Condensate depletion in two-species Bose gases: A variational Quantum Monte Carlo study

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We investigate two-species Bose gases in traps with various interactions using variational Quantum Monte Carlo (VMC) techniques at zero temperature. The bosons are represented by hard spheres (HS) whose diameter is equivalent to the s-wave scattering length in the low-energy and long-wavelength approximation. We explore the role of repulsive and attractive inter- or intraspecies interactions on the condensate properties of the mixtures, particularly the condensate fraction of each species as compared to the case when each species is in a separate trap of its own. We model the repulsive interactions by a hard core (HC) potential and the attractive interactions by a shallow model potential. The VMC density profiles and energies are evaluated at various interactions and two mass ratios of the species.

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I. INTRODUCTION

The interest in the investigation of two-species Bose-Einstein condensates (2BECs) in traps has grown substantially since their first experimental realization in 1997 [1]. Since then, the literature on 2BECs in traps has exploded [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20] and the interests are now drifting more strongly towards these mixtures [21, 22], which are the major theme of this paper.

In this paper we investigate the role of inter- and intraspecies interactions on the properties of two-species Bose gases (2BEC) in a tight isotropic harmonic trap at zero temperature using variational Quantum Monte Carlo (VMC) methods. A tight trap enables us to simultaneously use a low number of particles and achieve high densities since the volume of the trapped cloud is much smaller than the usual size [23, 24, 25], where $a_{ho} \sim 10^4 \text{Å}$.

Here $a_{ho} = \sqrt{\hbar/m\omega_{ho}}$ is the trap length where $m$ is the mass of the boson, $\omega$ the trapping frequency, and $\hbar$ Planck’s constant. We represent the bosons by hard spheres (HS) whose hard core (HC) diameter is equivalent to the s-wave scattering length in the low-energy and long wavelength approximation. In order to describe the interactions, we use a HS potential for repulsive, and a shallow two-body model potential for attractive interactions. Basing on this, we emphasize the qualitative nature of the present work and deemphasize comparisons with current experiments. The results stand alone as qualitative properties of the model system. A key point in our present research is that we do not use the scattering length in describing attractive interactions as is usually done in mean-field investigations, but rather the depth of a two-body model potential as justified later on. We thus vary the depth of the model potential and HC diameters of the bosons and investigate the resulting properties such as the VMC energies and density distributions. We particularly focus on the VMC condensate fractions and condensate density profiles in an -and to the best of our knowledge- unprecedented manner in the literature concerning mixtures of Bose gases. Another key point here is that we focus on the factors that enhance the condensate depletion of the 2BEC components. We find chiefly that the mixing of two Bose gases in a trap enhances the depletion of the condensates of each gas as compared to the case when either one is in a separate trap of its own. Thus the one-component Bose gas (1BEC) in our paper works chiefly as a reference system to which we compare our mixtures. Further we find that no phase separation can occur in the case of attractive interspecies interactions and that two Bose gases can not be mixed in the case of large repulsive interspecies interactions. Some of our findings are similar to those of Kim and Lee [20] and Shchesnovich et al. [4]. Our work is particularly related to the work of Ma and Pang [17] who did an investigation similar to ours except that they used repulsive interactions only, whereas we additionally use attractive interactions. We further evaluate the energies of the systems and check them against an approximate model calculation.

On the theoretical side, there have been many theories and investigations. For example Kim and Lee [20] examined the stability properties of the ground state of 2BECs as a function of interspecies interactions. One of the ground states that they found had a component localized at the center of the trap surrounded by the other component thereby forming a core and shell. Ho and Shenoy [6] discussed binary mixtures of alkali condensates and found that the heavier of the two components always enters into the interior of the trap and the lighter component is usually pushed towards the edges of the trap. Chui et al. [9] investigated the nonequilibrium spacial phase segregation process of a mixture of alkali BECs. Pu and Bigelow [7] presented theoretical studies of a 2BEC. They showed that a mixed Bose gas displays novel behaviour not found in a pure condensate and that the structure of the density profiles is very much influenced by the interactions.
On the experimental side, there also have been many investigations. For example Modugno et al. [21] reported the realization of a mixture of BECs of two different atomic species using potassium and rubidium by means of sympathetic cooling. Again Modugno et al. [22] reported on the Bose-Einstein condensation of potassium atoms achieved by sympathetically cooling the potassium gas with evaporatively cooled rubidium. Mudrich et al. [23] explored the thermodynamics in a mixture of two different ultracold Bose gases. They showed that a hot gas can be cooled to a lower temperature by mixing it with another colder gas. Maddaloni et al. [30] demonstrated an experimental method for a sensitive and precise investigation of the interaction between two condensates. They studied the effects of interaction by studying two completely overlapping condensates and found that the center-of-mass oscillations of the two condensates are damped if they are interacting and otherwise if they are noninteracting. Matthews et al. [31] presented the experimental realization and imaging of a vortex in a two-component BEC. They induced the vortices by a transition between two spin states by hyperfine splitting of $^{87}$Rb using a two photon microwave pulse. Again Matthews et al. [32] explored the dynamical response of a BEC due to a sudden change in the interaction strength and presented a method for the creation of condensate mixtures using radio frequency and microwave fields. Further they observed an oscillatory behaviour of the condensate sizes when the interactions are changed.

Although the above revealed some of the most important properties of ultracold mixed atomic systems in traps, an investigation of the condensate properties and energies is still missing. For example, what is the role of the hard core (HC) of the atoms in one component in determining the condensate fraction of the other component? In previous publications [23, 31], it has been shown that the hard core (HC) of the bosons plays a fundamental role in depleting the condensate of a one-species Bose gas in a trap. Another issue which has not been addressed before is the role of the mass-ratio of the bosons in a mixture in determining the condensate fractions and we briefly address this issue in this paper.

The paper is organized as follows. In Sec. II we present the method we used. In Sec. III we outline our results and in Sec. IV we discuss them and connect to the previous literature. In Sec. V we list our conclusions and in Appendix A we present a model for the estimation of the energies.

II. METHOD

We consider ultracold two-species Bose gases (2BEC) of $N_1$ and $N_2$ particles, masses $m_1$ and $m_2$, and HC diameters $a_c$ and $b_c$, respectively, confined in a spherically symmetric tight harmonic trap. The total number of particles $N = N_1 + N_2$ is kept fixed and we use small numbers of particles since larger ones increase the computational times substantially. We investigate the 2BECs using variational quantum Monte Carlo (VMC) methods at zero temperature. The program for VMC used in earlier publications [33, 34] and for the one-body-density-matrix (OBDM) [33] has been modified to accomodate 2BECs. We shall not explain the VMC technique as it can be found in a large number of references, rather we present our trial wave function and mention briefly how the particles are moved and how the densities are calculated.

A. Hamiltonian

The Hamiltonian of a two-component Bose gas is

$$H = \sum_{i=1}^{N_1} \left( -\frac{\hbar^2}{2m_1} \nabla^2_{r_1i} + \frac{1}{2}m_1\omega_1^2r_{1i}^2 \right) + \sum_{j=1}^{N_2} \left( -\frac{\hbar^2}{2m_2} \nabla^2_{r_2j} + \frac{1}{2}m_2\omega_2^2r_{2j}^2 \right) + \sum_{i<j} V^{\text{int}}_{11}(|r_{1i} - r_{1j}|) + \sum_{k<l} V^{\text{int}}_{22}(|r_{2k} - r_{2l}|) + \sum_{m,n} V^{\text{int}}_{12}(|r_{1m} - r_{2n}|)$$

(1)

where $m_1$ and $m_2$ are the individual masses of the atoms, $r_{\sigma 1},...,r_{\sigma N_\sigma}$ are the particle position-vectors from the center of the trap of components $\sigma = 1$ and 2, $\omega_1$ and $\omega_2$ are the trapping frequencies, $V^{\text{int}}_{11}$ and $V^{\text{int}}_{22}$ are the intraspecies interactions of species 1 and 2, respectively, and $V^{\text{int}}_{12}$ is the interspecies interaction.

