The rich physics of multi-species boson mixtures has attracted much attention since the first realization of the coexistence of the double condensates from two different spin states $|F = 2, m = 2\rangle$ and $|F = 1, m = -1\rangle$ of $^{87}\text{Rb}$ [1]. Some interesting properties, such as the stability of condensates, phase separation, and symmetry breaking, have been investigated both experimentally [1, 2] and theoretically [3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. It was found that $^{87}\text{Rb}$ in two hyperfine states can form two separate condensates with a spatial overlap [1] and this overlapping region can be adjusted by tuning the interspecies interaction. Theoretical studies including both the Thomas–Fermi approximation and numerical solutions of the Gross–Pitaevskii equation [3, 4, 7, 12] have also found that two overlapping condensates can be separated into a core at the trap center and a surrounding shell. This phase separation can be achieved by changing the interspecies interaction, the total number of particles, and the symmetry of the trapping potential. It is suggested that the system may become unstable for certain interaction strength [1], which may lead to a spontaneous symmetry breaking spatially [3, 12].

Most of the early theoretical efforts mentioned above only give the properties of condensates at zero temperature. In this Letter, we study a two-species hard-core boson system in a three-dimensional isotropic harmonic trap through the path-integral quantum Monte Carlo simulation, which allows us to probe such a system at finite temperature. Here we concentrate on the conditions under which the phase separation occurs.

The path-integral quantum Monte Carlo method has been successfully applied to the one-species boson systems in traps [13]. It provides the exact solution of a many-body system within a controllable variance. The total energy, density profile, specific heat, condensation fraction, and other quantities can all be evaluated [13].

The system considered here consists of two types of particles, marked as species 1 and species 2, respectively, with total particle numbers $N_1$ and $N_2$ and particle masses $m_1$ and $m_2$. For a realistic system, these two types of particles can be different elements, two different isotopes of the same element, or two different hyperfine states of identical atoms. The interactions between two like and unlike atoms are characterized by the s-wave scattering lengths $a_{11}$, $a_{22}$, and $a_{12}$. In the model studied here, $a_{11}$ and $a_{22}$ are the hard-core diameters of the particles in species 1 and 2, respectively, and $a_{12} = (a_{11} + a_{22})/2$.

The Hamiltonian for the system of $N = N_1 + N_2$ particles is given by

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \sum_{j > k = 1}^{N} V_{jk},$$

(1)

where

$$\mathcal{H}_i = -\frac{\hbar^2}{2m_i} \sum_{l=1}^{N_i} \nabla_l^2 + \sum_{l=1}^{N_i} U_i(r_l)$$

(2)

is the Hamiltonian of the noninteracting system of the $i$th species under the spherically symmetric trapping potential $U_i(r) = k_i r^2/2 = m_i \omega_i^2 r^2/2$. The interaction between any two particles $V_{jk}$ is assumed to be a hard-core potential.

The algorithm applied to the one-species systems [13] is generalized to study the two-species system here. We treat the two-species system as two subsystems, each of which contains one species and follows its own statistics. The permutations are only performed among the identical particles during a simulation. However, these two subsystems do not behave independently because of the interspecies interaction. The Monte Carlo steps are influenced by the interactions among all the particles as well as the permutations of the particles in each species.

In order to calculate the density profile, we divide the space into small shells along the radial direction. We choose the interval between two shells such that after averaging over a large number of Monte Carlo steps on the order of $10^6$, the finite-size error diminishes in comparison with the statistical error. The spatial density $\rho_i(r)$ can then be obtained by counting the number of particles from each species in a given shell. The normalization relation $\int \rho_i(r) \, d\mathbf{r} = N_i$ is used to check the...
convergence. For convenience, we use the dimensionless units with $\hbar = m_1 = \omega_1 = 1$.

We start the simulation with two species with an identical mass, hard-core radius, and total particle number to verify that the condensation does occur below a certain temperature. The two condensates show different critical temperatures as we change the ratios $a_{11}/a_{22}$ and $m_2/m_1$. The stronger the interaction is, the lower the critical temperature. The condensation favors the lighter particles because a heavier particle system has a lower critical temperature, which agrees well with the available experimental results.

Our main interest here is on the structures of the mixtures. We calculate the densities of two condensates at various parameters at temperature $T/T_0 = 0.1$ when both the species have undergone Bose–Einstein condensation. Here $T_0$ is the condensation/critical temperature under the mean-field approximation for species $1$ with a total number of particles $N$. The mixtures possess two distinct structures depending on the relationship between the external potentials on the two species. We have examined two cases, one with an equal energy spacing in the single-particle spectra and another with an identical external potential. We will elucidate the results for both cases.

We first consider the case with the same energy spacing in the single-particle spectra, that is, $\omega_1 = \omega_2$. Two identical condensates are found when $m_2/m_1 = 1$, $N_2/N_1 = 1$, and $a_{11}/a_{22} = 1$, as shown in Fig. 1(a). Comparing with the mean-field result on the one-species condensate, the double condensates in our simulation display the same expansion as $N a_{jk}$ is increased from $2$ to $40$.

In order to separate the two overlapped condensates, we perform simulations with various parameters $m_2/m_1$, $a_{11} = a_{22}$, and $N_2 = N_1$, respectively. Figures 1(a)–(i) show the density profiles of the two species in the system of these cases. There are two significant features in the density profiles as $m_2/m_1$ is increased from $1$ to $4$, as shown in Figs. 1(a)–(c): The heavier species remains to be concentrated at the central area of the trap while the lighter particles are pushed outward and finally form an outer shell surrounding the heavier species.

