

Studies of two-species Bose-Einstein condensation

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Abstract: We describe our recent progress on the investigation of two-species Bose-Einstein condensation. From a theoretical analysis we show that there is a new rich phenomenology associated with two-species Bose-Einstein condensates which does not exist in a single-species condensate. We then describe results of a numerical model of the evaporative cooling process of a trapped two-species gas.

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1. Introduction

The realization of Bose-Einstein condensation (BEC) in dilute alkali vapors¹⁻³ has opened the field of weakly-interacting degenerate Bose gases. During the past two and a half years, substantial experimental and theoretical progress has been made on the study of the properties of this new state of matter. Indeed, the physics of trapped diluted condensates has emerged as one of the most exciting fields of physics in this decade. Recently, the remarkable experimental realization of a condensate mixture composed of two spin states of ^{87}Rb ⁴ has prompted significant interest in the physics of a new class of quantum fluids: the two-species Bose-Einstein condensate (TBEC)⁵⁻¹². Multi-component and, particularly, multi-species condensates offer new degrees of freedom, which give rise to a rich set of new phenomena that do not exist in a one-species condensate. Furthermore, the TBEC offers new and interesting experimental challenges.

The investigation of a TBEC requires progress on several different fronts. On the theoretical side, our effort is rooted in the study of the properties of a set of coupled non-linear Schrödinger equations which can be used to describe the TBEC within the mean field limit. Of equal importance is our development of an experimental strategy for preparing a high-density laser cooled atomic mixture, for loading magnetic trap where evaporative cooling can be applied to form a condensate. We first discuss our contributions to the theoretical description of the TBEC with an emphasis on those phenomenological features which distinguish the TBEC from the single component BEC

and which are experimentally accessible. Finally, we describe results derived from a numerical model of the evaporative cooling process developed to help determine the optimal strategy for cooling into the doubly condensed phase.

In this paper we focus our discussion on the particular system composed of a mixture of sodium (Na) and rubidium (Rb) atoms. We have selected this system because (a) both species have been successfully Bose condensed and (b) because other candidate systems, such as a sodium-cesium mixture, have already been found by us¹³ to be less desirable due to large inter-species trap loss rates. We stress, however, that many of our results are generalizable to other atomic mixtures, spin-state mixtures and Fermi-Bose mixtures.

2. Properties of the TBEC: some theoretical predictions

In the following, we give a brief description of the novel properties of a TBEC confined in an isotropic spherical potential at zero temperature. Throughout our discussion, we assume that the effect of gravity can be compensated for by choosing appropriate atomic species and spin states or by using the proper magnetic/optical trapping fields. Neglecting gravitational effects not only simplifies our calculations, it allows us to focus on the more essential intrinsic couplings within the TBEC.

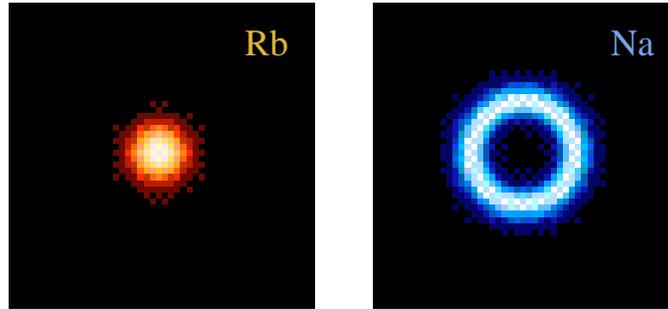


Figure 1. Density distribution of a Na-Rb TBEC for different values of a_{12} . In our calculations, we take ^{87}Rb as species 1 and ^{23}Na as species 2, with scattering lengths 6 and 3 nm, respectively. $N_1 = N_2 = 10^3$. The trapping frequencies are: $\omega_1 = 2\pi \times 160$ Hz and $\omega_2 = 2\pi \times 310$ Hz.

