Number and spin densities in the ground state of a trapped mixture of two pseudospin-$\frac{1}{2}$ Bose gases with interspecies spin-exchange interaction

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Abstract. We consider the ground state of a mixture of two pseudospin-$\frac{1}{2}$ Bose gases with interspecies spin exchange in a trapping potential. In the mean field approach, the ground state can be described in terms of four wavefunctions governed by a set of coupled Gross-Pitaevskii-like (GP-like) equations, which differ from the usual GP equations in the existence of an interference term due to spin-exchange coupling between the two species. Using these GP-like equations, we calculate such ground state properties as chemical potentials, density profiles and spin density profiles, which are directly observable in experiments. We compare the cases with and without spin exchange. It is demonstrated that the spin exchange between the two species lowers the chemical potentials, tends to equalize the wavefunctions of the two pseudospin components of each species, and, thus, homogenizes the spin density. The novel features of the density and spin density profiles can serve as experimental probes of this novel Bose system.

Keywords: quantum gases
Number and spin densities in the ground state of a mixture of two Bose gases

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1. Introduction

Multicomponent Bose–Einstein condensation (BEC) has been an active subject of research in recent years. People have considered BEC of a mixture of two different spinless species [1]–[8] and of spinor gases such as spin-1 [9]–[13] and pseudospin-$\frac{1}{2}$ gases [14]–[16]. More recently, a mixture of two distinct species of pseudospin-$\frac{1}{2}$ gases with interspecies spin exchange was investigated theoretically [17]–[23]. In such a mixture, there are $N_{a}$ atoms of species $a$ and $N_{b}$ atoms of species $b$, while each atom has a pseudospin degree of freedom with basis state $\sigma=\uparrow, \downarrow$. The particle number of each species $N_{\alpha}=N_{\alpha\uparrow}+N_{\alpha\downarrow}$ ($\alpha=a,b$) is conserved, but the particle number of each pseudospin component of each species $N_{\alpha\sigma}$ ($\sigma=\uparrow, \downarrow$) is not conserved because of the spin-exchange coupling between the two species. Note that for a pseudospin-$\frac{1}{2}$ gas, the total spin of each species is always a constant, $S_{\alpha}=N_{\alpha}/2$, while its $z$ component is $S_{\alpha z}=(N_{\alpha\uparrow}−N_{\alpha\downarrow})/2$.

The scatterings between any two atoms are now pseudospin dependent. For the scattering between an atom of species $\alpha$ coming in with pseudospin $\sigma_{1}$ and going out with pseudospin $\sigma_{4}$ and an atom of species $\beta$ coming in with pseudospin $\sigma_{2}$ and going out with pseudospin $\sigma_{3}$, the scattering length is denoted as $\xi_{\alpha\beta\sigma_{1}\sigma_{2}\sigma_{3}\sigma_{4}}$. Correspondingly, the effective interaction is $g_{\alpha\beta\sigma_{1}\sigma_{2}\sigma_{3}\sigma_{4}}=2\pi\hbar^{2}\xi_{\alpha\beta\sigma_{1}\sigma_{2}\sigma_{3}\sigma_{4}}/\mu_{\alpha\beta}$, where $\mu_{\alpha\beta}$ is the reduced mass of the two atoms. For convenience, we define the shorthand forms $g_{\alpha\sigma\sigma\sigma}=g_{\alpha\sigma\sigma\sigma\sigma\sigma}$ for the intraspecies scattering of the same pseudospins $\sigma$, $g_{\alpha\sigma\sigma}=2g_{\alpha\sigma\sigma\sigma}\sigma\sigma$ for the interspecies scattering of different pseudospins $\sigma \neq \sigma'$, $g_{\alpha\sigma\sigma'}=g_{\alpha\sigma\sigma\sigma'}\sigma\sigma'$ for the interspecies scattering without spin exchange, and $g_{c}\equiv g_{\alpha\sigma\sigma\sigma}$ for the interspecies spin-exchange scattering. We shall also use the shorthand forms $\xi_{\alpha\sigma\sigma}$ for $\xi_{\alpha\sigma\sigma\sigma\sigma\sigma}$, $\xi_{\alpha\sigma\sigma}$ for $2\xi_{\alpha\sigma\sigma\sigma\sigma\sigma}$, and $\xi_{\alpha\sigma\sigma'}$ for $\xi_{\alpha\sigma\sigma\sigma'}\sigma'$. In this paper, all these scattering lengths $\xi$ and thus the effective interaction...
strengths \( g \) are considered to be positive. Thus the many-body Hamiltonian density is [17, 18]