B. Units

We take length and energy in units of the trap $a_{ho} = \sqrt{\hbar/m\omega_{ho}}$ and $\hbar\omega_{ho}$, respectively, where $m = m_1$ and $\omega_{ho} = \omega_1$ are the mass and trapping frequency of component 1, respectively. Using these units ($H \rightarrow H/(\hbar\omega_{ho}) = \tilde{H}$, $r \rightarrow r/a_{ho} = \tilde{r}$), the Hamiltonian (1) can be rewritten in the form

$$\tilde{H} = \frac{1}{2} \sum_{i=1}^{N_1} \left( -\tilde{\nabla}^2_{r_{1i}} + \tilde{r}_{1i}^2 \right) + \frac{1}{2} \sum_{j=1}^{N_2} \left[ -\frac{m_1}{m_2} \tilde{\nabla}^2_{r_{2j}} + \frac{m_2}{m_1} \left( \frac{\omega_2}{\omega_1} \right)^2 \tilde{r}_{2j}^2 \right] + \sum_{i<j} \tilde{V}^{\text{int}}_{11}(\tilde{r}_{1i} - \tilde{r}_{1j}) + \sum_{k<l} \tilde{V}^{\text{int}}_{22}(\tilde{r}_{2k} - \tilde{r}_{2l}) + \sum_{m,n} \tilde{V}^{\text{int}}_{12}(\tilde{r}_{1m} - \tilde{r}_{2n})$$

(2)

thus introducing two ratios $(m_1/m_2)$ and $(m_2\omega_2^2/m_1\omega_1^2)$ into the Hamiltonian.
We model the two-body interactions by using a hard-core square well (HCSW) potential. Essentially, it is a hard core plus an attractive tail added to it. Figure 1 shows our model potential where $V(r)$ is the depth and $r$ the two-body interparticle distance, all in units of the trap. Here for the bosonic HC diameter is $a_c = 0.05$, the depth is $V_0 = -3$, and the range is $d = R - a_c$ which we keep fixed at 0.54. This range is of the same order of magnitude as that used in a previous work [35] for another potential and we return to this point in Sec. IV D. In this paper we are chiefly interested in using the depth of the HCSW to describe the interactions and not the associated scattering length. Nevertheless we check the stability of the systems at the first Feshbach resonance when $a \rightarrow \pm \infty$ in Sec. IV E later on.

### C. HCSW interactions

The general form of the trial wave function is

$$\Psi_T(\{r_1\}, \{\xi_{11}\}, \{\xi_{22}\}, \{\xi_{12}\}) = \prod_{m=1}^{N_1} \prod_{n=1}^{N_2} f_{12}(\{r_{1m} - r_{2n}\}) \times \prod_{\sigma} \prod_{i=1}^{N_\sigma} \prod_{j=1}^{N_\sigma} (1_{\sigma} - \{r_{\sigma i} - r_{\sigma j}\})$$

where $\{r_\sigma\} \equiv \{r_{\sigma 1}, \ldots, r_{\sigma N_\sigma}\}$, $g_\sigma(\xi_{\sigma i})$ are single particle wave functions for particles of type $\sigma = 1, 2$, and $f_{\sigma_1,\sigma_2}$ are pair correlation functions for intraspecies and interspecies interactions with variational parameters given by the sets $\{\xi_{\sigma_1,\sigma_2}\} = \{\beta_{\sigma_1,\sigma_2}, \gamma_{\sigma_1,\sigma_2}, \epsilon_{\sigma_1,\sigma_2}\}$. Here the pairs $\{\sigma_1, \sigma_2\}$ are \{11\} and \{22\} for intra- and \{12\} or \{21\} for interspecies interactions. There can be several choices for the Jastrow functions depending on the interatomic interactions. In our case we constructed a flexible Jastrow function inferred from the exact solution of two particles interacting via a HCSW potential,

$$f_{\sigma_1,\sigma_2}(r_{ij}) = \begin{cases} A_{\sigma_1,\sigma_2} \sin[\gamma_{\sigma_1,\sigma_2}(r_{ij} - a_{\sigma_1,\sigma_2})] & : r_{ij} \leq a_{\sigma_1,\sigma_2} \\ 1 + \beta_{\sigma_1,\sigma_2}^2 \exp[-\epsilon_{\sigma_1,\sigma_2}(r_{ij} - r_{\sigma_1,\sigma_2})^2] & : r_{ij} > r_{\sigma_1,\sigma_2} \end{cases}$$

where $r_{\sigma_1,\sigma_2}$ is the position of the maximum of the Jastrow function and $a_{\sigma_1,\sigma_2}$ is the HC diameter, where $a_{11} = a_c$, $a_{22} = b_c$, and $a_{12} = a_{21} = (a_c + b_c)/2$. The sinusoidal part is taken similar to the exact solution of two particles colliding inside a HCSW with relative energy $E_{\sigma_1,\sigma_2} = \hbar^2 k_{\sigma_1,\sigma_2}^2/(2\mu_{\sigma_1,\sigma_2})$ and HC diameter $a_{\sigma_1,\sigma_2}$ by replacing the HCSW wavevector $K_{\sigma_1,\sigma_2} = \sqrt{2\mu_{\sigma_1,\sigma_2}(V_{\sigma_1,\sigma_2} + E_{\sigma_1,\sigma_2})}/\hbar^2$ for each type of interaction of strength $V_{\sigma_1,\sigma_2}$ by a variational parameter $\gamma_{\sigma_1,\sigma_2}$. This is in order to decouple the Jastrow functions from their HCSWs and to introduce some flexibility to them. Another reason for this replacement is that we do not know the values of $E_{\sigma_1,\sigma_2}$ at the higher densities and we therefore allow $\gamma_{\sigma_1,\sigma_2}$ to vary slightly in order to indirectly imply a value for $E_{\sigma_1,\sigma_2}$. (Here $\mu_{11} = m_1$, $\mu_{22} = m_2$, and $\mu_{12} = m_1 m_2/(m_1 + m_2)$.) In our simulations, the optimized $\gamma_{\sigma_1,\sigma_2}$ are always very close to $K_{\sigma_1,\sigma_2}$ and $\gamma_{\sigma_1,\sigma_2} \geq K_{\sigma_1,\sigma_2}$. Thus attractive interaction between the particles is included in the Jastrow via $\gamma_{\sigma_1,\sigma_2}$. We then join the sinusoidal part at $r_{ij} = r_{\sigma_1,\sigma_2}$ to another function which decays to 1 in the long range. Note then that $r_{\sigma_1,\sigma_2}$ is not necessarily equal to $R_{\sigma_1,\sigma_2}$, the edge of the HCSW for each interaction type, and depending on the well depth it can be either inside or outside the HCSW. The reason for this construction is to provide smooth Jastrow functions whose maxima are at inter-

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**FIG. 1:** HCSW interatomic potential with $a_c = 0.05$, attractive well range $R - a_c = 0.54$ and a potential depth $V_0 = -3$. For $r \leq a_c$, $V(r)$ is infinite. All lengths and energies are in trap units, $a_{ho} = \sqrt{\hbar/m\omega_{ho}}$ and $\hbar\omega_{ho}$, respectively.

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$$V(r) = \begin{cases} V_0 & : r < a_c \\ V_0 - R & : r \geq a_c \end{cases}$$
The particles are moved according to

\[ r_{\sigma}^\prime = r_{\sigma} + \Delta r_{\sigma} \cdot (\eta - 0.5) \]

where \( r_{\sigma}^\prime \) are new positions, \( \eta \) is a random number between 0 and 1 and \( \Delta r_{\sigma} \) are step size vectors which are adjusted to obtain optimal diffusion through configuration space—i.e. to obtain a VMC acceptance rate of \( \approx 50\% \). After each update of the particle coordinates the proposed move is either accepted or rejected according to the (MRT)\(^2\) algorithm where the square of the trial wave-function is used as the probability distribution from which particle configurations are sampled.

**F. Minimization of the variance of the energy**

In order to optimize the trial wavefunction, we numerically minimize the variance of the energy \( \sigma_E \) with respect to the variational parameters of the trial wavefunction.

