0\right]^2 + M\omega\left[Q_N-Q_N^0\right]^2\right\}} \tag{5}$$

and

$$E = \frac{1}{2}\left[(N_1-1)\sqrt{\omega^2 + \frac{2}{m_1}(N_1\lambda_1 + N_2\lambda_{12})} + (N_2-1)\sqrt{\omega^2 + \frac{2}{m_2}(N_2\lambda_2 + N_1\lambda_{12})} + \right.$$

$$\left. + \sqrt{\omega^2 + 2\left(\frac{N_1}{m_2} + \frac{N_2}{m_1}\right)\lambda_{12}} + \omega + \frac{m_1 N_1 m_2 N_2}{M}\omega^2 L^2\left(1 - \frac{\omega^2}{\Omega_{12}^2}\right)\right]. \tag{6}$$

It is instructive to compare the structures of the wavefunction (5) and energy (6) to the solution of the problem for $L = 0$ [32]. In particular, the center-of-mass and relative center-of-mass are not centered anymore at their origins and a term proportional to L^2 is added to the energy. We shall analyze the implications of these structures shortly.

To translate the wavefunction to the laboratory frame, we plug in the mixture's Jacoby coordinates explicitly into (5). Furthermore, the shifts of the relative center-of-mass and center-of-mass coordinates (3) have to be 'translated' to corresponding coordinates' shifts x_0 and y_0 of the two species in the laboratory frame. Using the inverse relations $X_{N_1} = Q_N + \frac{m_2}{M}\sqrt{\frac{N_2}{N_1}}Q_{N-1}$ and $Y_{N_2} = Q_N - \frac{m_1}{M}\sqrt{\frac{N_1}{N_2}}Q_{N-1}$ the final result for the wavefunction is given by

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

$$\times e^{-\frac{\alpha_1}{2}\sum_{j=1}^{N_1}(x_j-x_0)^2 - \beta_1 \sum_{1 \le j < k}^{N_1}(x_j-x_0)(x_k-x_0)} e^{-\frac{\alpha_1}{2}\sum_{j=1}^{N_2}(y_j-y_0)^2 - \beta_2 \sum_{1 \le j < k}^{N_2}(y_j-y_0)(y_k-y_0)} \times$$

$$\times e^{+\gamma \sum_{j=1}^{N_1}\sum_{k=1}^{N_2}(x_j-x_0)(y_k-y_0)}, \tag{7}$$

where the coefficients α, β, and γ are collected in Appendix A. The shifts of the coordinates in the laboratory frame are given by the expectation values of the individual species' center-of-mass operators

$$x_0 = \langle\Psi|\hat{X}_{N_1}|\Psi\rangle = \frac{m_2 N_2}{M}\left(1 - \frac{\omega^2}{\Omega_{12}^2}\right)L, \quad y_0 = \langle\Psi|\hat{Y}_{N_2}|\Psi\rangle = \left[1 - \frac{m_1 N_1}{M}\left(1 - \frac{\omega^2}{\Omega_{12}^2}\right)\right]L. \tag{8}$$

We can now discuss the meaning of repulsion and attraction between the two condensates which becomes transparent within our model. When $\lambda_{12} = 0$, species 1 is localized at $x_0 = 0$ and species 2 at $y_0 = L$. For repulsive inter-species interaction the two species grow apart: x_0 decreases and y_0 increases; whereas for attractive inter-species interaction the two species come closer together: x_0 increases and y_0 decreases. Side by side, the term added to the energy [last term in (6)] takes on an appealing form as a function of the individual species' center-of-mass expectation values (8),

$$\frac{1}{2}\frac{m_1 N_1 m_2 N_2}{M}\omega^2 L^2\left(1 - \frac{\omega^2}{\Omega_{12}^2}\right) = \frac{1}{2}m_1 N_1 \omega^2 x_0^2 + \frac{1}{2}m_2 N_2 \omega^2 (y_0 - L)^2 + \lambda_{12}N_1 N_2 (x_0 - y_0)^2, \tag{9}$$

also see Appendix B. The added energy term (9) can be interpreted as the 'classical potential energy' of a N_1 particles of mass m_1 shifted by x_0 in a harmonic potential localized at the origin, N_2 particles of mass m_2 shifted by $y_0 - L$ in a harmonic potential localized at L, and the corresponding energy of their mutual harmonic interaction which scales like the square of their distance $(x_0 - y_0)^2$. We emphasis that all terms of the mixture's energy (6), except that originating from the center-of-mass, depend on the inter-species interaction λ_{12} and hence vary along the demixing pathway.

Let us proceed to many-body quantities derived from the many-particle wavefunction of the mixture (7). The all-particle density matrix of the mixture is defined by (here normalized to unity):

$$
\rho_{12}^{(N)}(x_1,\ldots,x_{N_1},y_1,\ldots,y_{N_2},x'_1,\ldots,x'_{N_1},y'_1,\ldots,y'_{N_2}) =
$$
$$
= \left(\frac{m_1\Omega_1}{\pi}\right)^{\frac{N_1-1}{2}} \left(\frac{m_2\Omega_2}{\pi}\right)^{\frac{N_2-1}{2}} \left(\frac{M_{12}\Omega_{12}}{\pi}\right)^{\frac{1}{2}} \left(\frac{M\omega}{\pi}\right)^{\frac{1}{2}} \times
$$
$$
\times e^{-\frac{\alpha_1}{2}\sum_{j=1}^{N_1}\left[(x_j-x_0)^2+(x'_j-x_0)^2\right]-\beta_1\sum_{1\le j<k}^{N_1}\left[(x_j-x_0)(x_k-x_0)+(x'_j-x_0)(x'_k-x_0)\right]} \times
$$
$$
\times e^{-\frac{\alpha_2}{2}\sum_{j=1}^{N_2}\left[(y_j-y_0)^2+(y'_j-y_0)^2\right]-\beta_2\sum_{1\le j<k}^{N_2}\left[(y_j-y_0)(y_k-y_0)+(y'_j-y_0)(y'_k-y_0)\right]} \times
$$
$$
\times e^{+\gamma\sum_{j=1}^{N_1}\sum_{k=1}^{N_2}\left[(x_j-x_0)(y_k-y_0)+(x'_j-x_0)(y'_k-y_0)\right]}.
\tag{10}
$$