\[
\hat{H}(r) = \sum_{\alpha \sigma} \tilde{\psi}_{\alpha \sigma}^\dagger \left[-\frac{1}{2m_\alpha} \nabla^2 + U_{\alpha \sigma}(r)\right] \tilde{\psi}_{\alpha \sigma} + \frac{1}{2} \sum_{\alpha \sigma \sigma'} g_{\alpha \sigma \sigma'} |\tilde{\psi}_{\alpha \sigma}|^2 |\tilde{\psi}_{\alpha \sigma'}|^2 \\
+ \sum_{\sigma \sigma'} g_{\sigma \sigma}|\tilde{\psi}_{\sigma \sigma}|^2 |\tilde{\psi}_{\sigma \sigma'}|^2 + g_c (\tilde{\psi}_{\alpha 1}^\dagger \tilde{\psi}_{\beta 1}^\dagger \tilde{\psi}_{\alpha 1} \tilde{\psi}_{\beta 1} + \tilde{\psi}_{\alpha 1}^\dagger \tilde{\psi}_{\beta 1}^\dagger \tilde{\psi}_{\alpha 1} \tilde{\psi}_{\beta 1}),
\]

(1)

where \( U_{\alpha \sigma}(r) \) is the external trapping potential, \( \tilde{\psi}_{\alpha \sigma} \equiv \tilde{\psi}_{\alpha \sigma}(r) \) is the Bose field operator for species \( \alpha \) with pseudospin \( \sigma \) \((\alpha = a, b, \sigma = \uparrow, \downarrow)\), and \( \sigma \) and \( \sigma' \) may or may not be equal. Expanded in terms of an orthonormal set of single-particle orbital basis states \( \{\phi_{\alpha \sigma, i}(r)\} \),

\[
\tilde{\psi}_{\alpha \sigma}(r) = \sum_i \tilde{a}_{\alpha \sigma, i} \phi_{\alpha \sigma, i}(r),
\]

(2)

where \( \tilde{a}_{\alpha \sigma, i} \) is the annihilation operator corresponding to \( \phi_{\alpha \sigma, i}(r) \). In \( \hat{H} \), the first two summations of interaction terms are the density–density interactions without spin exchange, as studied in previous models of Bose mixtures, and the last term is the spin-exchange interaction, which causes spin correlation or entanglement between the two species, and is also responsible for the novel features discussed in the present paper.

Under the usual approximation of a single orbital mode, Bose statistics and energetics imposes that all atoms of each species \( \alpha \) and with the pseudospin state \( \sigma \) occupy the single-particle orbital mode of lowest energy, here denoted as \( \phi_{\alpha \sigma}(r) \), and hence in the expansion (2) of the field operator \( \tilde{\psi}_{\alpha \sigma}(r) \), one only needs to consider one term \( \tilde{a}_{\alpha \sigma} \phi_{\alpha \sigma}(r) \), where \( \tilde{a}_{\alpha \sigma} \) is the annihilation operator corresponding to \( \phi_{\alpha \sigma}(r) \). Consequently, in each term of the many-body Hamiltonian \( \int d^3 r \hat{H}(r) \), there is an integration of a product of single-particle wavefunctions, which now becomes an effective coefficient. Therefore, under the approximation of a single orbital mode, the details of \( \phi_{\alpha \sigma}(r) \) are not needed in describing the many-body ground state in terms of creation and annihilation operators or, equivalently, the collective spin operators, although such simplification is lost when one goes beyond the approximation of a single orbital mode. In a broad parameter regime, the two species are quantum entangled in the particle numbers of the two pseudospin states or collective spins, that is, the two species do not undergo BEC separately; hence the ground state was dubbed entangled BEC.