The interaction dependence of the density profiles is given in Figs. 1(d)–(f). The interaction strength can dramatically affect the particle distribution. Here we show the results for the same number of particles in each species with $m_2/m_1 = 4$. The densities of both the species at the trap center decrease as the interaction strength is increased from $a_{ij} = 0.15$ to $0.3$. However, under a stronger interaction strength, the lighter particles are pushed out further away from the trap center. Heavier particles spread out with a less distance.

Figures 1(g)–(i) show the changes in the density distribution as the total number of particles increases from $200$ to $1600$ while keeping $N_2 = N_1$, $m_2/m_1 = 4$, and $a_{11} = a_{22} = 0.15$. The two condensates are always in partial overlap but with more the lighter particles going outward with a larger $N$. This means that when more particles are trapped in an experiment, the heavier particles can be caged inside the light particles with both the species forming condensates at the low energy levels of the single-particle spectra.

The condensation fraction in a species can be determined by counting the particles on the permutation rings. We have evaluated the condensation fractions for each species in the system with parameters shown in Fig. 1 and find them in the range of $0.8$–$0.95$. This means that a reasonable fraction of particles is not in phase coherence with the rest in that species. Furthermore, particles can accumulate in any single-particle state, for example, the first excited state, to form a condensate. In fact, in certain parameter regions, the particles can be completely driven out of the single-particle ground state by strong correlation.

To have a better picture of whether a particle is in its single-particle ground state or not, we further decompose the density of each species into that of the single-particle ground state and the corresponding excited states in Fig. 2.

We show here the percentages of the particles in each species in the single-particle ground states at different in-

![Figure 1: Density profiles of the double condensates with various parameters at $T/T_0 = 0.1$ and with $N_1 = N_2$. (a)–(c) show the changes of the density profiles at different mass ratios but with $N = 200$ and $a_{11} = a_{22} = 0.4$. (d)–(e) show the cases at different interaction strengths with $m_2/m_1 = 4$ and $N = 200$. (g)–(i) show the dependence of the total particle number with $m_2/m_1 = 4$ and $a_{11} = a_{22} = 0.1$.](image-url)
cause when one species is pushed away from the central area of the trap by the correlation, the particles in both the species are also driven away from the single-particle ground states by the same force. The distribution of the particles in the energy space is strongly influenced by the energy spacing and the scattering lengths. Therefore, no significant separation between the two species can happen in the energy space when $\omega_1 = \omega_2$ and $a_{11} = a_{22}$.

So far we have shown that the lighter particles can form an outer shell surrounding the heavier particles. A mass ratio far away from 1, strong interaction, and large number of particles are all the contributing factors for the particles to accumulate in the higher single-particle energy states and to cause a spatial separation between the two species. However, the structure of a mixture turns out to be very different if the external trapping potentials on the two species are different from those with $\omega_1 = \omega_2$. Let us consider the case with an identical external potential, that is, with $k_1 = m_1 \omega_1^2 = k_2 = m_2 \omega_2^2$. In Fig. (c) we compare the results under different external potentials. The percentage indicates the fraction of particles in the single-particle ground state. The simulation result shown in Fig. (c) under an identical external potential does not have any significant phase separation even though most particles are pushed out of the single-particle ground states. While keeping the same energy spacing, the spatial phase separation between the two species is obvious, as shown in Fig. (b).

More interestingly, the roles of the heavier and lighter species can be reversed under the identical potential case with the heavier particles forming an outer shell surrounding the lighter particles. To consider a possible experiment, we have performed the simulation with parameters appropriate to the $^{87}\text{Rb}$–$^{23}\text{Na}$ mixture. We set Na as species 1 and Rb as species 2. The total particle numbers $N_1 = N_2 = 100$ and the hard-core radii used in producing the results shown in Fig. (a) are equivalent to an actual mixture with $s$-wave scattering lengths of $3 \text{ nm}$.
and 6 nm, respectively, and a total particle number on the order of $10^4$. In Fig. 4, the density profiles of both the species under the same single-particle energy spacing and identical external potential are shown. The energy spacing in the single-particle spectrum of Rb is about half of that of Na for the data shown in Fig. 4(a) due to the difference in the trapping frequencies. The small energy gap and large scattering length make it much easier for Rb atoms to be driven out of the trap center or its single-particle ground state whereas most Na atoms stay at the trap center or in its single-particle ground state. This is totally counterintuitive and in disagreement with the mean-field results. No significant spatial separation is found when the single-particle energy spacings are the same, as shown in Fig. 4(b); but increasing either the interaction strength or the total number of particles can result in the spatial separation with an outer shell of Na.

Under the identical external potential, we have also found that the spatial separation of the two species is independent of the ratio $m_2/m_1$. Therefore, for a system containing any two species, it is energetically favorable to have the species with a larger scattering length to form a low-density outer shell surrounding the other with a smaller scattering length; this is consistent with the experimental observation for the mixture of $^{87}$Rb atoms with two distinct spin states. It is also possible for a future experiment to realize the separation in the energy space as predicted here.

Our simulations show that the external potentials can be used to tune the structure of a boson mixture. With the same trapping frequency for the two species, it is more likely for a system with a mass ratio close to 1 to form an outer shell of particles with a larger scattering length whereas for system with a mass ratio far away from 1 to form an outer shell of lighter particles. In the latter case, the large difference of external potentials between two species outweighs the moderate effect of the two-body interactions within a species. It is possible for the $^{87}$Rb–$^{41}$K mixture to form an outer shell of Rb atoms whereas for the $^{87}$Rb–$^{23}$Na mixture to form an outer shell of Na atoms and the future experiment will tell.

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