The variance is given by \( \sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \) where in general for any operator \( O \)

\[
\langle O \rangle = \frac{\int dr_1 dr_2 |\Psi_0|^2 \left( \frac{O \Psi_1}{\Psi_1} \right) |\Psi_1|^2}{\int dr_1 dr_2 |\Psi_0|^2 |\Psi_1|^2} \tag{8}
\]

with \( \Psi_0 = \sum_{\{\psi_1\}} \cdot \prod_{j=1} N_j \int dr_{11} \frac{d^3 r_{12} \cdots d^3 r_{2N}}{|\Psi_0|^2} \) and \( \Psi_1 = \sum_{\{\psi_2\}} \cdot \prod_{j=1} N_j \int dr_{11} \frac{d^3 r_{12} \cdots d^3 r_{2N}}{|\Psi_1|^2} \). Here \( |\Psi_1|^2/|\Psi_0|^2 \) are weights used for the reweighting process of the variational operator \( O \). \( \{\xi_{\sigma_1,\sigma_2}\} \) are the optimized sets of variational parameters. In the Gaussians we also use the initial \( \sigma_0^0 \) and the optimized \( \sigma_0 \).

**G. Condensate fraction**

In the systems considered here we have two condensate fractions \( n_0^{(1)} \) and \( n_0^{(2)} \) for components 1 and 2, respectively. The overall condensate fraction of the mixture is \( n_0^{(1)} N_1 + n_0^{(2)} N_2 \) but we only focus on the individual \( n_0^{(1)} \) and \( n_0^{(2)} \). The condensate fraction of each component is evaluated by calculating the eigenvalues of the natural orbitals using the one-body-density-matrix (OBDM) of each component in a manner similar to a calculation by DuBois and Glyde\(^3\). By using the trial wave function of Sec. \( \Pi \)D we evaluate the OBDM for components 1 and 2, respectively, as follows. In order to make the equations more compact, we define

\[
Q_1(r_{11}, \cdots) = \psi(r_{11}, r_{12}, \cdots, r_{1N_1}, \{\xi_{11}\}; \{\xi_{22}\}; \{\xi_{12}\})
\]

\[
Q_1(r_{11}', \cdots) = \psi(r_{11}', r_{12}, \cdots, r_{1N_1}, \{\xi_{11}\}; \{\xi_{22}\}; \{\xi_{12}\})
\]

\[
Q_2(r_{21}, \cdots) = \psi(r_{11}, r_{21}, r_{22}, \cdots, r_{2N_2}, \{\xi_{22}\}; \{\xi_{12}\})
\]

\[
Q_2(r_{21}', \cdots) = \psi(r_{11}, \{\xi_{11}\}; r_{21}', r_{22}, \cdots, r_{2N_2}, \{\xi_{22}\}; \{\xi_{12}\})
\]

Hence the OBDMs are written

\[
\rho_0(r_{11}, r_{11}') = \prod_{i=1}^{N_1} \int d^3 r_{i1} \prod_{j=1}^{N_2} \int d^3 r_{j1} Q_1(r_{11}, \cdots) Q_1(r_{11}', \cdots) < \psi | \psi >
\tag{9}
\]
leaving out the integration over $r_{11}$ and $r'_{11}$ and

$$\rho_b(r_1, r'_{11}) = \prod_{i=1}^{N_1} d^3r_1_i \prod_{j=2}^{N_2} d^3r_j Q_2(r_1, \cdots) Q_2(r'_{11}, \cdots)$$

where

$$\langle \psi | \psi \rangle = \int dr_1 \int dr_2 |\psi(r_1; \xi_1) \cdot \{\xi_1|; \{\xi_2; \{\{\xi_{12}\}}})|^2,$$

is the normalization factor and $\xi_{1,2}$ are the optimized variational parameters. Hence we extract the OBDM for each component from the two-body density matrix (TBDM) of the mixture by integrating out the contribution from the other component. In a manner similar to Ma and Pang \[17\] then, each component is essentially treated as a subspecies with its own properties but still it is not independent of the other species as a result of the interspecies interactions. The interspecies interactions are included in the OBDM through the interspecies Jastrow function $f_{12}$. From the trial wave function we can verify that Eqs. (9) and (10) reduce to the one-component case if the interspecies interactions are turned off. That is the interspecies Jastrow function $f_{12}$ becomes equal to 1 and the two components become independent of each other as they are now noninteracting.

### A. Stability of the mixtures as compared to one-species Bose gases

During the numerical optimization of the variational parameters as explained in Sec. IIIA we plot the energy $E_{VMC}/N$ versus the set of variational parameters $\{\xi_{1,2}\}$ used in our wave function. The numerical optimization process changes the variational parameters over several iterations and searches for a minimum in the energy variance which also leads to a minimum in the energy. After a number of iterations, we obtain plots such as those shown in the following figures. For example Fig. 2 displays the VMC energy $E_{VMC}/N$ vs one of the variational parameters $\alpha_1$ for a mixture with $a_c = 0.1$, $b_c = 0.2$ and repulsive HC interactions only (upper frame) and for a mixture with $a_c = 0.2$, $b_c = 0.3$, attractive (HCSW, $V_{12} = -10.0$) inter- and repulsive HC interspecies interactions (lower frame). The figure depicts clearly the presence of energy minima at $\alpha_1 \sim 0.25$ and $\sim 2.9$, respectively. The behavior of the energy versus the other variational parameters is the same as in Fig. 2 and all of them display energy minima. After the completion of the optimization process and in the final evaluation of the wavefunction for each system, we choose the variational parameters that correspond to the energy minimum, i.e., the ground state. All of our repulsive or attractive 2BECs display energy minima as above and we can therefore state safely that our mixtures are stable systems.

In comparison, Fig. 3 shows the VMC energy against $\alpha$ for a HCSW 1BEC of 20 particles, HCSW depth $V = -6$ and $a_c = 0.2$ using the same trial wavefunction (3) but set for one component only. The figure shows a peculiar result, namely the presence of two equal energy minima at $\alpha \sim 1.15$ and 1.2, i.e. a degeneracy. One of the minima is due to the single-particle, the other due to the Jastrow part of the trial wavefunction. The single-particle wavefunction is connected to the external trapping potential and the Jastrow function to the interparticle interactions and generates as such the energy minima due to these potentials. This plot has been generated from two VMC runs using different minimization directions \[37\] in order to ensure the presence of the two minima. We have seen this phenomenon in all the VMC runs for this particular system at various other HCSW depths. We do not understand at the present why this double minimum does not occur in 2BECs.

### B. Definitions of the densities

In order to describe the density of the systems, we used $na_b^3$ with $a_b$ the HS diameter of the bosons for component 1 and $nb_b^3$ with $b_b$ the HS diameter for the bosons of component 2. We thus describe the systems by the HC density only, even in the presence of attractive interactions. We define the total VMC spacial density distributions (condensate + normal parts) by $n_1(r)$ and $n_2(r)$ for components 1 and 2, respectively, and in units of $a_{ho}^3$.

### III. RESULTS

In what follows we present the results of our Monte Carlo simulations. We display and discuss the resulting VMC density profiles and the condensate fractions of our mixtures with various interactions. We further compare the condensate fractions of the mixtures with the condensate fractions of their components when either one is in a separate trap of its own. We compare our VMC energies with the results from an approximate mean-field model derived in Appendix A. We further reveal the role of the mass ratio $m_1/m_2$ in determining some properties of the Bose gases. The trapping frequency is set to be the same for both components ($\omega_1 = \omega_2$) and the mass ratio is arbitrarily chosen to be $m_1/m_2 = 1.200$. 

### H. Density profiles

The densities are calculated during a VMC run by dividing the space along the radial direction into spherical shells (bins) concentrated at the center of the trap and collecting the particles of each species in them as was done before by DuBois and Glyde \[33\].
In the interpretation of our results, we sometimes need to
interpretations. The total VMC density of a 1BEC is written
\( n_a(r) \) and \( n_b(r) \) are the VMC condensate density distributions. The total VMC density of a 1BEC is written \( n(r) \).

The goal of this and the following sections is to display the spacial VMC density profiles of 2BECs with various interaction parameters which have largely not been displayed before in the literature. Figure 2 displays the MC density profiles of 2BECs with attractive (HCSW) interspecies and repulsive (HC) intraspecies interactions. The points with error bars represent \( n_T(r) \) of the mixture, the open circles represent the density \( n_1(r) \) and the open triangles \( n_2(r) \). The thick and thin dashed lines are \( n_{0,1}(r) \) and \( n_{0,2}(r) \), respectively. The strength of the interspecies interactions is indicated by the depth of the HCSW, \( |V_{12}| \), and the range of the HCSW is kept fixed at 0.54. In all our mixtures, here and thereon, the components have \( N_1 = 20 \) and \( N_2 = 10 \) particles and in this section \( a_c = 0.2 \) and \( b_c = 0.3 \). There is a particular reason for the choice of the latter large \( a_c \) and \( b_c \) above, this is in order to enable substantial depletion of the condensates. We keep \( a_c \) and \( b_c \) fixed and increase \( V_{12} \) from 0 to −40 in the “negative” sense.