However, these four wavefunctions and the corresponding elementary excitations are important physical properties. For a uniform system, \( \phi_{\alpha \sigma}(r) \) is simply the constant \( 1/\sqrt{\Omega} \), where \( \Omega \) is the volume of the system. For convenience, we write the mean field value of the Bose field operator \( \langle \tilde{\psi}_{\alpha \sigma} \rangle \) as \( \psi_{\alpha \sigma} e^{i\gamma_{\alpha \sigma}} \), where \( \psi_{\alpha \sigma} > 0 \). This is the so-called condensate wavefunction. The condensate wavefunction for the pseudospin \( \sigma \) component of species \( \alpha \) is \( \psi_{\alpha \sigma} = n_{\alpha \sigma} \sqrt{N_{\alpha \sigma}}/\sqrt{\Omega} \), where \( N_{\alpha \sigma}^0 \) is the corresponding particle number in the many-body ground state of the system, determined by the many-body Hamiltonian, and \( n_{\alpha \sigma} = \pm \) is a sign. To minimize the energy, the signs of three components can be chosen to be + while that of the other one is chosen to be −.

In a trapping potential, which is an experimental necessity for BEC of cold atoms, the wavefunction \( \psi_{\alpha \sigma}(r) \) is dramatically different from a constant. Moreover, the details of \( \psi_{\alpha \sigma}(r) \) provide experimentally very important information, as their modular square is just the particle density, which is directly measurable and is a key observable.
In this paper, we consider such a pseudospin-$\frac{1}{2}$ mixture in a trapping potential, and find some interesting properties, especially the density and spin density profiles of the four orbital modes of lowest energy, $\{\phi_{\alpha\sigma}\}$. There have been many calculations on such properties in other kinds of BEC mixtures [3, 24], which demonstrated that a trapping potential brings in significant features absent in a homogeneous system.

The GP-like equations can be obtained by using the Euler–Lagrange equation

$$\frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{\psi}_{\alpha\sigma}} \right) - \frac{\partial \mathcal{L}}{\partial \psi_{\alpha\sigma}} = 0,$$

(3)

with $\mathcal{L} = i\sum_{\alpha\sigma}\psi_{\alpha\sigma}^* \dot{\psi}_{\alpha\sigma} - \langle \hat{H} \rangle$, and then replacing $i\partial_t$ with $\mu_{\alpha\sigma}$. One obtains

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U_{\alpha\sigma}(\mathbf{r})\right) \psi_{\alpha\sigma} + g^{aa}_{\sigma}\psi_{\alpha\sigma}^2 \psi_{\alpha\sigma} + g^{a\bar{a}}_{\sigma}\psi_{\alpha\sigma}\bar{\psi}_{\bar{\alpha}\bar{\sigma}} + g^{a\bar{a}}_{\bar{\sigma}}\bar{\psi}_{\bar{\alpha}\bar{\sigma}}^2 \psi_{\alpha\sigma} + g^{\bar{a}a}_{\bar{\sigma}}\bar{\psi}_{\bar{\alpha}\bar{\sigma}}^2 \psi_{\alpha\sigma} + g^{\bar{a}\bar{a}}_{\bar{\sigma}}\bar{\psi}_{\bar{\alpha}\bar{\sigma}}\bar{\psi}_{\bar{\alpha}\bar{\sigma}} = \mu_{\alpha\sigma} \psi_{\alpha\sigma},$$

(4)

where the $g_e$ term is due to the spin-exchange interaction, and is a new feature absent in previous models of Bose mixtures. The minus sign comes from the requirement that the phases $\gamma_{\alpha\sigma}$ of the four components should satisfy $\cos(\gamma_{\alpha1} - \gamma_{\alpha1} - \gamma_{b1} + \gamma_{b1}) = -1$ for the minimization of the energy. For $g_e > 0$, this spin-exchange interaction is like an attractive interaction in some way; counteracting the other interaction terms if the latter are repulsive. However, it is a new effect, as it depends on the wavefunctions rather than the densities.

When the $g_e$ term is negligible, the system behaves like the usual Bose mixtures with repulsive interactions. When the $g_e$ term is dominant, the system behaves in a similar way to an attractive mixture with the intraspecies interaction negligible. Moreover, to minimize the spin-exchange interaction energy $g_e \langle \hat{\psi}_{a1}^\dagger \hat{\psi}_{b1}^\dagger \hat{\psi}_{b1}^\dagger \hat{\psi}_{a1} \rangle = -2g_e \psi_{a1}^\dagger \psi_{a1}^\dagger \psi_{b1}^\dagger \psi_{b1}^\dagger \cos(\gamma_{a1} - \gamma_{a1} - \gamma_{b1} + \gamma_{b1}) = -2g_e \psi_{a1}^\dagger \psi_{a1}^\dagger \psi_{b1}^\dagger \psi_{b1}^\dagger$, the density profiles for the two pseudospin components of each species tend to be the same. To see this, note that each wavefunction can be real and positive [25]. The other terms in the Hamiltonian of course break this equality, as will be studied later in this paper.