The integration of (10) to the intra-species and inter-species reduced density matrices [52] follows the lines of [32, 34] and are not reproduced here. The final results for the lowest-order intra-species and inter-species reduced density matrices are given by

$$
\rho_1^{(1)}(x,x') = N_1\left(\frac{\alpha_1+C_{1,0}}{\pi}\right)^{\frac{1}{2}} e^{-\frac{\alpha_1}{2}\left[(x-x_0)^2+(x'-x_0)^2\right]}e^{-\frac{1}{4}C_{1,0}\left[(x-x_0)+(x'-x_0)\right]^2},
$$

$$
\rho_2^{(1)}(y,y') = N_2\left(\frac{\alpha_1+C'_{0,1}}{\pi}\right)^{\frac{1}{2}} e^{-\frac{\alpha_2}{2}\left[(y-y_0)^2+(y'-y_0)^2\right]}e^{-\frac{1}{4}C'_{0,1}\left[(y-y_0)+(y'-y_0)\right]^2},
$$

$$
\rho_{12}^{(2)}(x,x',y,y') = N_1N_2\left[\frac{(\alpha_1+C_{1,1})(\alpha_2+C'_{1,1})-D_{1,1}^2}{\pi^2}\right]^{\frac{1}{2}} e^{-\frac{\alpha_1}{2}\left[(x-x_0)^2+(x'-x_0)^2\right]} \times
$$
$$
\times e^{-\frac{\alpha_2}{2}\left[(y-y_0)^2+(y'-y_0)^2\right]} \times e^{-\frac{1}{4}C_{1,1}\left[(x-x_0)+(x'-x_0)\right]^2}e^{-\frac{1}{4}C'_{1,1}\left[(y-y_0)+(y'-y_0)\right]^2} \times
$$
$$
\times e^{+\frac{1}{2}D_{1,1}\left[(x-x_0)+(x'-x_0)\right]\left[(y-y_0)+(y'-y_0)\right]}e^{+\frac{1}{2}D'_{1,1}\left[(x-x_0)-(x'-x_0)\right]\left[(y-y_0)-(y'-y_0)\right]},
\tag{11}
$$

where the various coefficients $C_{1,0}$, $C'_{0,1}$, $C_{1,1}$, $C'_{1,1}$, $D_{1,1}$, and $D'_{1,1}$ are results of coupled recursive relations [32] and prescribed in Appendix A. The respective densities, i.e., the diagonals of the reduced density matrices (11), are given by

$$
\rho_1^{(1)}(x) = N_1\left(\frac{\alpha_1+C_{1,0}}{\pi}\right)^{\frac{1}{2}} e^{-(\alpha_1+C_{1,0})(x-x_0)^2},
$$

$$
\rho_2^{(1)}(y) = N_2\left(\frac{\alpha_2+C'_{0,1}}{\pi}\right)^{\frac{1}{2}} e^{-(\alpha_2+C'_{0,1})(y-y_0)^2},
$$

$$
\rho_{12}^{(2)}(x,y) = N_1N_2\left[\frac{(\alpha_1+C_{1,1})(\alpha_2+C'_{1,1})-D_{1,1}^2}{\pi^2}\right]^{\frac{1}{2}} e^{-(\alpha_1+C_{1,1})(x-x_0)^2} \times
$$
$$
\times e^{-(\alpha_2+C'_{1,1})(y-y_0)^2}e^{+2D_{1,1}(x-x_0)(y-y_0)}.
\tag{12}
$$

Clearly, the intra-species densities are localized around x_0 or y_0 whereas the inter-species density is localized both at x_0 and y_0. Since all these many-body quantities are given analytically, we can evaluate them explicitly at each point along the demixing pathway.

The extent to which the two condensates mix along the demixing pathway can be quantified using the spatial overlap between their corresponding densities (12). Explicitly, we consider the overlap of the square roots of the one-particle densities per particle,

$$
S_{12} = \int_{-\infty}^{+\infty} dx \sqrt{\frac{\rho_1^{(1)}(x)}{N_1}} \sqrt{\frac{\rho_2^{(1)}(x)}{N_2}} =
$$

$$
= \left(\frac{\sqrt{(\alpha_1 + C_{1,0})(\alpha_2 + C'_{0,1})}}{\frac{1}{2}[(\alpha_1 + C_{1,0}) + (\alpha_2 + C'_{0,1})]} \right)^{\frac{1}{2}} e^{-\frac{(\alpha_1 + C_{1,0})(\alpha_2 + C'_{0,1})}{2[(\alpha_1 + C_{1,0}) + (\alpha_2 + C'_{0,1})]}(x_0 - y_0)^2} =
$$

$$
= \left(\frac{\sqrt{(\alpha_1 + C_{1,0})(\alpha_2 + C'_{0,1})}}{\frac{1}{2}[(\alpha_1 + C_{1,0}) + (\alpha_2 + C'_{0,1})]} \right)^{\frac{1}{2}} e^{-\frac{(\alpha_1 + C_{1,0})(\alpha_2 + C'_{0,1})}{2[(\alpha_1 + C_{1,0}) + (\alpha_2 + C'_{0,1})]}\frac{\omega^4}{\Omega_{12}^4}L^2}. \tag{13}
$$

Definition (13) seems natural since it reduces to unity when the two densities are equal. Generally, when the distance between the two condensates $y_0 - x_0 = \frac{\omega^2}{\Omega_{12}^2}L$ increases, i.e., for $\frac{\Omega_{12}}{\omega} < 1$, their overlap decreases and vice versa. Of course, expression (13) gives the precise value of the two condensates' overlap as a function of all parameters; the masses, interaction strengths, and the number of particles of each species. Below, we obtain the analogous expression evaluated at the mean-field level of theory, in which the interplay between the intra-species and inter-species interactions can be straightforwardly analyzed.