The key features of Fig. 2 are as follows. The attractive forces enable full mixing of the two components. In frame (a) component 2 is slightly pushed out towards the edges of the trap due to the repulsive interspecies interactions arising by setting \( V_{12} = 0 \). That is when the attractive part of the HCSW is switched off, the HCSW changes to a repulsive HC potential. Then we note that although \( V_{12} = 0 \), full mixing of the two components is still possible. At the instant the HCSW is “switched on” as in frame (b), component 2 is pulled back towards the center of the trap with no remnant expulsion at the

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edges of the trap. The densities in frame (b) jump now above those in frame (a) and continue to rise as \( V_{12} \) is increased. In frames (a) and (b) the condensate densities \( n_{0,1}(r) \) and \( n_{0,2}(r) \) are similar in shape to their corresponding total densities \( n_1(r) \) and \( n_2(r) \), but in the rest of the frames (c-f) they are not. Rather they obtain a flat shape in frames (c) and (d) after which they are slightly pushed out towards the edges of the trap in frames (e) and (f). In any case, the attractive forces prevent the condensate from total expulsion towards the edges of the trap. We anticipate that as the density rises further with \( V_{12} \), the condensates will be pushed out further towards the surface of the cloud because the condensate seeks the lower density regimes of the cloud. The reason is because the lower cloud density at the edges of the trap causes a lesser local condensate depletion than the higher density towards the center. Note also that the total densities in frames (a-c) have a Gaussian shape, but then they divert from it somewhat. The densities rise also significantly with the increase of attractive interspecies interactions: \( n_T(r) \) rises by a factor of \( \approx 18 \) from frame (a) to frame (f) as the cloud radius shrinks in size by a factor of \( \approx 3 \).

We are also able to use large attractive interspecies interactions (\( V_{12} = -40 \)) at the energy scale of ultracold Bose gases and still obtain energetically stable systems.

2. Condensate fractions

The goal of this section is to display the effect of complete mixing on the depletion of each condensate in a 2BEC mixture as compared to the case when either condensate is in a separate trap of its own in which case it forms a 1BEC. For this purpose we consider the mixtures in Fig. 4. Figure 4 displays their condensate fractions as a function of \( n a_{HS}^3 \). The open and solid squares represent

**FIG. 4:** VMC density profiles and condensate properties of 2BECs with HCSW inter- and HC intraspecies interactions. \( V_{12} \) is the interspecies HCSW depth. Points with error bars: \( n_T(r) \), open circles and triangles: \( n_1(r) \) and \( n_2(r) \), respectively, thick and thin dashed lines: corresponding \( n_{0,1}(r) \) and \( n_{0,2}(r) \), respectively.
In what follows we investigate the condensate properties of 2BECs, this time with attractive intra- and repulsive interspecies interactions. This is somewhat the opposite case of Sec. III C where attractive inter- and repulsive intraspecies interactions are used. We chiefly aim at revealing the difference in the results when using different types of combinations of repulsive and attractive interactions. Figure 5 compares now the condensate fraction $n_0^{(1)}$ of the 2BEC of Fig. 4 (solid triangles) with HCSW intraspecies interactions (intra.) against $n_0^{(1)}$ of the 2BEC of Fig. 4 (open triangles) with HCSW interspecies interactions (inter.). The open circles display the condensate fraction $n_0$ of a HCSW 1BEC of $N = 20$ particles and $a_c = 0.2$ in a separate trap of its own, this is our reference system. Here the HCSW depth is varied in the range ($V = 0$ to $-16$).

The condensate fraction $n_0^{(1)}$ of the mixture with attractive interspecies interactions (intra.) shows the largest depletion, although the bosons in its shell have a smaller HC diameter than those in the mixture with attractive intraspecies interactions (intra.). It seems that the attractive intraspecies interactions boost the value of the condensate (solid triangles) beyond the HC intraspecies result (open triangles). It will be shown in Sec. III E below that for a number of purely repulsive mixtures with the same bosonic HC diameters in the cores but different HC diameters in the shells, the condensate depletion is larger in the 2BECs with larger bosons in the shell. Our reference shows again the smallest condensate depletion which is again a manifestation of the fact that mixing enhances the condensate depletion beyond the 1BEC result.

Substantial depletion is observed in Fig. 6 at $V_{ii} = -16$ ($\sim 50\%$ for $n_0^{(1)}$ and $\sim 60\%$ for $n_0^{(2)}$). If compared to Fig. 4 we can see that this amount of depletion sets in there at $V_{12} = -15$ (frame e), that is at a comparable (interspecies) HCSW depth. However, the density in the latter ($\sim 11$) is lower than the former ($\sim 14$) because the number of attracting pairs of two-species bosons is smaller in Fig. 4 than in our case here which leads to a slower rise in the density with HCSW depth.

2. Condensate fractions

D. Attractive intra- and repulsive interspecies interactions

1. Density profiles

Figure 5 displays density profiles as in Fig. 4 but with $a_c = 0.2$ and $b_c = 0.4$ with HCSW intra- and HC interspecies interactions ($V_{12} = 0$). We keep $a_c$ and $b_c$ fixed and vary the intraspecies HCSW depths ($V_{ii}$, $i = 1, 2$) in the range $V_{ii} = -4$ to $-16$ keeping $V_{11} = V_{22}$. As a result of the attractive intraspecies interactions, the core and the shell contract in volume and the density of the system grows substantially in response from $nT(0) \sim 2.5$ in frame (a) to $\sim 14$ in (d) as the radius of the cloud shrinks from $\sim 3$ to $1.5$. The shell is pushed radially inwards towards the center of the trap by the confining forces of the trap. Contrary to Fig. 4 the $n_{0,1}(r)$ and $n_{0,2}(r)$ profiles keep following the shape of their corresponding $n_1(r)$ and $n_2(r)$.

E. Repulsive inter- and intraspecies interactions

1. Density profiles

Figure 5 displays the VMC spacial density distributions of HC 2BECs with various interspecies interactions and the same definitions of points as in Fig. 4. Here $a_c$ is varied while $b_c$ is kept fixed at 0.3. We can see that mixing of the two components is enabled up to $a_c = 0.3$ before complete phase-separation sets in. On increasing $a_c$ beyond $b_c$ in frames (a-h), component 1 (of HC $a_c$) is gradually pushed out towards the edges of the trap with
the rise of interspecies repulsion \( (a_c + b_c)/2 \). This is contrary to our expectations because we thought that component 2 (of HC \( b_c \)) would be pushed out instead since it is the lighter of the two given that \( m_1/m_2 = 1.200 \) and \( \omega_1 = \omega_2 \). This can be explained as follows. Essentially, as the HC diameter of the bosons of one component increases, the Bose gas expands in size in order to accommodate the larger bosons. As a result, the component with lower intraspecies repulsion “falls” into the center of the trap seeking the minimization of the total repulsive potential energy. As the HC diameter \( a_c \) is increased, the interspecies repulsion rises pressurizing the core radially towards the center of the trap. As a result, the density of the core \( n_2(0) \) rises by a factor of \( \approx 2 \) from frame (a) to (h) and nearly as from frame (d) on, \( n_1(0) \) begins to approach zero and the two components begin to separate into a shell and a core. If we imagined removing the shell completely from the trap, the core will expand and become almost uniform in density and therefore “flat” in shape \([33, 34]\). We found that it is very hard to “squeeze” the core further to higher density by increasing \( a_c \) beyond 2. In frame (h) total phase separation has occurred leaving a dip at the boundary between the two components. One could imagine placing a third-species particle in that dip as it is a potential trap by itself. Contrary to the case of Figs. 4(d-f), the condensate density distributions of both components follow the shape of their total densities up to phase separation.

With repulsive interactions only in these mixtures, we can always have stable systems if there is sufficient repulsion between the bosons of the core counteracting the outer pressure arising from the shell. Otherwise a dilute
core collapses readily under the heavy pressure of a dense shell.