Below we shall describe the finding that the larger the interspecies spin-exchange $g_e$ is, the stronger the overlap between the density profiles of the two pseudospin components of each species is. Hence density profiles are very good experimental probes of the underlying interspecies correlations. On the other hand, by comparing the experimental and theoretical results on the number density and spin density profiles, one may estimate the spin-exchange interaction strength $g_e$. Experimentally, by studying the effect of $g_e$ on the density profiles, one can obtain information on such a mixture.

Up to now, there has not been a report on experimental studies of such a spin-exchange mixture of different species. However, the interspecies spin-exchange interaction is determined by the difference between the interspecies triplet and singlet scattering lengths, which has been found to be quite a few nanometers (nm) [26]. In this paper, the theoretical investigation using this parameter value clearly indicates interesting new
features. Hence our work also provides some motivation and methodology for experimental exploration of such a mixture.

In section 2, the numerical method is described. In section 3, we calculate the ground state properties, comparing the cases with and without spin exchange, and demonstrating the experimentally observable effects of interspecies spin exchange. Then we give a summary in section 4.

2. The numerical method

We assume the trapping potential to be

$$U_{\alpha\sigma}(r) = \frac{1}{2}M_\alpha\omega_\alpha^2(\rho^2 + \lambda^2 z^2),$$

(5)

where $\rho = \sqrt{x^2 + y^2}$, $\lambda$ represents the trap anisotropy, and $M_\alpha$ and $\omega_\alpha$ are the mass of the $\alpha$-atom and the trap frequency, respectively. $U_{\alpha\uparrow} = U_{\alpha\downarrow}$. For a magnetic trap, $M_\alpha\omega_\alpha^2 = \gamma_\alpha\mu_B B_0$, with $\gamma_\alpha$ being the $g$ factor of the $\alpha$-atom, and $B_0$ being the central magnetic field multiplied by a normalized factor. In order to have the parameter values close to the experimental data, we imagine species $a$ as $^{87}$Rb and species $b$ as $^{23}$Na; then $M_a\omega_a^2/M_b\omega_b^2 = \gamma_a/\gamma_b = 1$, i.e. $U_{a\sigma} = U_{b\sigma}$. Define $\kappa \equiv \omega_b/\omega_a\sqrt{M_a/M_b} = \sqrt{87/23}$. In our calculation, we use the parameter values $\omega_a = 2\pi \times 75$ Hz, $\omega_b = \kappa\omega_a$ and $\lambda = \sqrt{8}$. The values of the scattering lengths are set to be $\xi_{\alpha\uparrow\uparrow} = 8$ nm, $\xi_{\alpha\uparrow\downarrow} = 6.7$ nm, $\xi_{\alpha\downarrow\downarrow} = 3.7$ nm, $\xi_{\uparrow\downarrow}^{bb} = 4$ nm, $\xi_{\downarrow\downarrow}^{bb} = 2$ nm, $\xi_{\uparrow\uparrow}^{bb} = 1.7$ nm, $\xi_{\downarrow\downarrow}^{bb} = 1.2$ nm, $\xi_{\uparrow\downarrow}^{ab} = 0.67$ nm, $\xi_{\downarrow\downarrow}^{ab} = 1.9$ nm. We vary the value of $\xi_\sigma$ and study its effect on the number densities and the spin densities.

We expand $\psi_{\alpha\sigma}$ in terms of the $N_{\text{basis}}$ eigenfunctions of the non-interacting Schrödinger equation in an anisotropic harmonic potential (5), that is,

$$\psi_{\alpha\sigma}(r) = \sum_{r=0}^{N_{\text{basis}}} A_{\alpha\sigma}^r R_{mr}(\rho) \Phi_{mr}(\varphi) Z_{w_r}(z),$$

(6)

where $R_{mr}(\rho)$, $\Phi_{mr}(\varphi)$ and $Z_{w_r}(z)$ correspond to the cylindrical coordinates $\rho$, $\varphi$ and $z$, respectively, and $A_{\alpha\sigma}^r$ is the expanding coefficient under the condition $\sum_{r=0}^{N_{\text{basis}}}(A_{\alpha\sigma}^r)^2 = N_{\alpha\sigma}$. For the ground state, only eigenfunctions with $m_r = 0$ are relevant.