Let us move to the mean-field solution for demixing which is obtained analytically as follows. The derivation generalizes that in [32, 34, 41]. The Gross-Pitaevskii ansatz for the mixture's wavefunction is

$$
\Phi(x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2}) = \prod_{j=1}^{N_1} \phi_1(x_j) \prod_{k=1}^{N_2} \phi_2(y_k). \tag{14}
$$

The orbitals $\phi_1(x)$ and $\phi_2(y)$ have to be determined self consistently. Sandwiching the many-body Hamiltonian (1) with the mean-field ansatz (14) one gets the Gross-Pitaevskii energy functional. Minimizing the latter with respect to the shapes of the two normalized orbitals $\phi_1(x)$ and $\phi_2(y)$, one obtains the coupled nonlinear integro-differential equations

$$
\left\{ -\frac{1}{2m_1}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m_1\omega^2 x^2 + \Lambda_1 \int dx' |\phi_1(x')|^2 (x - x')^2 + \right.
$$

$$
\left. +\Lambda_{21} \int dy |\phi_2(y)|^2 (x - y)^2 \right\} \phi_1(x) = \mu_1 \phi_1(x),
$$

$$
\left\{ -\frac{1}{2m_2}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m_2\omega^2 (y - L)^2 + \Lambda_2 \int dy' |\phi_2(y')|^2 (y - y')^2 + \right.
$$

$$
\left. +\Lambda_{12} \int dx |\phi_1(x)|^2 (x - y)^2 \right\} \phi_2(y) = \mu_2 \phi_2(y), \tag{15}
$$

where μ_1 and μ_2 stand for the respective chemical potentials and the mean-field interaction parameters are given by $\Lambda_1 = \lambda_1(N_1 - 1)$, $\Lambda_2 = \lambda_1(N_2 - 1)$, $\Lambda_{12} = \lambda_{12}N_1$, and $\Lambda_{21} = \lambda_{12}N_2$.

Recall that within the Gross-Pitaevskii treatment of demixing only the interaction parameters Λ_1, Λ_2, Λ_{12}, and Λ_{21} appear.

The coupled Gross-Pitaevskii equations (15) admit an analytic solution. This is intriguing in itself, as we are not aware of other analytical mean-field solutions for demixing of two spatially-inhomogeneous Bose-Einstein condensates. The final result for the orbitals reads

$$\phi_1(x) = \left(\frac{m_1}{\pi} \sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})} \right)^{\frac{1}{4}} e^{-\frac{m_1}{2}\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})}(x-x_0)^2},$$

$$\phi_2(y) = \left(\frac{m_2}{\pi} \sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})} \right)^{\frac{1}{4}} e^{-\frac{m_2}{2}\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})}(y-y_0)^2}, \tag{16}$$

where further details are collected in Appendix B. Finally, the Gross-Pitaevskii energy of the mixture takes on the following form, expressed as a function of the interaction parameters only:

$$\varepsilon^{GP} = \frac{E^{GP}}{N} = \frac{1}{2} \frac{\Lambda_{12}\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})} + \Lambda_{21}\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})}}{\Lambda_{12} + \Lambda_{21}} +$$

$$+\frac{1}{2}\frac{\Lambda_{12}m_1\omega^2 x_0^2 + \Lambda_{21}m_2\omega^2(y_0 - L)^2}{\Lambda_{12} + \Lambda_{21}} + \frac{\Lambda_{12}\Lambda_{21}(x_0 - y_0)^2}{\Lambda_{12} + \Lambda_{21}}. \tag{17}$$

Indeed, the first line in (17) is the mean-field energy as if the two harmonic traps overlap ($L = 0$), see [32], and the second line is precisely the 'potential-energy-and-interaction' term added at the many-body level of theory to describe the demixing for $L \neq 0$, see (6) and (9).

Let us intermediately summarize. We have put forward an exactly-solvable model for demixing of two Bose-Einstein condensates, whose many-body and mean-field ground-state solutions are given in closed and analytical forms. We can now ask further questions, on energetics, condensation, correlations, and on other properties, first at the many-body level of theory and than at the mean-field level of theory, and investigate the respective differences. From what we have depicted so far above, the model (1) looks sufficiently rich such that a detailed account can only find sufficient room beyond the present paper. We hence proceed with exploration of just two additional selected quantities.

We return to the degree of mixing of the two condensates characterized by their spatial overlap (13), but now at the mean-field level. The Gross-Pitaevskii densities per particle are nothing but $\phi_1^2(x)$ and $\phi_2^2(y)$ [the orbitals (16) are real-valued functions]. Consequently, we readily find

$$S_{12}^{GP} = \int_{-\infty}^{+\infty} dx\, \phi_1(x)\phi_2(x) = \left(\frac{\sqrt{m_1 m_2 \sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})}}\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})}}{\frac{1}{2}\left[m_1\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})} + m_2\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})} \right]} \right)^{\frac{1}{2}} \times$$

$$\times e^{-\frac{m_1 m_2 \sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})}\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})}}{2\left[m_1\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})} + m_2\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})} \right]}(x_0 - y_0)^2}, \tag{18}$$

where $x_0 - y_0 = -\frac{\omega^2}{\Omega_{12}^2}L$ just like in the many-body case, see Appendix B. Equation (18) shows in a transparent manner the dependence of the spatial overlap between the two condensates on the masses, m_1 and m_2, and intra-species Λ_1, Λ_2 and inter-species Λ_{12}, Λ_{21} interaction parameters. One can push the analysis further in the case the parameters of both species are equal, i.e., $m_2 = m_1$, $\Lambda_2 = \Lambda_1$, and $\Lambda_{12} = \Lambda_{21}$. Then, $S_{12}^{GP} = e^{-\frac{m_1}{4}\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})}\frac{\omega^4}{\Omega_{12}^4}L^2}$. For a given intra-species interaction Λ_1, attraction or repulsion, the overlap decreases monotonously with inter-species repulsion and increases monotonously with inter-species attraction. Furthermore, for a

given inter-species interaction Λ_{21}, attraction or repulsion, the overlap increases monotonously with intra-species repulsion and decreases monotonously with intra-species attraction. The latter reflects the common wisdom that it is more difficult to spatially-separate condensates when they are made of repulsive species.