Figure 8 displays the MC density distributions of a 2BEC with HC interactions only where $a_c$ and $b_c$ are both increased at a fixed ratio $a_c : b_c = 1 : 2$. In this case the density of the core $n_1(0)$ decreases because both $a_c$ and $b_c$ are increased. A peculiar result is that even at very large values of the interspecies repulsions no complete phase separation is observed as it occurs in Fig. 5a. Some uniformity in the density distribution of the core arises at the larger $a_c$.

In Fig. 10 we make comparisons between densities at the center of the trap as a function of the interaction parameter $N_1a_c$ for various systems with repulsive interactions. The crosses are for a HC 1BEC of 20 particles in a separate trap of its own and the same trap length as

![Figure 8](image-url)
before $a_{ho} = \sqrt{\hbar/m_1\omega_1}$. The open circles and triangles are, respectively, for the core in Fig. 8 and an additional mixture with $a_c : b_c = 1 : 3$ whose density profiles we do not reveal. The solid diamonds are for the core in Fig. 9 and an additional mixture with $a_c : b_c = 1 : 2$. Thus the goal is to show the effect of mixing a HC 1BEC with various other 1BECs on the central core density of the system. The density $n(0)$ of the HC 1BEC drops as it is mixed with another component, and for a larger ratio of $b_c$ relative to $a_c$ the core density drops further. The density of the core with one of the HCs fixed ($b_c = 0.3$) varies only slightly as $a_c$ increases. Note that the values of the core density at $r = 0$, except for the latter case, converge at the higher $N_1 a_c$.

FIG. 9: As in Fig. 8 but with the HC diameters both varying at a fixed ratio of $a_c : b_c = 1 : 2$. 

$N_1 = 20 \quad a_c = 0.1$
$N_2 = 10 \quad b_c = 0.2$

$n_0^{(1)} = 95.44\%$
$n_0^{(2)} = 91.93\%$

(a)

$N_1 = 20 \quad a_c = 0.2$
$N_2 = 10 \quad b_c = 0.4$

$n_0^{(1)} = 88.04\%$
$n_0^{(2)} = 80.40\%$

(b)

$N_1 = 20 \quad a_c = 0.3$
$N_2 = 10 \quad b_c = 0.6$

$n_0^{(1)} = 79.27\%$
$n_0^{(2)} = 68.04\%$

(c)

$N_1 = 20 \quad a_c = 0.4$
$N_2 = 10 \quad b_c = 0.8$

$n_0^{(1)} = 70.82\%$
$n_0^{(2)} = 57.56\%$

(d)

$N_1 = 20 \quad a_c = 0.5$
$N_2 = 10 \quad b_c = 1.0$

$n_0^{(1)} = 62.89\%$
$n_0^{(2)} = 48.69\%$

(e)

$N_1 = 20 \quad a_c = 0.6$
$N_2 = 10 \quad b_c = 1.2$

$n_0^{(1)} = 54.32\%$
$n_0^{(2)} = 40.81\%$

(f)

$N_1 = 20 \quad a_c = 0.7$
$N_2 = 10 \quad b_c = 1.4$

$n_0^{(1)} = 48.09\%$
$n_0^{(2)} = 34.84\%$

(g)

$N_1 = 20 \quad a_c = 0.8$
$N_2 = 10 \quad b_c = 1.6$

$n_0^{(1)} = 40.04\%$
$n_0^{(2)} = 28.58\%$

(h)
2. Condensate fraction

Figure 11 compares the condensate fraction \( n_{0}^{(2)} \) of Fig. 8 \((a_{c}: b_{c} = 1 : 2)\) to two other systems. The open circles display \( n_{0} \) for a HC 1BEC of 10 particles in a separate trap of its own and the same trap length as before \( a_{ho} = \sqrt{\hbar/m_{1}\omega_{1}} \). The solid triangles display \( n_{0}^{(2)} \) for the HC 2BEC of Fig. 8 with \( b_{c} \) fixed and \( a_{c} \) varying. The open triangles display \( n_{0}^{(2)} \) for the HCSW 2BEC of Fig. 9 with \( a_{c} \) and \( b_{c} \) varied and \( V_{12} \) varying. We note that the condensate depletion is highest in the HC 2BEC of Fig. 8. The depletion of the condensate in the HCSW 2BEC is less pronounced. This reveals that the repulsive interspecies interactions play a more pronounced role in depleting the condensates of the mixture than attractive interspecies interactions. The attractive interspecies interactions boost the condensate somewhat above the HC-interspecies interactions result. The depletion of the condensate is lowest for a 1BEC. Thus the mixing of condensates enhances their depletion due to the presence of interspecies interactions of various strengths as compared to the case when they are separate, each in a trap of its own.

Figure 12 displays chiefly the condensate fractions of the components as a function of \( n a_{ho}^3 \) at the center of the trap in various HC systems compared to a reference. The open squares represent the condensate fraction \( n_{0} \) of a HC 1BEC of 20 particles \((reference)\). The open triangles represent the condensate fraction \( n_{0}^{(1)} \) of the 2BEC of Fig. 8 where \( a_{c} \) and \( b_{c} \) are varied at a constant ratio of 1:2 and the solid triangles that at a ratio of 1:3, respectively. In addition, and for further comparison, the open and solid circles represent \( n_{0}^{(2)} \) of the latter two mixtures, respectively. We can see that \( n_{0}^{(1)} \) is lower for \( a_{c} : b_{c} = 1 : 3 \) than for 1:2 and the same is true for \( n_{0}^{(2)} \). The latter values of \( n_{0}^{(1)} \) are lower than those of HC 1BEC displayed for comparison. This shows again that mixing and a larger interspecies interaction enhance the depletion of the condensates in each component beyond the 1BEC result.

F. Energies

In this section we compare our VMC energies for HC 2BECs against the energies calculated by an approximate
The estimate that we obtained for the total energy of the mixture \( E^{MFA} \) is given by Eq. (A10) where \( MFA \) stands for mean-field approximation.

Figure 13 displays our VMC energies for the repulsive mixtures investigated in Figs. 9 with \( a_c : b_c = 1 : 2 \) (open triangles) and 8 with \( b_c = 0.3 \) (solid circles). The open diamonds show the additional VMC calculations for HC 2BECs with \( a_c : b_c = 1 : 3 \) similar to Fig. 9. The crosses, times, and open circles display \( E^{MFA} \) for the systems indicated by the open triangles, diamonds, and solid circles, respectively. We note that there is good agreement between the energies \( E^{MFA} \) and the VMC results at the lower \( n a_c^3 \) but then they begin to diverge somewhat at the higher densities. The same is true for \( E_{1:3}^{MFA} \) and \( E_{b_c=0.3}^{MFA} \) largely do not agree with the VMC results but show the same trend in their values. This might be chiefly due to the fact that the TF radius of the core is not a good representation of the cloud radius for this particular case because the two components completely phase-separate at the higher inter-species repulsions. In all cases, the energies rise with the HC densities. The rise is steepest when \( b_c \) is fixed and \( a_c \) varied, the reason being due to the fact that the core density varies slowly with the rise of \( a_c \) (see Fig. 8). That is as the shell is expelled towards the edges of the trap, the potential energy rises faster than the change in \( n_2(0)b_c^3 \) compared to the other systems.

The points are larger than the error bars.

FIG. 13: VMC energies and energies of Eq. (A10) \( (E^{MFA}/N) \) versus the HC density \( n a_c^3 \). Open triangles: mixture in Fig. 9 \( (a_c : b_c = 1 : 2) \), open diamonds: the mixture with \( a_c : b_c = 1 : 3 \), and solid circles: mixture in Fig. 8 \( (b_c = 0.3) \). Crosses, times, and open circles: corresponding estimates \( E^{MFA}/N \) in the same order. The points are larger than the error bars.

G. Effect of mass ratio

In this section we present the role of the mass ratio \( m_{ratio} = m_1/m_2 \) in determining the properties of mixed Bose gases. We consider two mass-ratios, the previous \( m_{ratio} = 1.2 \) and a new \( m_{ratio} = 5 \) and in order to keep the trap length unchanged, we only change \( m_2 \). We further note that changing \( m_{ratio} \) changes the energy of the system since \( m_1/m_2 \) and \( m_2/m_1 \) appear explicitly in the Hamiltonian (2).

