

Miscibility of Binary Bose-Einstein Condensate Mixture with Competing s - and p -Wave Interaction

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Abstract: Combining two Bose-Einstein condensates (BECs) may result in a miscible or immiscible mixture. In this study, we investigate the miscibility-immiscibility transition of binary BEC mixture trapped in an isotropic harmonic potential, with both inter-species s -wave and p -wave scattering interaction included. The mean-field Gross-Pitaevskii equations with p -wave interaction term are numerically solved to obtain the ground-state phase diagram. Due to the p -wave interaction competing with isotropic s -wave interaction, the spatial density profile of binary BEC mixtures transforming from immiscible phase to miscible phase is observed. The p -wave interaction caused miscibility can be observed in current experiments of Bose-Bose mixture tuned near a p -wave Feshbach resonance.

Key words: Bose-Einstein condensate (BEC); p -wave; s -wave; miscibility-immiscibility transition

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0 Introduction

Quantum gas mixtures have been a subject of intensive study in recent years. Combining two-species degenerate atom gases, besides of two different hyperfine states of homonuclear atoms^[1], such as Bose-Bose^[2-6], Bose-Fermi^[7-8] and Fermi-Fermi^[9] heteronuclear combinations are extensively explored. Important properties of these binary mixtures, such as miscibility, are mainly determined by the relative intensity between the inter- and intra-species interactions.

For cold collisions between atoms, the s -wave scattering interaction with isotropic spatial dependence is dominant and higher partial wave channels with anisotropic spatial dependence are negligibly small or forbidden by quantum statistics, such as for a single-component Bose-Einstein condensate (BEC), p -wave scattering between identical parti-

cles is forbidden by bosonic statistics^[10]. While for BEC mixture of heteronuclear atoms, non- s -wave scattering channels are allowed but usually weak at low temperature with ignored scattering phase shift, as the centrifugal barrier existed for high-partial waves. On the other hand, interactions beyond the s -wave pseudopotential, such as anisotropic scattering with p -, d - or higher partial waves, often lead to more novel physical effects. Exploring the properties of cold atomic systems with higher partial wave scattering interactions has inspiring interests not only from experimental physicists but also from theoretical physicists.

The effective interactions between ultracold atoms can be controlled with the magnetic or optical Feshbach resonances (FRs) in current experiments^[11-12]. Taking advantage of the different magnetic moments between atomic state and molecular state, one can tune two atoms into a FR by chang-

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ing magnetic fields, and atoms interact strongly with each other near a FR. Of particular experimental interest, searching and exploring non- s -wave broad FRs, with open-channel dominated characteristics, between ultracold atoms reveals more versatile tuning of atomic interactions and can deepen our understanding of ultracold collisions.

The study of ultracold collisions near broad FRs of non- s -wave has limited witness although predicted to exhibit richer physics which is nonexistent only with s -wave interactions. An extensive theoretical search of broad s -, p - and d -wave FRs in all possible combinations of stable alkali-metal atoms are demonstrated in Ref. [13] using analytical multi-channel quantum-defect theory (MQDT). Broad s -wave FR in fermionic atomic mixture of ^6Li and ^{40}K , featuring small two-body and three-body collision losses, has been reported^[11,14] experimentally and predicted in theory^[15]. Low-field s -wave FRs in ^{23}Na - ^{87}Rb mixture^[16-17] and several broad p - and d -wave FRs are reported in bosonic ^{85}Rb - ^{87}Rb mixtures^[18-19] and ^{41}K atoms^[20]. Motivated by the experimental finding of broad s - and p -wave FRs in ^{85}Rb - ^{87}Rb ultracold mixture^[18], we explore the property of miscibility in binary BEC mixture with both inter- and intra-species s - and p -wave scattering interactions included.