At zero temperature, the self-consistent nonlinear Schrödinger equations, known as Gross-Pitaevskii equations (GPEs), for a TBEC can be written as^{5,6,10,11}:

$$i\hbar \frac{\partial \psi_1(r, t)}{\partial t} = \left[-\frac{\hbar^2}{2m_1} \nabla^2 + \frac{1}{2} m_1 \omega_1^2 r^2 + N_1 U_1 |\psi_1|^2 + N_2 U_{12} |\psi_2|^2 \right] \psi_1, \quad (1)$$

$$i\hbar \frac{\partial \psi_2(r, t)}{\partial t} = \left[-\frac{\hbar^2}{2m_2} \nabla^2 + \frac{1}{2} m_2 \omega_2^2 r^2 + N_2 U_2 |\psi_2|^2 + N_1 U_{12} |\psi_1|^2 \right] \psi_2, \quad (2)$$

where $\psi_i(r, t)$ denotes the macroscopic condensate wave function for species i , with r being the radial coordinate. N_i , m_i and ω_i are particle number, mass and trap frequency, respectively. The interaction between particles are described by a self-interaction term $U_i = 4\pi\hbar^2 a_i/m_i$ and a term that corresponds to the interaction between different species $U_{12} = 2\pi\hbar^2 a_{12}/m$ (with m being the reduced mass of the two species), where a_i is the scattering length of species i and a_{12} between species 1 and 2. The time-independent form of the nonlinear Schrödinger equations are obtained by replacing the left hand sides of Eqs. (1),(2) with $\mu_i \psi_i(r)$ ($i=1,2$), with μ_i being the chemical potential.

The ground state wavefunctions ψ_1 and ψ_2 can be obtained¹⁰ by solving the coupled GPEs (Eqs. (1) and (2)) iteratively. For negative a_{12} (i.e., attractive inter-species interaction), both wave functions are compressed as compared to the case of two inde-

pendent condensates (i.e., $a_{12} = 0$). If the magnitude of a_{12} becomes larger than a certain value, the condensates mixture will eventually collapse. By contrast, for small positive a_{12} , two coupled, interpenetrating condensates are formed and each of the individual condensate wavefunctions become somewhat flattened due to the mutual repulsion between the species. However, for large positive a_{12} , the ground state is no longer necessarily a mixture of two overlapping condensates. Instead, the system “phase separates” into two distinct condensates^{5,10}: one forming a core at the center of the trap and the other forming a surrounding shell. Fig. 1 illustrates the ground state density distribution of a Na-Rb condensates mixture at different values of a_{12} . At large a_{12} , we see a phase separated TBEC with a Rb core and a Na shell. Another interesting phenomenon arising from a large repulsive inter-species interaction is the possibility of the formation of a metastable state of the TBEC¹¹. Our simulations (see below) show that, in the Na-Rb system, the Na condensate will form prior to the Rb condensate such that the Rb atoms condense in the presence of the repulsive Na condensate core into a metastable shell around the Na. However, from previous calculations, we know that the more stable state in this case should be comprised of a Rb core and a Na shell as shown in Fig. 1. We investigate the mechanical stability of this Na-core/Rb-shell system by externally perturbing the trapping potential and find that it is indeed not unconditionally stable: under a sufficiently strong external perturbation it will make a *macroscopic quantum jump* to the more stable Rb-core/Na-shell system. These macroscopic metastable states arise from the inter-species interactions and hence are unique for the multi-component condensates.