We consider the systems depicted in Fig. 9 with \( m_{ratio} = 1.2 \) and compare its properties with those of exactly these same systems evaluated at \( m_{ratio} = 5.0 \). Figure 14 displays the condensate fractions of the latter systems vs \( n a_c^3 \) where the condensate fraction \( n_0^{(1)} \) (and \( n_0^{(2)} \)) is the same for both values of \( m_{ratio} \). Therefore \( m_{ratio} \) has no influence on the relation between condensate fraction and HC density. The scenario is however different if one plots the condensate fractions as a function of the HC interaction parameter \( N_1a_c \) as in Fig. 15. The crosses and open circles show \( n_0^{(1)} \) and the open and solid triangles \( n_0^{(2)} \) each for \( m_{ratio} = 5 \) and 1.2, respectively. We can see that the condensate fractions for \( m_{ratio} = 5 \) are higher than for 1.2 because the central HC densities are lower for 5. Effectively, as \( m_2 \) is reduced to increase \( m_{ratio} \), the trapping forces confining the shell \( -\nabla\cdot\nabla m_2\omega^2r_c^2 \) are reduced accordingly. Thus, the cloud of the mixture expands as the pressure of the shell on the core is lifted causing the central densities to decline in favor of an increase of the condensate fractions. Figure 16 displays \( n a_c^3 \) as a function of \( N_1a_c \) for the latter systems where \( n a_c^3 \) for \( m_{ratio} = 5 \) is lower than for 1.2 at higher \( N_1a_c \) as explained above. As we increase \( m_{ratio} \), the energy of the system rises as demonstrated in Fig. 17 where \( E_{VMC}/N \) is plotted against \( n a_c^3 \) for two \( m_{ratio} \) values and \( a_c : b_c = 1 : 2 \).
IV. DISCUSSION

We discuss now important details on the results of our calculations and connect to the previous literature. We elaborate on the mixing and phase separation of components, stability of the mixtures and the origins of the enhanced condensate depletion. First of all, however, we mention briefly the work of Ma and Pang [17] which is most relevant to ours.

A. The work of Ma and Pang

Ma and Pang [17] investigated HC 2BECs trapped in a three-dimensional isotropic trap at finite temperature using path-integral quantum Monte Carlo simulations. Their main interest was in the structure of the mixtures, i.e., the densities and their profiles. They particularly concentrated on the conditions under which phase separation occurs and treated the two-species system as two subsystems each of which contains one species with its own statistics. However, the two species do not behave independently of each other due to the interspecies interactions. They found that by changing the mass ratio of the components $m_2/m_1$ the lighter particles are pushed outward and form a shell surrounding the heavier core. Further, the density and condensate fractions of the mixture drop with a rise of the interspecies interactions. When identical external potentials are used, no phase separation is observed, but when they are different phase separation occurs. They also found that the spatial phase separation is independent of $m_2/m_1$ and that the species with the larger scattering length favors the formation of a low-density outer shell.

Now in our work here we conducted our calculations at zero temperature and we simulated two-species Bose gases with both attractive and repulsive interactions. We particularly concentrated on the role of the inter- and intraspecies interactions on the enhancement of the condensate depletions in the mixture as compared to the case when each component is in a separate trap of its own. We followed Ma and Pang in treating each component as a subsystem with its own properties. In addition to their investigations on the effect of the mass ratio, we additionally investigated its effect on the energies and condensate fractions.

B. Mixing and demixing

In the case of intercomponent attraction as in Fig. 11, no phase separation occurs because the two gases attract each other. Note that the attractive interspecies interactions at some point overwhelm the repulsive intraspecies interactions as identified by the large increase in the overall density $n_T(r)$ of the system. That is, the repulsive intraspecies interactions do not become attractive, they just get overwhelmed similar to a case discussed by Chui...
and Ryzhov \cite{38}. Further, the two gases are now trapped by the attractive potential of each other such that the importance of the external trap is underplayed. Since in all our calculations the minima of the two confining potentials coincide, the two components interpenetrate completely \cite{12} and are drawn together into what resembles a 1BEC system acting similarly to it. We conclude that in this case, the attractive interspecies interactions play a more pronounced role than the repulsive ones in determining the properties of the systems. Therefore the condensates are able to migrate towards the edges of the trap at the higher densities \( na_\text{HS}^3 \) as in the case of a HC 1BEC \cite{33}. In the somewhat opposite case of Fig. 9 the intercomponent repulsion pushes the condensate of the core towards the center of the trap.

In the case of Figs. 8 and 9 we find chiefly that full mixing is impossible at large repulsive interspecies interactions. Larger interspecies repulsion leads to full phase separation as in Fig. 5a and even though the shell there has a much lower density than the core, substantial depletion \( \sim 20\% \) is still observed which is attributed to the presence of large bosons in the shell. Note that it is hard to define a density \( na_\text{HS}^3 \) for the shell as it is expelled towards the edges of the trap.

An investigation of the detailed nature of the overlap region between the shell and core is also important since it influences properties such as the ground state energy, the excitation spectrum and the collisional relaxation rates as outlined earlier by Barankov \cite{11}. He explored the boundary between two repulsively interacting condensates in the weak and strong separation limits and found that the asymptotic behaviour of each condensate far from the boundary is determined by its correlation (healing) length. In the case of strong separation, he found that there exists a hollow in the total density profile which is very deep. The latter allows the investigation of one-particle excitations at the boundary between the components as well as surface wave excitations due to the surface tension \cite{11}. As a result of the full separation in Fig. 5 we also observe a hollow in the total density profile between shell and core as discussed by Barankov. In the future one could add one foreign particle to be trapped by this hollow and investigate its energy as a function of some property of the mixture using the Monte Carlo method. Such a hollow is however not observed in Fig. 9 because no complete phase-separation occurs. The reason is because as the HC diameters of the bosons in the core are increased, the bosons spread out and the core expands. As a result, these bosons penetrate into the shell which is pushed in the opposite direction towards the center of the trap by the confining forces of the external potential. This is however not the case in Fig. 5 as the HC diameters of the bosons in the core are kept fixed and that of the shell increased. Thus complete phase-separation is only possible when the size of the bosons in only one component is increased. This has also been confirmed by Ma and Pang previously.

Two length scales can be used to characterize a two-component BEC \cite{10}: one is the penetration depth, the other is the healing length. The penetration depth is a measure for the width of the overlap region and, as we can see from above, a function of the interspecies interactions. It is largest in the case of attraction between the two components as it is equal to the radius of the cloud whereas in the case of large intercomponent repulsion it is smaller than the radius of the cloud. The penetration depth is reduced as the intercomponent repulsion rises. Nevertheless, complete mixing is still possible at moderate repulsive interspecies forces as demonstrated in Figs. 8 and 9. Since the density profile of the core in the latter two systems is very much influenced by the presence of a shell, we anticipate that the healing length of a 1BEC changes upon mixing with a shell. In what follows, we discuss some of the previous literature in connection to our current observations.

Shchesnovich et al. \cite{4} studied a \(^{85}\text{Rb}\) and \(^{87}\text{Rb}\) 2BEC by varying the interspecies interactions. They found that these two components would not separate if the interspecies interactions are attractive and in this paper we have verified this point as well. They argued that a separation of the two species takes place when the energy gain due to the attractive intraspecies interactions overwhelms the quantum pressure at the interface of the two species.

Cornell et al. \cite{12} reviewed some early results on mixed condensates and provided a qualitative exegesis of the theoretical and experimental techniques that are involved. They found that there is a critical value for the interaction term \( a_{12} = \sqrt{a_1 a_2} \) beyond which phase separation occurs with little spatial overlap. This is when the scattering length \( a_1 \) of component 1 becomes larger than \( a_2 \) of component 2, causing atoms 1 to move favorably towards the edges of the cloud forming a spherical shell around the core consisting of atoms 2. Our results are in line with those of Cornell et al. \cite{12} and also Hall et al. \cite{14} as we also observe that the component with the larger bosonic hard core diameter migrates to the edges of the trap.

Shi et al. \cite{10} studied the phase separation of two-species trapped and untrapped Bose gases at finite temperature and found that the interspecies interactions affect the formation and depletion of the two condensates and lead to spatial phase-separation of the mixture. They argued that the shell is trapped in an effective potential which has a minimum away from the center of the trap close to the surface of the core. This effective trap is a combination of the traps confining the mixture and the interspecies interactions. According to Shi et al. then, condensation of the shell happens at the surface of the core and indeed we observe a condensate in the shell as displayed in Figs. 8 and Figs. 9.
C. Why do we use a HCSW?