Therefore, GP-like equation (4) is transformed to the following nonlinear equation:

$$\begin{align*}
(E_{\alpha\sigma}^d - \mu_{\alpha\sigma})A_{\alpha\sigma}^d &+ g_{\alpha\sigma}^d \sum_{ijk} A_{\alpha\sigma}^i A_{\alpha\sigma}^j A_{\alpha\sigma}^k I(i, j, k, \alpha, l) \\
&+ g_{\alpha\sigma}^d \sum_{ijk} A_{\alpha\sigma}^i A_{\alpha\sigma}^j A_{\alpha\sigma}^k I(i, j, \alpha, k, l) \\
&+ g_{\alpha\sigma}^d \sum_{ijk} A_{\alpha\sigma}^i A_{\alpha\sigma}^j A_{\alpha\sigma}^k I(i, \alpha, j, \alpha, k, l) \\
&+ g_{\alpha\sigma}^d \sum_{ijk} A_{\alpha\sigma}^i A_{\alpha\sigma}^j A_{\alpha\sigma}^k I(i, \alpha, j, \alpha, k, \alpha, l) \\
&- g_e \sum_{ijk} A_{\alpha\sigma}^i A_{\alpha\sigma}^j A_{\alpha\sigma}^k I(i, j, \alpha, k, \alpha, l) = 0, 
\end{align*}$$

(7)

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where $E_{i\alpha}^l = ((2n_i + m_i + 1) + (w_i + 1/2)\lambda)\hbar\omega_{\alpha}$.

\[
I(i, j, k, l, \sigma) = \frac{1}{2\pi} \int_0^\infty R_{ni}^m(\eta_{\alpha\sigma}^2\rho^2) R_{nj}^m(\eta_{\beta\sigma}^2\rho^2) R_{nk}^m(\eta_{\beta\sigma}^2\rho^2) R_{nl}^m(\eta_{\alpha\sigma}^2\rho^2) \rho \, d\rho \\
\times \int_{-\infty}^{+\infty} Z_{w_i}(\eta_{\alpha\sigma} z) Z_{w_j}(\eta_{\alpha\sigma} z) Z_{w_k}(\eta_{\beta\sigma} z) Z_{w_l}(\eta_{\beta\sigma} z) \, dz,
\]

where $m_r$ ($r = i, j, k, l$) should be 0. There are various algorithms for determining the solutions of the nonlinear equation set, such as fixed-point iteration and the Newton method. We use the Broyden method to obtain the solutions of equation (7) because of its high speed and precision.

3. Calculations

We shall use the GP-like equations (4) to study the effect of interspecies spin exchange on the number densities

\[
n_{\alpha\sigma} = |\psi_{\alpha\sigma}(r)|^2,
\]

and the spin densities

\[
S_{\alpha \sigma}(r) = \frac{1}{2}[|\psi_{\alpha \sigma}(r)|^2 - |\psi_{\alpha \bar{\sigma}}(r)|^2].
\]

For simplicity, we assume that the atom numbers of the two species are equal, i.e. $N_\alpha = N_\beta = N$. Although the cases of $N \leq 1000$ may not be experimentally realistic, they serve as a theoretical demonstration of the dilute limit, in which the interaction energy is small, especially in comparison with the cases with larger $N$.

3.1. The case without interspecies spin exchange

First we consider the case of $\xi_\epsilon = 0$, in which the system reduces to a mixture of four spinless condensates. The results for this case are summarized in figures 1–6. They are all consequences of minimizing the repulsive interactions among the four components, as detailed in the following.

We have $\mu_{\alpha \bar{\sigma}} > \mu_{\alpha \sigma}$ under the present parameter values, as indicated in figure 1, which shows the chemical potential $\mu_{\alpha \sigma}$ as a function of $N$, $\mu_{\alpha \sigma}$ and $\mu_{\alpha \bar{\sigma}}/\hbar\omega_\alpha - \mu_{\beta \sigma}/\hbar\omega_\beta$ increase with $N$. The difference between $\mu_{\alpha \bar{\sigma}}$ and $\mu_{\alpha \sigma}$ is due to the spin dependence of the various scattering lengths. This result can be confirmed by a calculation based on the Thomas–Fermi approximation, which leads to $\mu_{\alpha \sigma} = 1/\Omega[\int U_{\alpha \sigma} \, dr + g_{\alpha \sigma}^a N_{\alpha \sigma} + g_{\beta \sigma}^a N_{\beta \sigma} + g_{\alpha \beta}^a N_{\alpha \beta} + g_{\beta \alpha}^a N_{\beta \alpha}]$. In a sense, $\mu_{\alpha \sigma}$ represents the average energy of one atom of species $\alpha$ with pseudospin $\sigma$. We can observe that $\mu_{\alpha \sigma}/\hbar\omega_\alpha$ decreases with $N$, towards the single-particle value $1 + \lambda/2 = 2.414$.