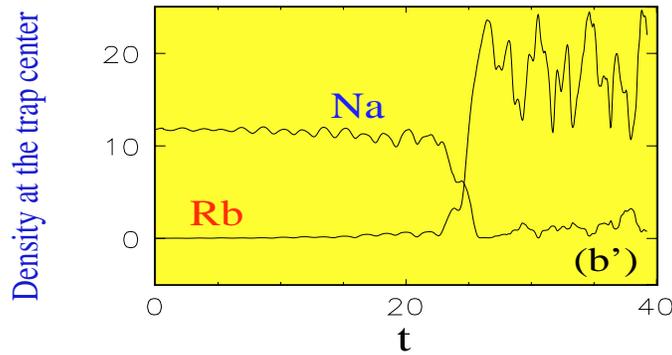


Figure 2. Density at the center of the trap as functions of time under a sinusoid modulation of the trapping potential. The units for time, length and density are: $1/\omega_1$, $\xi = \sqrt{\hbar/2m_1\omega_1}$ and ξ^{-3} , respectively. $a_{12} = 9.6$ nm. Other parameters are the same as in Fig. 1. A macroscopic quantum jump occurs at about $t=25$.

One of the fundamental properties of the confined condensate lies in the nature of the collective excitations. Excitation frequencies of a single-species Rb or Na condensate have been experimentally measured^{14,15} and theoretically calculated^{16–19}, and good agreement has been found between the two. We have generalized the standard Bogoliubov-Hartree theory²⁰ for one-species BEC to the case of the TBEC¹¹ and find that inter-species coupling dramatically modifies the excitation spectrum. We identified two types of isotropic breathing modes: in-phase and out-of-phase modes. We have also found that for large repulsive coupling, some non-isotropic modes possess imaginary frequencies indicating that the TBEC is unstable⁷. Recently, Öhberg²¹ showed that, under these conditions, a symmetry-breaking state is more stable and hence might represent

the true ground state. However, that work is done for a 2d condensate with a very small number of particles, and the relative energy difference between the symmetric and un-symmetric states is only a few percent. More detailed studies with realistic parameters in a 3d trap is needed for the full understanding the dynamics of the transition between a symmetric and non-symmetric state. The recent observation of Feshbach resonance²² provides us with the exciting possibility of tuning the value of a_{12} and studying such transitions experimentally. The instability induced by large repulsive coupling is reminiscent of the cross-phase modulation (XPM) instability in nonlinear optics²³. In fact, the GPEs for BEC are very similar to the nonlinear Schrödinger equations describing wave propagation inside optical fibers. When one light field is present, a modulation instability occurs in the case of anomalous group velocity dispersion, analogous to the negative scattering length instability for a one-species BEC. When two light fields co-propagate, instability can be induced by XPM in both the anomalous- and normal-dispersion regimes. Such modulation instability can lead to the break up of intense cw radiation into ultrashort pulses and formation of solitons. Extensive work in the field of nonlinear optics may then help us understand the physics of BEC, such as the detailed dynamics of how quantum fluctuations will affect a TBEC with imaginary modes.

For a more rigorous treatment of the TBEC fluctuation and stability character, we must go beyond the mean-field theory. Starting from a second quantized grand canonical Hamiltonian, we have identified an eigenvalue associated with the TBEC which plays the same role as the sign of the scattering length in a one-species BEC in that it is the determiner of condensate stability⁹. We predict that there is a finite range of inter-species interaction strengths in which a Na-Rb double condensate can be stable in a harmonic trap, beyond this range, however, we find that the TBEC is unstable against particle number fluctuations. A phenomenon closely related to fluctuations is the diffusion of quantum phases of the condensate wavefunctions²⁵. We have found that at the exact boundary of the stable/unstable region, the relative phase of the two condensate components of the TBEC can become locked, evolving without relative diffusion, while the individual phases continue to diffuse over time¹².

As an important property of superfluidity, quantum vortices in alkali BEC have attracted several theoretical investigations. In his recent work, Rokhsar argued that a vortex state is unstable in a one-species condensate due to the presence of a bound core state²⁴. In the case of a Rb-Na TBEC, one may produce a system comprised of a vortex-free Rb condensate at the center of the trap surrounded by a Na condensate in a vortex state such that a repulsive inter-species interaction may prevent the existence of the bound state and hence, stabilize the system. A detailed study of vortices in the TBEC is currently under way. In the above, we have briefly discussed some novel properties of the TBEC. There are still many open questions. More theoretical investigations are in progress to deepen our understanding of this unique macroscopic quantum system. Of equal importance is the realization of an experiment that will test these theoretical predictions.