The properties of BEC mixture with only s -wave interaction have been studied more clearly^[21-22]. Under the Thomas Fermi approximation, the phase separation region is $g_{12}^2 \geq g_1 g_2$, where g_1 and g_2 are the intra-species interactions of components 1 and 2, respectively, while g_{12} is the inter-species interaction between them. When the repulsive interaction between the two BECs is large enough, the two components repel each other so that they separate into two distinct clouds with small spatial overlap, corresponding to the immiscible phase. When the effect of interspecies interactions is weak compared with the intra-species interactions, the two components are miscible and overlap with each other at the center of the trapping potential. In the presence of p -wave, BEC phase separation has new characteristics different from the usual s -wave

case. Moreover, we find that the two kinds of BEC with original phase separation can be mixed by adjusting the p -wave interaction. This is helpful to adjust the mixing properties of BEC experimentally.

1 Theoretical Model

According to the form of p -wave interaction^[23], the mean field approximation is made for the two-component boson system, and the properties of Bose-Einstein condensate are approximately described by the mean field equation^[10,24]. The mean field equation is the Gross-Pitaevskii (GP) equation^[24]. We denote ψ_i ($i = 1, 2$) as the condensate wave function of species i , the total energy of BEC mixture in three-dimensional space can be written in the following form^[10,25]

$$E = \int d\mathbf{r} \sum_{i=1}^2 \left(\frac{\hbar^2}{2m_i} |\nabla \psi_i|^2 + V_T^i |\psi_i|^2 + \frac{g_i}{2} |\psi_i|^4 \right) + \int d\mathbf{r} \left(g_{12} |\psi_1|^2 |\psi_2|^2 + \frac{\pi \hbar^2 \nu_p}{m_r} |\psi_2 \nabla \psi_1 - \psi_1 \nabla \psi_2|^2 \right) \quad (1)$$

By differentiating the energy function, we obtain the mean field equations of the ground state of the two components^[26-27], shown as

$$\begin{aligned} \mu_1 \psi_1 = & \left(-\frac{\hbar^2 \nabla^2}{2m_1} + V_T^1 + g_1 |\psi_1|^2 + g_{12} |\psi_2|^2 \right) \psi_1 - \\ & \frac{\pi \hbar^2 \nu_p}{m_r} \left(|\psi_2|^2 \nabla^2 \psi_1 - \psi_2^* \psi_1 \nabla^2 \psi_2 + 2\psi_2 \nabla \psi_2^* \cdot \nabla \psi_1 - \right. \\ & \left. 2\psi_1 \nabla \psi_2^* \cdot \nabla \psi_2 \right) \end{aligned} \quad (2)$$

$$\begin{aligned} \mu_2 \psi_2 = & \left(-\frac{\hbar^2 \nabla^2}{2m_2} + V_T^2 + g_2 |\psi_2|^2 + g_{12} |\psi_1|^2 \right) \psi_2 - \\ & \frac{\pi \hbar^2 \nu_p}{m_r} \left(|\psi_1|^2 \nabla^2 \psi_2 - \psi_1^* \psi_2 \nabla^2 \psi_1 + 2\psi_1 \nabla \psi_1^* \cdot \nabla \psi_2 - \right. \\ & \left. 2\psi_2 \nabla \psi_1^* \cdot \nabla \psi_1 \right) \end{aligned} \quad (3)$$

where $\mu_{1(2)} = \partial E / \partial N_{1(2)}$ is the chemical potential for two species, $V_T^{1(2)} = m_{1(2)} \omega_{1(2)}^2 (x^2 + y^2 + z^2) / 2$ the harmonic trap potential, $g_{1(2)} = 4\pi \hbar^2 a_{1(2)} / m_{1(2)}$ the intra-species s -wave interaction strength, and $g_{12} = 2\pi \hbar^2 a_{12} / m_r$ the inter-species s -wave interaction strength. The first term on the right of the equation is the kinetic energy term. The second is the harmonic oscillator potential term. The third term which is intra-species interaction and the fourth

which is inter-species interaction both are s -wave interaction terms. The last term is the p -wave interaction term. N_i , m_i , ω_i , a_i are the number of particles, mass, trap frequency, and s -wave scattering length for the i -th species, and a_{12} , ν_p , m_r are s -wave scattering length between species 1 and 2, p -wave scattering volume, reduced mass, respectively.