Now we take a look at the spatial dependence of the atom densities $n_{\alpha\sigma}(r) = |\psi_{\alpha\sigma}(r)|^2$. The density profiles for several different values of $N$ are shown in figure 2, where the distributions along the $\rho$ and $z$ directions are depicted. These plots display some interesting features. Obviously $n_{\alpha\bar{\sigma}}$ and $n_{\alpha\sigma}$ are complementary, because of the normalization condition $\int (n_{\alpha\bar{\sigma}} + n_{\alpha\sigma}) \, dr = N$. When $N$ is small, $n_{\alpha\bar{\sigma}}$ and $n_{\alpha\sigma}$ are close to each other, because the interaction energy is small. But with increase of $N$, the difference between $n_{\alpha\bar{\sigma}}$ and $n_{\alpha\sigma}$ increases in order to lower the interaction energy. When $N$ is large enough, two or more peaks may appear in some density profiles, due to the inclusion of

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Figure 1. Reduced chemical potential $\mu_{\alpha\sigma}/\hbar\omega_\alpha$ varying with the atom number $N$ of each species, at a generic parameter point without interspecies spin exchange, i.e. $\xi_e = 0$. $\mu_{\alpha\sigma}$ and $\mu_{a\sigma}/\hbar\omega_a - \mu_{b\sigma}/\hbar\omega_b$ increase with $N$.

Figure 2. Density $n_{\alpha\sigma} = |\psi_{\alpha\sigma}|^2$ for each pseudospin component of each species, at a generic parameter point with $\xi_e = 0$, as defined in the text, for $N = 100, 1000, 5000, 10000$. $N$ is the atom number of each species. The upper plots are profiles along the $\rho$ direction with $z = 0$. The lower plots are profiles along the $z$ direction with $\rho = 0$. More than one peak appears in some plots, due to the inclusion of higher order eigenfunctions in the expansion (6) when the interaction energy becomes important.
Figure 3. Profiles of the total density \( n_\alpha = n_{\alpha \uparrow} + n_{\alpha \downarrow} \), for each species, along the \( \rho \) direction with \( z = 0 \), and along the \( z \) direction with \( \rho = 0 \), at a generic parameter point with \( \xi_e = 0 \), as defined in the text, for \( N = 100, 1000, 5000, 10000 \). Not all components coexist in every region; this is in order to minimize the total energy under the given parameter values. The density profiles are more extended in the \( \rho \) direction than in the \( z \) direction, as the trapping in the \( z \) direction is stronger than that in the \( \rho \) direction.

higher order eigenfunctions in the expansion (6) when the interaction energy becomes important.

The profiles of the total density for each species, \( n_\alpha = n_{\alpha \uparrow} + n_{\alpha \downarrow} \), are shown in figure 3. We can see that not all components coexist in every region, in analogy with the two-component BEC [3]; this is in order to minimize the total energy under the given parameter values.

The density profiles are more extended in the \( \rho \) direction than in the \( z \) direction, as exhibited in figure 2 and in figure 3. The reason is that the trapping in the \( z \) direction is stronger than that in the \( \rho \) direction.

We have also plotted the two-dimensional density profiles with \( \rho \) and \( z \) as the two coordinates, as shown in figure 4 for \( \lambda = \sqrt{8} \), and in figure 5 for \( \lambda = 1 \), both with \( N = 10000 \). The complementarity between the two pseudospin components of each species is very clear. In the former case, as \( \lambda \neq 1 \), the profiles are asymmetric between the \( \rho \) and \( z \) directions. In the latter case, as \( \lambda = 1 \), the profiles are symmetric between the \( \rho \) and \( z \) directions.
Figure 4. Two-dimensional density profiles on a cross section including the z-axis, with \( \rho \) and \( z \) as the coordinates, at a generic parameter point defined in the text, with \( \xi_e = 0 \), \( \lambda = \sqrt{8} \) and \( N = 10000 \). The profiles are asymmetric between the \( \rho \) and \( z \) directions as \( \lambda \neq 1 \).