3. Models of forced evaporative cooling in the Na-Rb system

Schematically, Bose-Einstein condensation in trapped alkalis is realized via the following steps: first, a large laser cooled sample of atoms is prepared in a magneto-optical trap (MOT); next this sample is loaded into a magnetic trap; and then finally forced evaporative cooling is used to increase the phase space density up to the critical values where the condensate forms. To date, we have made significant progress on the first two steps in this process - namely, we have produced a dense heteronuclear alkali vapor using a MOT and, most recently, we have successfully magnetically trapped this ultra-cold mixture. A detailed account of these achievements is however beyond the scope of the

present work. In this review, we will concentrate on our numerical model of the evaporative cooling process in the Na-Rb system and show that efficient cooling can happen in a time scale that is satisfactory for the production of a TBEC. To investigate the the two-species evaporative cooling process we have developed a numerical model based on Bird's method for fluid dynamics²⁸ which is very similar to that employed by Wu, Arimondo and Foot to study evaporative cooling and Bose condensation in the single species case²⁹. The method can be described as follows: two atomic samples, each at a given temperature, are generated and accordingly accommodated by a harmonic trap (with possibly different characteristic frequencies). The samples are then separated into cells according to their position. Collisions are carried out at each cell for a time δt , much smaller than the average collision time. These are hard-sphere collisions such that pairs of atoms with high relative velocity have higher probability of collision. After that, the atoms are allowed to evolve in the trap with their post-collision velocities during the same time δt . Evaporative cooling is modeled by requiring that atoms with a distance from the center of the trap larger than $R_{in} \exp(-t/\tau)$ are ejected. We used $R_{in}=0.4$ cm and $\tau=12$ s.

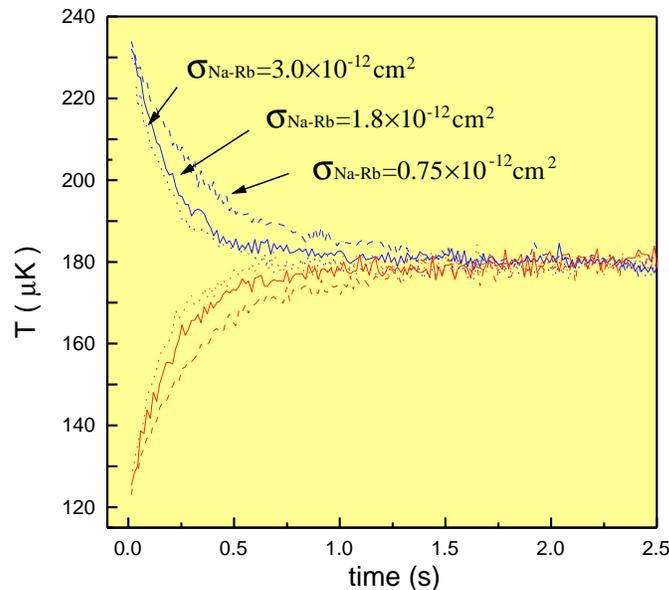


Figure 3. Thermal relaxation of a mixture of Na and Rb atoms. Trap frequencies for Na: $\omega_x = \omega_y = 2 \times \omega_z = 100 \times 2\pi \text{ rad/s}$; for Rb: $\omega_x = \omega_y = 2 \times \omega_z = 52 \times 2\pi \text{ rad/s}$. Other parameters are: densities $n_{Rb} = n_{Na} = 8 \times 10^8 \text{ cm}^{-3}$, intra-species cross-sections $\sigma_{Na} = 2 \times 10^{-12} \text{ cm}^2$, $\sigma_{Rb} = 9 \times 10^{-12} \text{ cm}^2$.