Perhaps, the most obvious difference between the many-body and mean-field wavefunctions of the mixture, equations (7) and (14), respectively, is that in the many-body treatment the two species are entangled whereas in the mean-field description, using the separable product state, the two species are obviously not entangled. Thus, finally, we move to the Schmidt decomposition of the many-body wavefunction, thereby generalizing recent results in the specific case of a symmetric mixture [35]. We begin from and employ Meher's formula which can be written as follows:

$$
\left(\frac{s}{\pi}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\frac{(1+\rho^2)s}{1-\rho^2}\left(x^2+y^2\right)} e^{+\frac{2\rho s}{1-\rho^2}xy} =
$$

$$
= \sum_{n=0}^{\infty} \sqrt{1-\rho^2}\rho^n \frac{1}{\sqrt{2^n n!}} \left(\frac{s}{\pi}\right)^{\frac{1}{4}} H_n(\sqrt{s}x)e^{-\frac{1}{2}sx^2} \frac{1}{\sqrt{2^n n!}} \left(\frac{s}{\pi}\right)^{\frac{1}{4}} H_n(\sqrt{s}y)e^{-\frac{1}{2}sy^2}, \quad (19)
$$

where the parameters $s > 0$, $1 > \rho \geq 0$ for Schmidt decomposition of the wavefunction, and H_n are the Hermite polynomials. The wavefunction (7) is rewritten in terms of the Jacoby coordinates of each of the species, including the shifts of the coordinates x_0 and y_0,

$$
\Psi(\bar{X}_1,\ldots,\bar{X}_{N_1},\bar{Y}_1,\ldots,\bar{Y}_{N_2}) = \left(\frac{m_1\Omega_1}{\pi}\right)^{\frac{N_1-1}{4}} \left(\frac{m_2\Omega_2}{\pi}\right)^{\frac{N_2-1}{4}} \left(\frac{M_{12}\Omega_{12}}{\pi}\right)^{\frac{1}{4}} \left(\frac{M\omega}{\pi}\right)^{\frac{1}{4}} \times
$$

$$
\times e^{-\frac{1}{2}\left(m_1\Omega_1\sum_{k=1}^{N_1-1}\bar{X}_k^2 + m_2\Omega_2\sum_{k=1}^{N_2-1}\bar{Y}_k^2\right)} \times
$$

$$
\times e^{-\frac{1}{2}\left(m_1\frac{m_2 N_2\Omega_{12}+m_1 N_1\omega}{M}\bar{X}_{N_1}^2 + m_2\frac{m_1 N_1\Omega_{12}+m_2 N_2\omega}{M}\bar{Y}_{N_2}^2\right)} e^{+\frac{m_1 m_2\sqrt{N_1 N_2}}{M}(\Omega_{12}-\omega)\bar{X}_{N_1}\bar{Y}_{N_2}}, \quad (20)
$$

where we denote for brevity here and hereafter $\bar{X}_k = \frac{1}{\sqrt{k(k+1)}}\sum_{j=1}^{k}[(x_{k+1}-x_0)-(x_j-x_0)]$, $1 \leq k \leq N_1-1$; $\bar{Y}_k = \frac{1}{\sqrt{k(k+1)}}\sum_{j=1}^{k}[(y_{k+1}-y_0)-(y_j-y_0)]$, $1 \leq k \leq N_2-1$; $\bar{X}_{N_1} = \frac{1}{N_1}\sum_{j=1}^{N_1}(x_j-x_0)$; and $\bar{Y}_{N_2} = \frac{1}{N_2}\sum_{j=1}^{N_2}(y_j-y_0)$. Furthermore, in (20) it is convenient to treat first the case of mixing, i.e., of attractive inter-species interaction $\Omega_{12} > \omega$; the slight modifications in the treatment of demixing, i.e., for repulsive inter-species interaction $\Omega_{12} < \omega$, are put forward below. Clearly, the wavefunction (20) boils down to that of the symmetric mixture when the parameters of species 1 and species 2 bosons are equal and for $L = 0$. On the other hand, unlike the Schmidt decomposition of the symmetric mixture [35] and before Mehler's formula (19) can be applied, equation (20) would require a squeeze mapping of $\bar{X}_{N_1}$ and $\bar{Y}_{N_2}$. Thus, defining

$$
\widetilde{X}_{N_1}^2 \equiv \bar{X}_{N_1}^2 \sqrt{\frac{m_1(m_2 N_2\Omega_{12}+m_1 N_1\omega)}{m_2(m_1 N_1\Omega_{12}+m_2 N_2\omega)}}, \quad \widetilde{Y}_{N_2}^2 \equiv \bar{Y}_{N_2}^2 \sqrt{\frac{m_2(m_1 N_1\Omega_{12}+m_2 N_2\omega)}{m_1(m_2 N_2\Omega_{12}+m_1 N_1\omega)}} \quad (21)
$$