For convenience, we use β_i to replace the coefficient before the interaction terms on the right side of the equations. For example, $\beta_p = \pi \hbar^2 \nu_p / m_r$ is the p -wave interaction strength, $\beta_{1(2)} = g_{1(2)}$ is the interaction strength of BEC itself, and $\beta_{12} = g_{12}$ is the interaction strength between two groups of BEC.

Before starting the numerical calculation, we discuss the meaning of the terms in Eq.(1). If the s -wave interaction and p -wave interaction are small, the kinetic energy term and potential energy term dominate the properties of the mixture. Generally speaking, the potential energy term tends to keep both clusters of BEC at the bottom of the well and in the ground state of the harmonic oscillator, while the kinetic energy term wants the wave function to be extended as much as possible, which makes them more inclined to mix. Therefore, both kinetic energy term and potential energy term tend to mix BEC together^[28]. The s -wave interaction energy of each BEC is directly proportional to the density. Therefore, more extended the wave function is, lower the interaction energy of BEC is. Consequently, it also tends to mix. The s -wave interaction between BEC is different, which tends to separate them.

For p -wave interaction, we need to consider the symbol of ν_p and the specific form of ϕ_i . When the two condensates are in miscible phase, their density profiles are similar in space, so $|\phi_2 \nabla \phi_1 - \phi_1 \nabla \phi_2|^2$ is small. As they move away in space, this item will gradually increase. But when they hardly overlap in space, this term will be reduced to zero. Therefore, when $\nu_p > 0$, p -wave interaction tends to make BEC either mixed or completely separated. When $\nu_p < 0$, the partially mixed configuration has the lowest p -wave interaction energy.

2 Numerical Results

In order to quantitatively describe the variation of phase separation with interaction parameters, two order parameters are defined^[29-31]. One of them is as follows.

$$\eta = \int d\mathbf{r} |\phi_1| |\phi_2| \quad (4)$$

It is the density overlapping integral of two species of BEC, which is used to distinguish the miscible phase from the separated phase. However, η cannot distinguish the separated phases with different symmetries. Therefore, the center distance between the two species is defined as

$$d = \left| \int d\mathbf{r} (|\phi_1|^2 - |\phi_2|^2) \mathbf{r} \right| \quad (5)$$

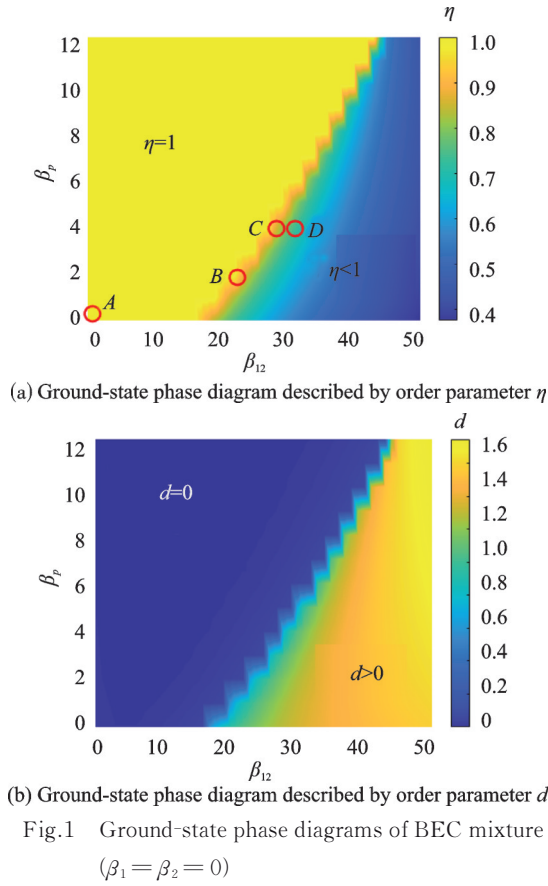
Two Gaussian wave functions whose centers do not coincide are selected as the initial trial wave functions, and the imaginary time evolution of two components of BEC mixture is carried out to find the ground state^[32].