In order to perform the simulations, we used an estimate for the cross-section between Na and Rb obtained from our experimental studies of the inter-species²² collisions. From our result, the sodium loss rate due to the collision with rubidium is $\beta^* n_{Rb} \sim 0.1/\text{s}$ (with a density of $n_{Rb} = 8 \times 10^8 \text{ cm}^{-3}$). And using a relative velocity of ~ 15 cm/s, we obtain the estimated Na-Rb cross section $\sigma_{Na-Rb} = 1.8 \times 10^{-12} \text{ cm}^2$. However, it should be noted that, even though this estimate is the best that can be inferred from the available data from two-species experiments, the true value of the inter-species cross-section is dependent on the yet undetermined inter-species scattering length. If the actual cross-section is much smaller than our estimate, the evaporative cooling process may need to be carried out at a slower rate in order to allow for efficient thermalization of the atomic samples during the evaporation process. As a first step in this investiga-

tion, we have modeled the thermalization of the two atomic clouds assuming that they are loaded into the magnetic trap with each species at its respective Doppler limited temperature (240 μK for Na and 120 μK for Rb). As shown in Fig. 3, we find that thermal relaxation occurs in a few hundred ms. Naturally, larger the inter-species cross section σ_{Na-Rb} is, the faster the system reaches its equilibrium.

The results of the evaporative cooling for the Na-Rb system are shown in Fig. 4. In Fig. 4(a), we see that after 50s (approximately 500 average collision times), more than 1% of the initial number of atoms remain in the trap. In Fig. 4(b), we note that due to the inter-species interaction, the system remains in equilibrium while evaporation takes place (except during the first second, where sympathetic cooling takes place). Fig. 4(c) displays the time dependence of the size of the samples together with the RF cut-off modeled in the manner described above. In Fig. 4(d), we show the time evolution of phase-space density ($n\lambda_{dB}^3$) for the Na-Rb system undergoing evaporative cooling.