(satisfying $\widetilde{X}_{N_1}\widetilde{Y}_{N_2} = \bar{X}_{N_1}\bar{Y}_{N_2}$), the last row of the wavefunction (20) transforms and reads

$$
e^{-\frac{1}{2}\frac{m_1 m_2\sqrt{N_1 N_2}}{M}\sqrt{(\Omega_{12}+\omega)^2 + \frac{(m_1 N_1 - m_2 N_2)^2}{m_1 N_1 m_2 N_2}\Omega_{12}\omega}\left(\widetilde{X}_{N_1}^2 + \widetilde{Y}_{N_2}^2\right)} e^{+\frac{m_1 m_2\sqrt{N_1 N_2}}{M}(\Omega_{12}-\omega)\widetilde{X}_{N_1}\widetilde{Y}_{N_2}}. \quad (22)
$$

Now, with equation (22), Mehler's formula can be directly applied. The final result for the

Schmidt decomposition reads

$$\Psi(\bar{X}_1,\ldots,\widetilde{X}_{N_1},\bar{Y}_1,\ldots,\widetilde{Y}_{N_2}) = \sum_{n=0}^{\infty} \sqrt{1-\rho^2}\rho^n \Phi_{1,n}(\bar{X}_1,\ldots,\widetilde{X}_{N_1})\Phi_{2,n}(\bar{Y}_1,\ldots,\widetilde{Y}_{N_2}),$$

$$\Phi_{1,n}(\bar{X}_1,\ldots,\widetilde{X}_{N_1}) = \left(\frac{m_1\Omega_1}{\pi}\right)^{\frac{N_1-1}{4}} e^{-\frac{1}{2}m_1\Omega_1\sum_{k=1}^{N_1-1}\bar{X}_k^2} \frac{1}{\sqrt{2^n n!}}\left(\frac{s}{\pi}\right)^{\frac{1}{4}} H_n\left(\sqrt{s}\widetilde{X}_{N_1}\right) e^{-\frac{1}{2}s\widetilde{X}_{N_1}^2},$$

$$\Phi_{2,n}(\bar{Y}_1,\ldots,\widetilde{Y}_{N_2}) = \left(\frac{m_2\Omega_2}{\pi}\right)^{\frac{N_2-1}{4}} e^{-\frac{1}{2}m_2\Omega_2\sum_{k=1}^{N_2-1}\bar{Y}_k^2} \frac{1}{\sqrt{2^n n!}}\left(\frac{s}{\pi}\right)^{\frac{1}{4}} H_n\left(\sqrt{s}\widetilde{Y}_{N_2}\right) e^{-\frac{1}{2}s\widetilde{Y}_{N_2}^2}, \quad (23)$$

where the Schmidt parameters are

$$\rho = \frac{\left[\frac{\sqrt{\left(\frac{\Omega_{12}}{\omega}+1\right)^2 + \frac{(m_1 N_1 - m_2 N_2)^2}{m_1 N_1 m_2 N_2}\frac{\Omega_{12}}{\omega}}+\left(\frac{\Omega_{12}}{\omega}-1\right)}{\sqrt{\left(\frac{\Omega_{12}}{\omega}+1\right)^2 + \frac{(m_1 N_1 - m_2 N_2)^2}{m_1 N_1 m_2 N_2}\frac{\Omega_{12}}{\omega}}-\left(\frac{\Omega_{12}}{\omega}-1\right)}\right]^{+\frac{1}{2}} - 1}{\left[\frac{\sqrt{\left(\frac{\Omega_{12}}{\omega}+1\right)^2 + \frac{(m_1 N_1 - m_2 N_2)^2}{m_1 N_1 m_2 N_2}\frac{\Omega_{12}}{\omega}}+\left(\frac{\Omega_{12}}{\omega}-1\right)}{\sqrt{\left(\frac{\Omega_{12}}{\omega}+1\right)^2 + \frac{(m_1 N_1 - m_2 N_2)^2}{m_1 N_1 m_2 N_2}\frac{\Omega_{12}}{\omega}}-\left(\frac{\Omega_{12}}{\omega}-1\right)}\right]^{+\frac{1}{2}} + 1}, \qquad s = \sqrt{m_1 m_2 \omega \Omega_{12}}. \quad (24)$$

Finally, the case of repulsive inter-species interaction $\Omega_{12} < \omega$ implies the assignments of, e.g., $\bar{Y}_{N_2} \to -\bar{Y}_{N_2}$ in (20) and $\rho \to -\rho$ in (24), similarly to [35].

Equation (24) quantifies precisely as a function of the mixture's parameters the entanglement between the two species along the demixing pathway. It is instrumental to discuss a few limiting cases. Without inter-species interaction, i.e., when $\Omega_{12} = \omega$, one has $\rho = 0$ and the two species are, of course, not entangled; The condensates themselves can possess strong intra-species interactions though. When Ω_{12} is very large (strong inter-species attraction) or very small (strong inter-species repulsion), ρ increases more and more towards unity and a high degree of entanglement emerges. Hence, within our model, a high degree of entanglement accompanies both mixing and demixing. Last but not least, when a very large asymmetry between the two species exists, explicitly, say, $m_1 N_1 \gg m_2 N_2$, ρ decreases more and more towards zero, implying the entanglement diminishes further and further, see in this context the situation for $L = 0$ [31]. As can be expected, for symmetric mixtures and $L = 0$ some of the above-obtained results boil down to those in [35]. This is a suitable place to stop the current investigation.

3. Concluding Remarks
In the present work a solvable model mimicking demixing of two Bose-Einstein condensates at the many-body level of theory is devised and investigated. The wavefunction, energy, reduced density matrices, densities, spatial overlap, and entanglement between the two condensates expressed as the Schmidt decomposition of the many-particle wavefunction are given in closed form along the demixing pathway. The connection between the center-of-mass and in particular relative center-of-mass coordinates and demixing is elucidated, within our model. Furthermore, the model is also solved analytically at the mean-field level of theory, and the above-computed properties are expressed in closed form also at the mean-field level of theory. A short discussion on the differences between properties computed at the many-body and mean-field levels of theory along the demixing pathway is made.