Figure 5. Two-dimensional density profiles on a cross section including the z-axis, with \( \rho \) and \( z \) as the coordinates, at a generic parameter point defined in the text, with \( \xi_e = 0 \), \( \lambda = 1 \) and \( N = 10000 \). The profiles are symmetric between the \( \rho \) and \( z \) directions as \( \lambda = 1 \).
Now we consider the spin density $S_{\alpha z}(r) = \frac{1}{2}(|\psi_{\alpha \uparrow}(r)|^2 - |\psi_{\alpha \downarrow}(r)|^2)$. The spin density profiles are shown in figure 6 for $N = 100, 1000, 5000, 10000$. It can be seen that along the $\rho$ direction, the spin density increases from a negative value at the center to a positive value at a certain radius, and then gradually decreases to zero. Both the radius with the positive maximal spin density and the radius where the spin density becomes zero increase with $N$. This feature can be understood in terms of the difference between the densities of $\uparrow$ and $\downarrow$ atoms shown in figure 2. The spin density being negative in inside regimes while it is positive in outside regimes occurs because we have assumed that $\xi_{\uparrow \uparrow} > \xi_{\downarrow \downarrow}$, and consequently more $\uparrow$ atoms tend to stay in the outside regime where the density is lower because of the trapping potential, while more $\downarrow$ atoms tend to stay in the inside regime, in order to lower the total energy. Of course the spin density approaches zero for large enough $\rho$, as the densities of $\uparrow$ and $\downarrow$ atoms both approach zero. Along the $z$ direction with $\rho = 0$, the spin density is mostly negative, also because more $\uparrow$ atoms than $\downarrow$ atoms stay in the larger $\rho$ regime. This effect weakens with increase of $z$, because the trapping potential increases, and consequently the difference between the numbers of $\downarrow$ and $\uparrow$ atoms decreases. There is only a very small regime where the spin density becomes positive but the values are too small to be visible on the plots. This feature is unlike that of the profiles along the $\rho$ direction, as there must be some regime of $\rho$ with more $\uparrow$ atoms.
Figure 7. Reduced chemical potential $\mu_{\alpha\sigma}/\hbar\omega_\alpha$ varying with $N$ for four different values of $\xi_e$. The chemical potential is lowered by the spin-exchange energy, which is attractive. $d\mu_{\alpha\sigma}/dN$ remains positive.

3.2. The case with interspecies spin exchange

Now we come to the effect of interspecies spin exchange, i.e. the case of $\xi_e \neq 0$. We have chosen $\xi_e = 0.53, 1.07, 2.03, 4.27$ nm. As stated in the Introduction, the mean field spin-exchange interaction energy

$$-2g_e\psi_{a\uparrow}\psi_{a\downarrow}\psi_{b\downarrow}\psi_{b\uparrow} \quad (8)$$

is an interference term and acts like an attractive interaction among the four orbital wavefunctions in some way, but it depends on the wavefunctions rather than the densities. This interference effect is manifested in the number and spin density profiles.

The spin exchange lowers the chemical potential, as is evident in figure 7, which is the numerical result for $\mu_{\alpha\sigma}$ as a function of $N$ for four values of $\xi_e$. It can be seen from the plots that the larger $\xi_e$ is, the lower $\mu_{\alpha\sigma}$ is. However, in all of these cases, $d\mu_{\alpha\sigma}/dN$ remains positive.

The interference among the four orbital wavefunctions is also manifested in the density profiles, as shown in figures 8–10. The spin-exchange energy (8) is minimized when $\psi_{a\uparrow} = \psi_{a\downarrow}$ for each species $\alpha$. It is competitive with the other interactions. If it dominates the energy, in order to lower the energy, the wavefunctions of the two pseudospin components of each species tend to be close to each other, compared with the case without spin exchange. Indeed, this tendency can be observed in figures 8 and 9, which show the density profiles for each pseudospin component of each species, in the $\rho$ direction with
Figure 8. Density profile $n_{\alpha\sigma} = |\psi_{\alpha\sigma}|^2$ for each pseudospin component $\sigma$ of each species $\alpha$ along the $\rho$ direction on the plane $z = 0$ for $N = 100$, 1000, 5000, 10000 and several values of $\xi_e$. Other parameter values are given in the main text. The larger $\xi_e$, the stronger the overlap among the four wavefunctions.