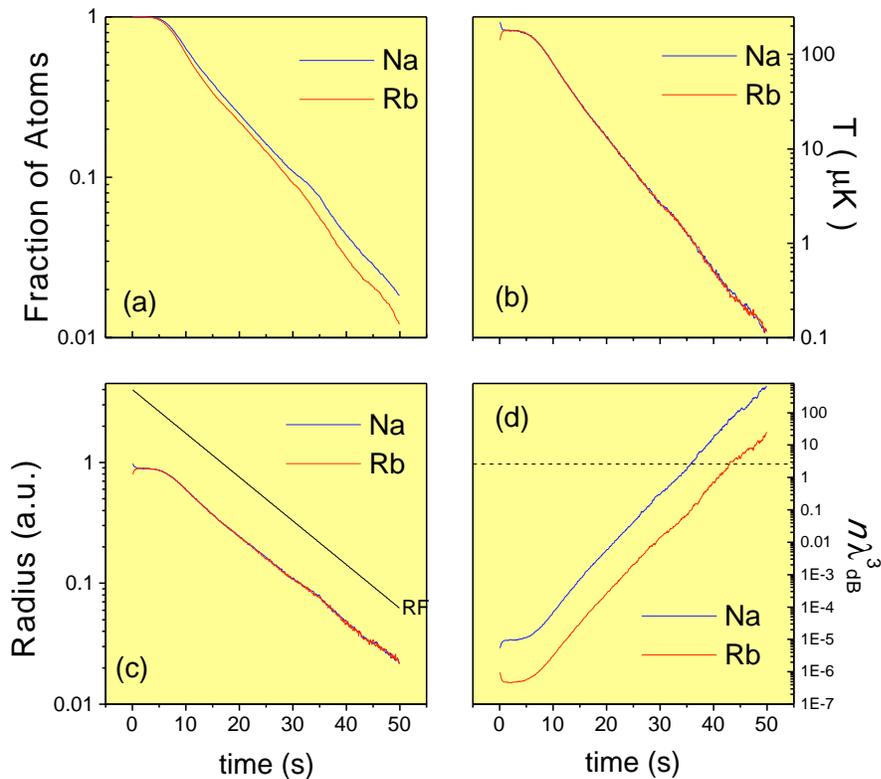


Figure 4. Evaporative cooling of a sample containing initially an equal number of Na and Rb atoms. (a) Fraction of atoms remaining as the evaporation takes place; (b) evolution temperature of the Na and Rb atoms; (c) average radius of the samples together with the cut-off imposed by the RF-field; (d) phase space density ($n\lambda_{dB}^3$) for each sample. The dashed line indicates the BEC border. Inter-species cross-section $\sigma_{Na-Rb} = 1.8 \times 10^{-12} \text{cm}^2$. Other parameters are the same as in Fig. 3.

The model described here assumes purely classical hard-sphere collisions and does not take into account the $(1+N)$ Bose-Einstein enhancement factor²⁹. Hence the penetration into the critical BEC boundary (defined by $n\lambda_{dB}^3 = 2.61$) should be considered as a conservative estimate. In sum, our simulations clearly indicate that evaporative

cooling has the power to increase phase-space density enough to expect that TBEC formation will occur for such conditions. In the animation (Fig. 5), the evaporative cooling path can be followed in phase space (temperature vs. density) so that the effectiveness of the process can be fully appreciated.

In order to more realistically study the formation of the two-species condensate, a version of the code that includes Bose statistics (which affect the collisional rate²⁹) is currently being utilized. Moreover, we are also taking full advantage of our multi-species capability to model the physics of sympathetic cooling, formation of Fermi-Bose mixtures and mixtures of Bose gases with various combinations of scattering lengths.

4. Conclusions and prospects

In summary, we have discussed some of the properties of the TBEC. We have shown that the nonlinear coupling between the two components gives rise to a rich set of new phenomena. We also modeled a two-species evaporative cooling process, indicating that it can lead to the formation of a TBEC. The territory of two inter-penetrating quantum fluids is still wide open and we believe that many exciting and unexpected new phenomena are waiting to be discovered.

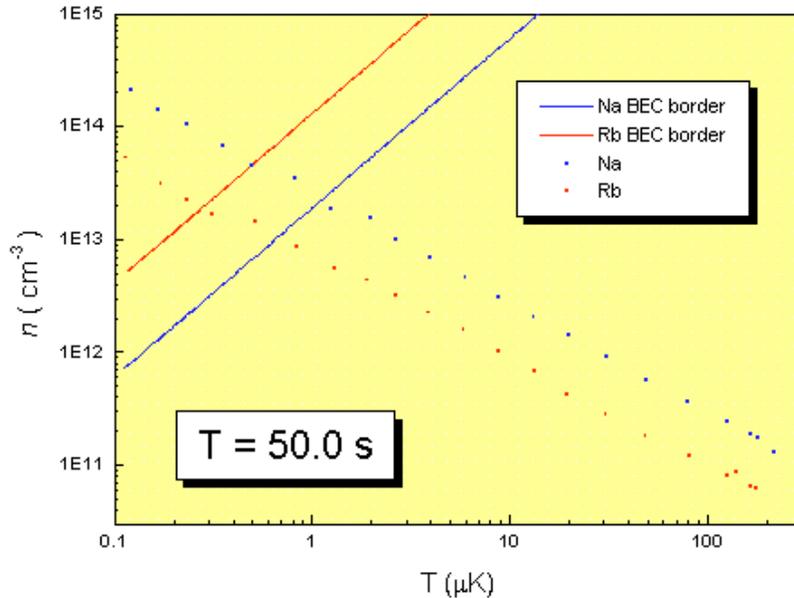


Figure 5. Evolution of the Na and Rb samples in phase space (density vs. temperature). The lines indicate the BEC boundary for Na and Rb. Parameters are the same as in Fig. 4.

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