There are several research directions the present investigation can lead to, of which we list the following three. An immediate study would be a comprehensive comparison between many-body and mean-field descriptions of demixing at the limit of an infinite number of particles. Therein, some properties, like the energy per particle and densities per particle, would exactly

coincide and other properties, like variances per particle of many-particle observables and the overlap between the many-body and mean-field wavefunctions, can differ substantially [53-65]. For finite mixtures, the fragmentation [66] along the demixing pathway would be instrumental to follow. Another research venue that is worth pursuing is benchmarking multiconfigurational time-dependent Hartree methods [67-70] and other numerical approaches for bosonic mixtures along the demixing pathway. Finally, a more distant but rewarding challenge would be the emulation and subsequent investigation of many-body effects when scattering attractive bosonic clouds from a potential barrier, or off each other, fully analytically [71-74].

Acknowledgments

Appendix A. Coefficients of the inter-species and intra-species reduced density matrices

It can be shown that the parameters of the wavefunction (7) in the laboratory frame entering the reduced density matrices are those of the wavefunction without the coordinates' shifts x_0 and y_0, and therefore are given by [32]:

$$\alpha_1 = m_1 \Omega_1 + \beta_1, \qquad \beta_1 = m_1 \left[-\Omega_1 \frac{1}{N_1} + (m_2 N_2 \Omega_{12} + m_1 N_1 \omega) \frac{1}{MN_1} \right],$$

$$\alpha_2 = m_2 \Omega_2 + \beta_2, \qquad \beta_2 = m_2 \left[-\Omega_2 \frac{1}{N_2} + (m_1 N_1 \Omega_{12} + m_2 N_2 \omega) \frac{1}{MN_2} \right],$$

$$\gamma = \frac{m_1 m_2}{M} (\Omega_{12} - \omega). \tag{A.1}$$

Correspondingly, since the various integrations of the all-particle density matrix (10) are taken along the variables $(x'_j - x_0) = (x_j - x_0)$ and $(y'_k - y_0) = (y_k - y_0)$, and hence, upon these integrations, the coordinates' shifts x_0 and y_0 can be eliminated, the coefficients of the inter-species reduced density matrix (11) are also those of the corresponding reduced density matrix without coordinates' shifts [32]:

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

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

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

$$D'_{1,1} = \gamma. \tag{A.2}$$

Analogously, the coefficients of the intra-species reduced density matrices (11) are given by [32]:

$$\alpha_1 + C_{1,0} = (\alpha_1 - \beta_1) \frac{[(\alpha_1 - \beta_1) + N_1 \beta_1][(\alpha_2 - \beta_2) + N_2 \beta_2] - \gamma^2 N_1 N_2}{[(\alpha_1 - \beta_1) + (N_1 - 1)\beta_1][(\alpha_2 - \beta_2) + N_2 \beta_2] - \gamma^2 (N_1 - 1) N_2},$$

$$\alpha_2 + C'_{0,1} = (\alpha_2 - \beta_2) \frac{[(\alpha_1 - \beta_1) + N_1 \beta_1][(\alpha_2 - \beta_2) + N_2 \beta_2] - \gamma^2 N_1 N_2}{[(\alpha_2 - \beta_2) + (N_2 - 1)\beta_2][(\alpha_1 - \beta_1) + N_1 \beta_1] - \gamma^2 (N_2 - 1) N_1}. \tag{A.3}$$

Of course, all these coefficients depend explicitly on the masses m_1, m_2, interaction strengths λ_1, λ_2, λ_{12}, and the numbers of particles N_1, N_2, and vary along the demixing pathway.

Appendix B. Further details of the solution of the coupled Gross-Pitaevskii equations and the coordinates' shifts

It is useful to rewrite (15) in terms of shifts of the coordinates x_0 and y_0, which themselves have to be determined explicitly within mean-field theory. Making use of the normalization of $\phi_1(x)$ and $\phi_2(y)$ and that they are even functions with respect to x_0 and y_0 [see the obtained self-consistent solution (16) given in the main text], one finds

$$
\begin{aligned}
&\left\{ -\frac{1}{2m_1}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m_1\omega^2(x-x_0)^2 + \Lambda_1 \int dx' |\phi_1(x')|^2 \left[(x-x_0) - (x'-x_0)\right]^2 + \right. \\
&\left. + \Lambda_{21} \int dy |\phi_2(y)|^2 \left[(x-x_0) - (y-y_0)\right]^2 \right\} \phi_1(x) = \left[\mu_1 - \frac{1}{2}m_1 x_0^2 - \Lambda_{21}(x_0-y_0)^2 \right] \phi_1(x), \\[8pt]
&\left\{ -\frac{1}{2m_2}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m_2\omega^2(y-y_0)^2 + \Lambda_2 \int dy' |\phi_2(y')|^2 \left[(y-y_0) - (y'-y_0)\right]^2 + \right. \\
&\left. + \Lambda_{12} \int dx |\phi_1(x)|^2 \left[(x-x_0) - (y-y_0)\right]^2 \right\} \phi_2(y) = \left[\mu_2 - \frac{1}{2}m_2(y_0-L)^2 - \Lambda_{12}(x_0-y_0)^2 \right] \phi_2(y),
\end{aligned}
$$
(B.1)

where, for the terms linear in $(x-x_0)$ and $(y-y_0)$ to drop out, x_0 and y_0 must obey

$$
\begin{aligned}
m_1\omega^2 x_0 + 2\Lambda_{21}(x_0-y_0) &= 0, \\
m_2\omega^2(y_0-L) - 2\Lambda_{12}(x_0-y_0) &= 0.
\end{aligned}
$$
(B.2)

The solution of the linear system (B.2) is $x_0 = \frac{2\Lambda_{21}}{m_1\Omega_{12}^2}L$ and $y_0 = \left(1 - \frac{2\Lambda_{12}}{m_2\Omega_{12}^2}\right)L$, where $\Omega_{12} = \sqrt{\omega^2 + 2\left(\frac{\Lambda_{12}}{m_2} + \frac{\Lambda_{21}}{m_1}\right)}$, hence $x_0 - y_0 = \left[2\left(\frac{\Lambda_{12}}{m_2} + \frac{\Lambda_{21}}{m_1}\right)\frac{1}{\Omega_{12}^2} - 1\right]L$. These are exactly the same values found within the many-body solution, see (8). Intriguingly, the frequency of the relative center-of-mass Jacoby coordinate in the many-body treatment is obtained (in the mean-field treatment) from re-expressing the mean-field equations using the coordinates' shifts x_0 and y_0.