Particularly the HCSW is a suitable potential to describe the attractive interactions between the HS bosons in this work, since it is a HC contact interaction plus an attractive tail added to the HC and the HC diameter is the same as the HS diameter of the bosons. Another reason for choosing the HCSW is to simulate a Feshbach resonance. This is because the HCSW has a well defined range, width, and depth and via these parameters one can easily tune the scattering length to be at the Feshbach resonance using Eq. (11) below when \( a \to \pm \infty \) in order to check any instabilities (or stabilities) arising from this. In terms of designing the trial wave function, the exact solution of the two-body Schrödinger equation interacting via a HCSW lead us in the construction of a flexible Jastrow function for HS bosons with attractive interactions as mentioned in Sec. [11]D.

D. HCSW parameters used

Our main purpose for the choices of the previous values of the HCSW parameters in this work was to provide a qualitative study of the properties of trapped Bose-gas mixtures with attractive interactions and to reach a qualitative understanding of the role of the interatomic interactions in these properties. We first remind the reader that the values of the HC diameters have been chosen to enable substantial depletion of the condensate.

1. Range

The range of the HCSW (\( R = 0.599a_h \)) used in this work is of the same order of magnitude as that used by Astrakharchik et al. [35] for another model potential of the form \( V(r) = -V_0/\cosh^2(r/r_0) \). Here \( r_0 \) determines the range and they set \( r_0 = 0.1a_p \) where \( a_p \) is the transverse oscillatory trap length for a highly elongated trap. Their \( a_p \) is small because of tight confinement along the transverse direction, similarly our \( a_h \) is also considered to be small since we use a tight trap.

2. Depth

We use a shallow HCSW which is much weaker than a realistic interatomic potential [39, 40], drawing our justification from what has been noted before by Gao [41]. He discussed improved interatomic model interactions beyond the HS potential or delta function pseudopotential used in Gross-Pitaevskii theory. These model potentials are simple in a sense that they are shallow and are applicable in quantum few-body and many-body systems.

One of the most important points relevant to our work mentioned by Gao is that a real interatomic potential can simply become unmanageable if used in few-body or many-body calculations. A key conclusion in his paper is that the real potential in a many-body system around the threshold, such as a BEC state, no matter how deep this potential might be, can be replaced by an effective shallow potential that supports only one or two bound states. Gao shows that by using shallow model potentials, much weaker than the real potentials, the results are in good agreement with those using a real interatomic potential.

E. Artificial stability of the mixtures, Feshbach resonance, and negative energies

The HC potentials used in this investigation, whether attractive or repulsive, prevent real collapse and therefore the mixtures are always stable and can not collapse to a singularity. In that sense, we speak of an “artificial stability” [42]. This HC is present in the HCSW potential since upon “switching on” a HCSW one effectively adds to the HC potential an attractive tail, well defined in width and depth. Thus whatever the depth of the HCSW is, the bosons will not be able to approach each other to distances lesser than the HC diameter of the interactions \( (a_c, b_c, (a_c + b_c)/2) \) as imposed by the Jastrow functions. As mentioned in Section [11]D, the Jastrow function of the HCSW has a short-range repulsive and a long-range attractive part. The short-range part of the HCSW Jastrow keeps the bosons at some average distance away from each other, whereas the attractive part tries to bring them closer together. The balance between the repulsive and attractive parts, keeps the system in equilibrium. In the case of repulsive interactions only, the system is primarily balanced by the repulsive HC and the external confining potential.

1. At the Feshbach resonance

If one should increase the HCSW depths to values up to the first Feshbach resonance and beyond, the systems begin to shrink to very high densities. At this stage their energy is mainly potential (negative) and a large fraction of the bosons reside inside the HCSW. However they still show the artificial stability discussed above. For example in Fig. [18] we demonstrate how the stability of a two-species Bose gas of \( N_1 = 20, N_2 = 10 \) particles, \( d = 0.54 \), and HS diameters \( a_c = 0.01, b_c = 0.02 \), respectively, shifts to higher \( \alpha \) values as \( V_{12} \) is increased from shallow to deep values, even up to the first Feshbach resonance at \( V_{12} = -8.462 \) and beyond. The intraspecies interactions are repulsive HCs. The HCSW depth corresponding to a Feshbach resonance is obtained from the condition that \( a \to \pm \infty \), where \( a \) is the s-wave scattering length of the HCSW. And according to Giorgini et al. [43] \( a \) is given by
mixture), \( R_b \) contracted and its density has risen substantially as in Figs. 2, 3, and 18. The liquid density is set by the range of values of the scattering length and potential depth. This of the Bose gas since when the energy becomes negative, there is a cost in kinetic energy increase if the bosons move closer together. Thus the density of the liquid saturates eventually to a value set by the range of the HCSW (and less so by the HC diameter).

There is a large energy release on condensation of the Bose gas to the dense liquid state. In Fig.18 we show how the energy drops from \( E/N \approx 1.6 \) at \( V_{12} = 0 \) to \( E/N \approx -90 \) at \( V_{12} = -10.0 \). Thus energy is released at a degree that is proportional to the well depth \( V \). Upon condensation, there is substantial depletion of the condensate so that a large percentage of the atoms lie in states above the condensate. Thus the condensation process is characterized by large increase in the density of the system, a large drop in the energy of the system until there is a large release of condensation, and a substantial depletion of the condensate.

\[ a = R_c + (R - R_c) \left\{ 1 - \frac{\tan[K_0(R - R_c)]}{K_0(R - R_c)} \right\}, \tag{11} \]

where \( R_c \) is the HC diameter (in our case \( a_c \) for component 1, \( b_c \) for component 2, or \( (a_c + b_c)/2 \) for the mixture), \( R \) the edge, and \( K_0 = \sqrt{\omega_0 m/\hbar^2} \) the wave vector of the HCSW. In trap units \( R_c \to R_c/\omega_0 = \bar{R}_c \) and similarly for \( R, \tilde{V}_0 \to V_0/\omega_0 = \bar{V}_0 \), and thus \( K_0 \to \sqrt{\bar{V}_0 \omega_0 m/\hbar^2} = \bar{K}_0 \).

In Fig.18 at \( V_{12} = -10 \) the wave function is very much contracted and its density has risen substantially as indicated by a large Gaussian variational parameter \( \sim 10 \). Note that one still obtains a deep negative energy minimum at the first Feshbach resonance manifesting the strong stabilizing factor of the HCs. Thus even if we reach the Feshbach resonance and surpass it while varying the HCSW depth, the systems remain artificially stable. Going back to the previous Fig.14 for example, we crossed a Feshbach resonance while increasing \( V \), but no sharp density profile indicative of a collapse can be seen. In the next section, we shall explain the occurrence of the negative energies to be the result of a liquefaction process of the Bose gas since when the energy becomes negative, energy is released from the system.

2. Liquefaction of Bose gases (negative energies)

The bosons can condense to a dense liquid at critical values of the scattering length and potential depth. This is signified by the occurrence of negative energies as in Figs.14 and 18. The liquid density is set by the range of the attractive well since there is a large energy incentive for a boson to lie in the attractive well of its neighbours but no further potential energy incentive to lie closer than that. There is a cost in kinetic energy increase if the bosons move closer together. Thus the density of the liquid saturates eventually to a value set by the range of the HCSW (and less so by the HC diameter).

In this section we explore possible reasons for the enhanced depletion of the condensates in the mixtures. We believe that due to mixing the reduction in free volume between the HS bosons available for condensate formation in each species is a common ground for enhanced depletion in all types of mixtures. The magnitude of reduction in free volume varies however with the types and strengths of interactions. As the free volume between the HS bosons decreases, the probability for relocating a boson at a certain site, say \( r_1 \) and energy \( \epsilon_0 \) to another location at \( r_1' \) and the same energy \( \epsilon_0 \) is reduced. This is because the chance of finding a site between the bosons large enough to accommodate a boson becomes lower.

Going back to Fig.7 then, the reason the mixtures with interspecies attraction (Fig.6) indicated by (inter.) show a larger depletion for component 1 (with HC \( a_c \)) than the mixtures with interspecies repulsion (Fig.5) indicated by (intra.) is because the former are completely mixed as compared to partial mixing of the latter. In the case of complete mixing the available volume for condensate formation is severely reduced and smaller than the case of partial mixing. Further, since both components in Fig.6 are localized at the center of the trap, they contribute to their mutual condensate depletion where the density is highest, namely at the center of the trap. In the case of partial mixing the shell contributes to the depletion chiefly at the edges of the trap and does not influence the condensate at the center of the trap very much. There could also be other reasons that explain the enhancement in the depletion.