In our calculation, we set $m_1 = m_2$, $N_1 = N_2$, $V_1 = V_2$, and assume that the potential well is isotropic. The iteration error is taken as 1×10^{-6} . When the energy error between two adjacent time periods is less than the iteration error, the propagation will stop. In this case, it is a miscible phase when $\eta = 1$ and an immiscible phase when $\eta < 1$. It is not difficult to understand that it is a miscible phase when $d = 0$ and an immiscible phase when $d > 0$.

For simplicity, we assume that the s -wave interaction of each BEC is zero, and only consider the phase transition caused by the s -wave interaction between the two BECs and p -wave interaction β_p .

We obtain the three-dimensional ground-state phase diagram of BEC mixture with p -wave interaction, as shown in Fig.1. Figs.1(a) and (b) are the ground-state phase diagrams described by order parameters η and d , respectively. Here we take $\beta_1 = \beta_2 = 0$. It can be seen from the figure that the p -wave interaction can enhance the mixing of BEC, while the interaction β_{12} between BEC tends to separate them.

We select several points in different regions cir-



cled with red in Fig.1 (a) and compared their density images. The results are shown in Fig.2. The first row to the fourth row are density images when $\eta = 1, 0.9, 0.8, 0.7$, corresponding to four points A, B, C and D in Fig.1(a), respectively. The first and second columns represent the ground state density of component 1 and component 2. Obviously, we can see that when $\eta = 1$, the centers of the two groups of BEC coincide, and their shapes are the same, which is a miscible state. When $\eta < 1$, their centers gradually move away, and they occupy different areas in the space, which is immiscible. This is consistent with the image presented by the order parameter d .

The above results are obtained when the conditions of the two components are the same. When some conditions are different, the mixture may have different properties and show more and richer results. When only s -wave interaction exists, adjusting the particle number ratio of the two atoms, in addition to the two phases mentioned above, there will be a symmetric immiscible phase^[31]. If some