Consequently, the Gross-Pitaevskii solution for the demixing scenario ($L \neq 0$) can be related to the solution of the coupled equations without the shifts of coordinates ($L = 0$). The self-consistent orbitals are given in the main text, see (16), and the respective chemical potentials read

$$
\begin{aligned}
\mu_1 &= \frac{1}{2}\left(\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})} + \frac{\Lambda_1}{\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})}} + \frac{\Lambda_{21}}{\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})}} \right) + \\
&\quad + \frac{1}{2}m_1 x_0^2 + \Lambda_{21}(x_0-y_0)^2, \\[8pt]
\mu_2 &= \frac{1}{2}\left(\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})} + \frac{\Lambda_2}{\sqrt{\omega^2 + \frac{2}{m_2}(\Lambda_2 + \Lambda_{12})}} + \frac{\Lambda_{12}}{\sqrt{\omega^2 + \frac{2}{m_1}(\Lambda_1 + \Lambda_{21})}} \right) + \\
&\quad + \frac{1}{2}m_2(y_0-L)^2 + \Lambda_{12}(x_0-y_0)^2.
\end{aligned}
$$
(B.3)

The total Gross-Pitaevskii energy (17) for demixing is equivalently obtained from the chemical potentials and the interaction energy, $E^{GP} = N_1\mu_1 + N_2\mu_2 - \frac{N_1}{2}\left[\Lambda_1 \int dx dx' |\phi_1(x)|^2 |\phi_1(x')|^2(x-\right.$

$x')^2 + \Lambda_{21} \int dxdy |\phi_1(x)|^2 |\phi_2(y)|^2 (x - y)^2 \Big] - \frac{N_2}{2} \Big[\Lambda_2 \int dydy' |\phi_2(y)|^2 |\phi_2(y')|^2 (y - y')^2 + \Lambda_{12} \int dxdy |\phi_1(x)|^2 |\phi_2(y)|^2 (x-y)^2 \Big].$

Finally and for completeness, it is instructive to re-express the Hamiltonian in the laboratory frame (1) using the shifts of the coordinates x_0 and y_0,

$$
\begin{aligned}
\hat{H}(x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2}) &= \sum_{j=1}^{N_1} \left[-\frac{1}{2m_1} \frac{\partial^2}{\partial x_j^2} + \frac{1}{2} m_1 \omega^2 (x_j - x_0)^2 \right] + \\
&+ \sum_{j=1}^{N_2} \left[-\frac{1}{2m_2} \frac{\partial^2}{\partial y_j^2} + \frac{1}{2} m_2 \omega^2 (y_j - y_0)^2 \right] + \lambda_1 \sum_{1 \le j < k}^{N_1} [(x_j - x_0) - (x_k - x_0)]^2 + \\
&+ \lambda_2 \sum_{1 \le j < k}^{N_2} [(y_j - y_0) - (y_k - y_0)]^2 + \lambda_{12} \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} [(x_j - x_0) - (y_k - y_0)]^2 + \\
&+ \frac{1}{2} m_1 N_1 \omega^2 x_0^2 + \frac{1}{2} m_2 N_2 \omega^2 (y_0 - L)^2 + \lambda_{12} N_1 N_2 (x_0 - y_0)^2 . \quad \text{(B.4)}
\end{aligned}
$$

Equation (B.4) admits an appealing physical interpretation of demixing and its energetics, within our model, as discussed in the main text.

References

[1] Ho T-L and Shenoy V B 1996 *Phys. Rev. Lett.* **77** 3276
[2] Esry B D, Greene C H, Burke J P Jr and Bohn J L 1997 *Phys. Rev. Lett.* **78** 3594
[3] Pu H and Bigelow N P 1998 *Phys. Rev. Lett.* **80** 1130
[4] Timmermans E 1998 *Phys. Rev. Lett.* **81** 5718
[5] Esry B D and Greene C H 1999 *Phys. Rev. A* **59** 1457
[6] Alon O E, Streltsov A I and Cederbaum L S 2006 *Phys. Rev. Lett.* **97** 230403
[7] Liu X P 2007 *Phys. Rev. A* **76** 053615
[8] Sakhel A R, DuBois J L and Glyde H R 2008 *Phys. Rev. A* **77** 043627
[9] Zöllner S, Meyer H-D and Schmelcher P 2008 *Phys. Rev. A* **78** 013629
[10] Oleś B and Sacha K 2008 *J. Phys. A* **41** 145005
[11] Papp S B, Pino J M and Wieman C E 2008 *Phys. Rev. Lett.* **101** 040402
[12] Navarro R, Carretero-González R and Kevrekidis P G 2009 *Phys. Rev. A* **80** 023613
[13] Hao Y and Chen S 2009 *Phys. Rev. A* **80** 043608
[14] Malet F, Kavoulakis G M and Reimann S M 2010 *Phys. Rev. A* **81** 013630
[15] Girardeau M D and Astrakharchik G E 2010 *Phys. Rev. A* **81** 043601
[16] Gautam S and Angom D 2010 *J. Phys. B* **43** 095302
[17] Mason P and Aftalion A 2011 *Phys. Rev. A* **84** 033611
[18] Sabbatini J, Zurek W H and Davis M J 2011 *Phys. Rev. Lett.* **107** 230402
[19] Wen L, Liu W M, Cai Y, Zhang J M and Hu J 2012 *Phys. Rev. A* **85** 043602
[20] García-March M Á and Busch T 2013 *Phys. Rev. A* **87** 063633
[21] Gautam S and Adhikari S K 2014 *Phys. Rev. A* **90** 043619
[22] Mistakidis S I, Katsimiga G C, Kevrekidis P G and Schmelcher P 2018 *New J. Phys.* **20** 043052
[23] Han J and Tsubota M 2019 *Phys. Rev. A* **99** 033607
[24] Richaud A, Zenesini A and Penna V 2019 *Sci. Rep.* **9** 6908
[25] Richaud A and Penna V 2019 *Phys. Rev. A* **100** 013609
[26] Chen T, Shibata K, Eto Y, Hirano T and Saito H 2019 *Phys. Rev. A* **100** 063610
[27] Sowiński T and García-March M Á 2019 *Rep. Prog. Phys.* **82** 104401
[28] Hejazi S S S, Polo J, Sachdeva R and Busch T 2020 *Phys. Rev. A* **102** 053309
[29] Warner C, Lam A Z, Bigagli N, Liu H C, Stevenson I and Will S 2021 *Phys. Rev. A* **104** 033302
[30] Osadchii M S and Muraktanov V V 1991 *Int. J. Quant. Chem.* **39** 173
[31] Bouvrie P A, Majtey A P, Tichy M C, Dehesa J S and Plastino A R 2014 *Eur. Phys. J. D* **68** 346
[32] Alon O E 2017 *J. Phys. A* **50** 295002
[33] Armstrong J R, Volosniev A G, Fedorov D V, Jensen A S and Zinner N T 2015 *J. Phys. A* **48** 085301
[34] Alon O E 2020 *Entropy* **22** 1342