The scenario is however different for component 2. In Fig.11 the depletion is larger for the 2BEC with interspecies repulsion (Fig.3) than the 2BEC with interspecies attraction (Fig.4). The reason may be because the boson sizes \( a_c \) of the HC 2BEC are increased far above those of the HCSW 2BEC which remain fixed thus outweighing the role of the HCSW in the depletion (free-volume reduction).
G. Ground state solutions

Trippenbach et al. \cite{16} identified all possible classes of solutions for 2BECs and found that, in the case of isotropic harmonic trapping potentials, many spherically-symmetric phase-separated geometries are possible. In addition, symmetry breaking solutions do exist but within the TF approximation the ground state cannot be one with broken symmetry. Similarly, our mixtures are spherically symmetric in their ground states.

V. CONCLUSIONS

In summary then, we have investigated the effect of intra- and interspecies interactions on the properties of ultracold 2BECs in tight harmonic traps using VMC. The repulsive inter- or intraspecies interactions were modelled by a HC contact potential, the radius of which being equivalent to the s-wave scattering length in the low-energy and long-wavelength approximation. The attractive interactions were modelled by a HC repulsive part plus a shallow attractive well, the HCSW. We did not describe the attractive interactions by the HCSW scattering length $a$, but rather the depth of the HCSW in order to avoid the large fluctuations in the value of $a$. We calculated the energies, density distributions and condensate density distributions. We further obtained the condensate fractions of the components from the OB-DMs. A key point is that we chiefly focused on the role of interactions in enhancing the condensate depletion of each component in a mixture as compared to the case when each component is in a separate trap of its own. To the best of our knowledge, this has not been done in the previous literature on mixed Bose gases up to this date. We present novel physics associated with the effect of intra- and interspecies interactions on the condensate properties of mixed Bose gases. We find that:

a) the mixing of two Bose gases in a trap enhances the condensate depletion of each gas as compared to the case when either one is in a separate trap of its own. In both cases of attractive and repulsive interactions the reduction in the available volume for condensate formation due to mixing plays a key role in the enhancement of the depletion. In the case of attractive interspecies interaction the enhanced depletion may be further driven by the liquefaction of the Bose gases at the higher densities and the release of energy.

b) when the condensates are phase separated due to strong repulsive interspecies interactions, the core remains stable and is not “squeezed” substantially by the shell. Complete mixing is still possible up to some repulsion threshold.

c) according to Refs. \cite{16}, our mixtures are stable because they are spherically symmetric.

d) we anticipate that the healing length of a 1BEC changes upon mixing it with a second component into the system.

e) in the case of complete phase-separation, although the density of the shell is much smaller than the core, substantial depletion is still observed in the shell triggered by the presence of large bosons in the shell.

f) in the case of intercomponent attraction a 2BEC behaves similarly to a 1BEC as the two components are completely mixed and allow the condensates of either component to migrate towards the edges of the trap at the higher densities. This is contrary to the somewhat opposite case of repulsive interspecies interactions where the condensate of the core is pushed back towards the center of the trap.

g) finally the HC potentials provide a strong stabilizing mechanism for the Bose gases with attractive interactions.

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APPENDIX A: MEAN-FIELD MODEL FOR THE ESTIMATION OF THE MIXTURE-ENERGIES

We consider two mixed Bose gases of $N_1$ and $N_2$ particles, HC diameters $a_1$ and $a_2$, and bosonic masses $m_1$ and $m_2$, respectively, where initially the interspecies interactions are set to zero. That means the two Bose gases are initially independent of each other and both of them are concentric spheres at the trap center. We then construct a rough model that describes the energy of a boson-boson mixture by using the following assumptions. In our estimate for the energies, we derive our concepts from a paper by Ao and Chui \cite{15} who gave a simplified expression for the total energy of an inhomogeneous binary Bose gas,

\[
E = \frac{1}{2} \left( G_{11} \frac{N_1^2}{V} + G_{22} \frac{N_2^2}{V} + \sqrt{G_{11}G_{22}} \cdot \frac{N_1N_2}{V} \right)
\]

(A1)

where $G_{ij} = 4\pi\hbar^2a_{ij}/m_{ij}$ are the interaction parameters, $a_{12}$ the inter- and $a_{ii}$ the intraspecies s-wave scattering lengths, $m_{ii}$ the mass of a boson in one component and $m_{12}$ the reduced mass and $V$ is the volume of the gas. This expression neglects the kinetic energy (quantum pressure) of each component. We modify this expression by replacing the first two terms on the right-hand-side by the Thomas-Fermi (TF) energy of each component. We use trap units in terms of component 1, i.e.
the shell is becomes a shell. An estimate for the potential energy of gains additional potential energy beyond the interspecies interactions. As a result, component 2 shell formed at the edges of the trap after switching on an approximate potential energy for the particles of the components are localized at the center of the trap and its initial TF energy when both mutually noninteracting late its energy, we therefore assume a superposition of the cloud in largely determined by the core in the case that of component 2. The TF radius of component 1 is \[ R_{TF,1} = (15N_1 a_c)^{1/5} \] and that of component 2 \[ R_{TF,2} = (15N_2 b_c)^{1/5} \]. 

Imagine now switching the interspecies interactions on such that the Bose gas with the larger HC diameter is expelled towards the edges of the trap and forms a shell. The shell would then lie approximately at the TF radius of the core away from the center of the trap. The volume of the cloud is then approximately \( V = 4\pi R_{TF,1}^3/3 \) if \( a_c < b_c \) and \( 4\pi R_{TF,2}^3/3 \) if \( a_c > b_c \). Thus the size of the cloud in largely determined by the core in the case of moderate repulsive interactions. In order to calculate its energy, we therefore assume a superposition of its initial TF energy when both mutually noninteracting components are localized at the center of the trap and an approximate potential energy for the particles of the shell formed at the edges of the trap after switching on the interspecies interactions. As a result, component 2 gains additional potential energy beyond \( E_{TF,2} \) when it becomes a shell. An estimate for the potential energy of the shell is

\[
E_{trap} = \frac{1}{2} N_1 m_1 \omega_{ho}^2 R_{TF,2}^2 / \hbar \omega_{ho} = \frac{1}{2} N_1 \left( \frac{m_1}{m_2} \right)^{4/5} (15N_2 b_c)^{2/5} \] (A5)

if component 1 forms a shell and

\[
E_{trap} = \frac{1}{2} N_2 m_2 \omega_{ho}^2 R_{TF,1}^2 / \hbar \omega_{ho} = \frac{1}{2} N_2 \left( \frac{m_2}{m_1} \right) (15N_1 a_c)^{2/5} \] (A6)

if component 2 forms a shell. That is we used

\[
\sum_{i=1}^{N_1} m_1 r_{1i}^2 = \langle r_1^2 \rangle \approx R_{TF,2}^2 \] (A7)

and

\[
\sum_{i=1}^{N_2} m_2 r_{2i}^2 = \langle r_2^2 \rangle \approx R_{TF,1}^2 \] (A8)

in estimating the radius of gyration of the core. Note that \( \sum_{k=1}^{N_k} m_k = N_k m_k \) \((k = 1 \text{ or } 2)\) is the total mass of either component as all the particles in a component have the same mass. The interspecies interactions can be calculated according to [A1]

\[
E_{int} = \sqrt{G_{11}G_{22}} \frac{N_1 N_2}{V} \] (A9)

Gathering all the previous terms together, the total energy of the mixture is then

\[
E^{MFA} \cdot (N_1 + N_2) \approx \frac{5}{15} \left[ N_1 (15N_1 a_c)^{2/5} + N_2 (15N_2 b_c)^{2/5} (m_2/m_1)^{1/5} \right] + 3[a_c b_c (m_1/m_2)]^{1/2} \cdot N_1 N_2 \left\{ \begin{array}{ll}
R_{TF,1}^{-3} : & a_c < b_c \\
R_{TF,2}^{-5} : & a_c > b_c 
\end{array} \right.
\] (A10)

where as a reminder \( \omega_1 = \omega_2 \).

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