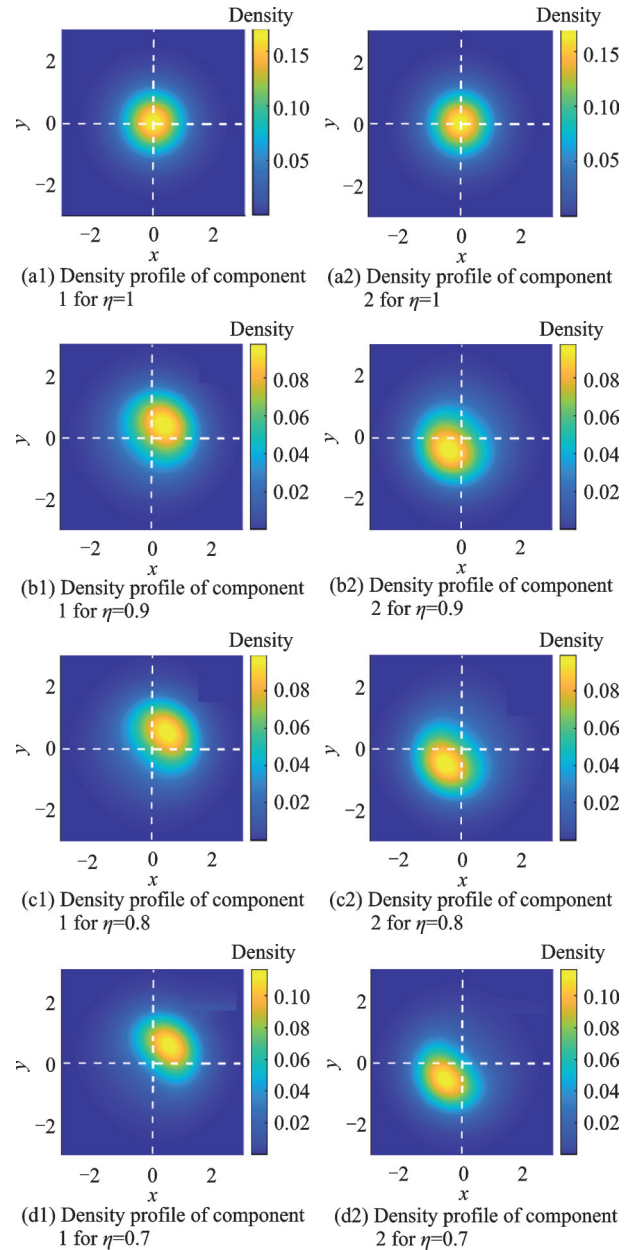


Fig.2 Ground-state density of BEC mixture in different regions

conditions are adjusted in the presence of p -wave interaction, a similar phenomenon may be seen.

In addition, another characteristic is observed. For simplicity, we assume that the s -wave interaction of each BEC is zero, and only consider the phase transition caused by the s -wave interaction between the two BECs and p -wave interaction β_p . We can find that the miscibility-immiscibility properties of BEC are not changed when the s -wave interaction between two BECs is zero or not zero. When the interaction is not zero, only the region of the miscible phase becomes larger, as we can see in Fig.3,

where the blue circle line represents the miscible phase boundary when $\beta_1 = \beta_2 = 0$, and the red square line represents the miscible phase boundary when $\beta_1 = \beta_2 = 1$. This also shows that the repulsive intra-species interactions try to expand the condensates and against the phase separation^[28, 33-34].

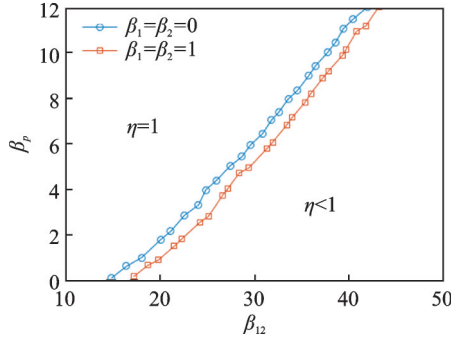


Fig.3 Miscible phase boundary when $\beta_1 = \beta_2 = 0$ and $\beta_1 = \beta_2 = 1$

3 Conclusions

We mainly study the miscibility properties of binary BEC mixtures with both inter-species s - and p -wave scattering interaction, and obtain their ground-state phase diagrams. When s -wave and p -wave interactions exist at the same time, they compete with each other, and will show richer characteristics than when there is only a single s -wave interaction. We find that p -wave interaction can enhance the miscibility of BEC mixture. Therefore, by adjusting the p -wave interaction, the two kinds of BEC separated from the original phase can be mixed, which provides a new pathway to adjust the mixing properties of BEC mixtures experimentally. Our study can be observed in current experiments of ^{85}Rb - ^{87}Rb ultracold mixture when the magnetic field tuned around 260 Gauss with both s - and p -waves Feshbach resonances existed^[17].

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Author contributions Miss PANG Jinghan and Dr. DENG Min contributed to code and data analysis. Miss PANG Jinghan, Dr. XUE Ming and Prof. LI Jinbin contributed to the discussion and background of the study and wrote the manuscript. All authors commented on the manuscript draft and approved the submission.

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具有竞争性 s 波和 p 波相互作用的二元玻色-爱因斯坦凝聚体混合物的混溶性

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摘要: 混合两种玻色-爱因斯坦凝聚体 (Bose-Einstein condensates, BECs) 可能会产生混溶或不混溶混合物。本文研究了束缚在各向同性谐振子势中的二元 BEC 混合物的混溶-非混溶转变, 其中包括组分间的 s 波和 p 波散射相互作用。通过数值求解包含 p 波相互作用项的平均场 Gross-Pitaevskii 方程, 获得基态相图。由于 p 波相互作用与各向同性 s 波相互作用相互竞争, 观察到二元 BEC 混合物从不混溶相转变为混溶相的空间密度分布。同时在 p 波 Feshbach 共振附近调控的玻色-玻色混合物的当前实验中可以观察到由 p 波相互作用引起的混溶性。

关键词: 玻色-爱因斯坦凝聚体; p 波; s 波; 混溶-不混溶转变