[35] Alon O E 2021 *Atoms* **9** 92
[36] Pruski S, Maćkowiak J and Missuno O 1972 *Rep. Math. Phys.* **3** 227
[37] Pruski S, Maćkowiak J and Missuno O 1972 *Rep. Math. Phys.* **3** 241
[38] Robinson P D 1977 *J. Chem. Phys.* **66** 3307
[39] Hall R L 1978 *J. Phys. A* **11** 1227
[40] Hall R L 1978 *J. Phys. A* **11** 1235
[41] Cohen L and Lee C 1985 *J. Math. Phys.* **26** 3105
[42] Załuska-Kotur M A, Gajda M, Orłowski A and Mostowski J 2000 *Phys. Rev. A* **61** 033613
[43] Yan J 2003 *J. Stat. Phys.* **113** 623
[44] Gajda M 2006 *Phys. Rev. A* **73** 023603
[45] Armstrong J R, Zinner N T, Fedorov D V and Jensen A S 2011 *J. Phys. B* **44** 055303
[46] Armstrong J R, Zinner N T, Fedorov D V and Jensen A S 2012 *Phys. Rev. E* **86** 021115
[47] Kościk P and Okopińska A 2013 *Few-Body Syst.* **54** 1637
[48] Schilling C 2013 *Phys. Rev. A* **88** 042105
[49] Benavides-Riveros C L, Toranzo I V and Dehesa J S 2014 *J. Phys. B* **47** 195503
[50] Schilling C and Schilling R 2016 *Phys. Rev. A* **93** 021601(R)
[51] Klaiman S, Streltsov A I and Alon O E 2017 *Chem. Phys.* **482** 362
[52] Coleman A J and Yukalov V I 2000 *Reduced Density Matrices: Coulson's Challenge (Lectures Notes in Chemistry vol 72)* (Berlin: Springer)
[53] Castin Y and Dum R 1998 *Phys. Rev. A* **57** 3008
[54] Lieb E H, Seiringer R and Yngvason J 2000 *Phys. Rev. A* **61** 043602
[55] Lieb E H and Seiringer R 2002 *Phys. Rev. Lett.* **88** 170409
[56] Yukalov V I 2011 *Phys. Part. Nucl.* **42** 460
[57] Klaiman S and Alon O E 2015 *Phys. Rev. A* **91** 063613
[58] Klaiman S and Cederbaum L S 2016 *Phys. Rev. A* **94** 063648
[59] Anapolitanos I, Hott M and Hundertmark D 2017 *Rev. Math. Phys.* **29** 1750022
[60] Michelangeli A and Olgiati A 2017 *Anal. Math. Phys.* **7** 377
[61] Cederbaum L S 2017 *Phys. Rev. A* **96** 013615
[62] Klaiman S, Streltsov A I and Alon O E 2018 *J. Phys.: Conf. Ser.* **999** 012013
[63] Sakmann K and Schmiedmayer J 2018 arXiv:1802.03746v2 [cond-mat.quant-gas]
[64] Alon O E 2019 *Symmetry* **11** 1344
[65] Michelangeli A, Nam P T and Olgiati A 2019 *Rev. Math. Phys.* **31** 1950005
[66] Mueller E J, Ho T L, Ueda M and Baym G 2006 *Phys. Rev. A* **74** 033612
[67] Alon O E, Streltsov A I and Cederbaum L S 2007 *Phys. Rev. A* **76** 062501
[68] Krönke S, Cao L, Vendrell O and Schmelcher P 2013 *New J. Phys.* **15** 063018
[69] Cao L, Krönke S, Vendrell O and Schmelcher P 2013 *J. Chem. Phys.* **139** 134103
[70] Lévêque C and Madsen L B 2018 *J. Phys. B* **51** 155302
[71] Weiss C and Castin Y 2009 *Phys. Rev. Lett.* **102** 010403
[72] Streltsov A I, Alon O E and Cederbaum L S 2009 *Phys. Rev. A* **80** 043616
[73] Cederbaum L S, Streltsov A I, Band Y B and Alon O E 2007 *Phys. Rev. Lett.* **98** 110405
[74] Gertjerenken B, Billam T P, Blackley C L, Le Sueur C R, Khaykovich L, Cornish S L and Weiss C 2013 *Phys. Rev. Lett.* **111** 100406