$z = 0$ and in the $z$ direction with $\rho = 0$ respectively. The larger $\xi_e$ is, the more dominant the spin-exchange interaction is, and then the closer $\psi_{\alpha\uparrow}$ and $\psi_{\alpha\downarrow}$ are to each other. When $\xi_e$ is large enough, the overlapping effect becomes very visible. Nevertheless, the overlap is not complete, because of other terms in the energy.

Figure 10 depicts the profile of the total density of each species, which can be compared with the plot for the same $N$ in figure 3; it can be seen that the overlap regime of the two species is also enhanced by the spin exchange, because of the effect of the spin-exchange term (8).

Moreover, we have also calculated the spin density profile, as shown in figure 11 for $N = 10000$. The spin density $S_{\alpha z} = \frac{1}{2} (|\psi_{\alpha\uparrow}| - |\psi_{\alpha\downarrow}|)^2$ is proportional to the difference between the densities of the two pseudospin components, so it is a quantification of...
the overlap between the two pseudospin components. Evidently, with increase of $\xi_e$, the variation of the spin density with the radius decreases. In other words, both the spin density $S_{z\alpha}$ of each species and the total spin density $S_z$ are homogenized by the spin exchange. When $\xi_e$ is large enough, each spin density tends to vanish. The underlying reason is also that $\psi_{\alpha\uparrow}$ and $\psi_{\alpha\downarrow}$, whose difference gives the spin density of species $\alpha$, tend to be close to each other in order to lower the spin-exchange energy. Consequently the spin density of each species $\alpha$ tends to vanish. In both the case without spin exchange and the case with spin exchange, the location on the $z$-axis where the spin density becomes zero is much smaller than that along the $\rho$ direction. Compared with the case without spin exchange, another notable feature is that when $\xi_e$ and $N$ are large enough, in the spin density profile along the $z$ direction with $\rho = 0$, the regime with positive spin density becomes more visible (figure 11). This is because the negative sign of the spin-exchange

Figure 9. Density profile $n_{\alpha\sigma} = |\psi_{\alpha\sigma}|^2$ for each pseudospin component $\sigma$ of each species $\alpha$ along the $z$ direction on the line $\rho = 0$ for $N = 100$, 1000, 5000, 10 000 and several values of $\xi_e$. Other parameter values are given in the main text. The larger $\xi_e$, the stronger the overlap among the four wavefunctions.
4. Summary

This paper concerns the ground state properties of a mixture of two species of pseudospin-$1/2$ Bose gases with interspecies spin-exchange interaction in a trapping potential. We have numerically calculated the four orbital condensate wavefunctions, each of which corresponds to a pseudospin component of each species, by using the GP-like equations. We set the atom number of each species to be $N$. Using these wavefunctions, the number and spin densities are obtained. When the spin-exchange scattering length is zero, this mixture reduces to a mixture of the usual type, with four components. Various features appear as consequences of minimizing the density–density interaction. For example, with increase of $N$, the difference between $n_{\alpha \uparrow}$ and $n_{\alpha \downarrow}$ for each species $\alpha$ increases.

If there exists interspecies spin-exchange scattering, novel features absent in the usual mixtures emerge. As the spin-exchange interaction is negative as a consequence of minimizing the energy, it acts like an attractive interaction. Nevertheless, it depends on the overlap among the four wavefunctions. It lowers the chemical potentials and makes the densities of the two pseudospin components of each species tend to be close to each other, and thus the spin density tends to be homogenized, and even tends to vanish when

\[ \xi_e = 0.53 \text{nm} \]
\[ \xi_e = 1.07 \text{nm} \]
\[ \xi_e = 2.03 \text{nm} \]
\[ \xi_e = 4.27 \text{nm} \]

**Figure 10.** Profiles of the total density $n_\alpha$ for each species $\alpha$ along the $\rho$ direction on the plane $z = 0$ and on the line $\rho = 0$ for atom number $N = 10000$ and several values of $\xi_e$. The larger $\xi_e$, the closer the profiles of the two species.

interaction counteracts the trapping potential, even though the trapping is stronger in the $z$ direction than in the $\rho$ direction.
the spin-exchange scattering length is so large that it dominates over the density–density interaction. Therefore as experimentally measurable quantities, the number and spin density profiles of such a mixture with interspecies spin exchange are effective probes of the novel many-body ground state of this system.

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