"Stability Signature" in Two-Species Dilute Bose-Einstein Condensates

C. K. Law,[1] H. Pu,[1,2] N. P. Bigelow,[2] and J. H. Eberly[1]
[1]Rochester Theory Center for Optical Science and Engineering and Department of Physics and Astronomy,
University of Rochester, Rochester, New York 14627
[2]Laboratory for Laser Energetics and Department of Physics and Astronomy, University of Rochester,
Rochester, New York 14627

(Received 4 June 1997)

We identify an eigenvalue associated with a dilute two-species Bose-Einstein condensate as the determiner of condensate stability. It plays the same role as the sign of scattering length in a one-species condensate. We predict that there is a range of interspecies interaction strength in which a sodium-rubidium mixture can be stable in a harmonic trap. [S0031-9007(97)04343-3]

PACS numbers: 03.75.Fi

The recent realization of condensates of trapped rubidium atoms in two different spin states [1] has opened the field of two-species Bose-Einstein condensation. The problems of controlling condensate mixtures of two different atomic species, such as sodium and rubidium, are expected to be a future challenge for both theoretical and experimental studies. A unique feature of a two-species condensate is the presence of interspecies interactions, and several authors have indicated that condensate wave functions may exhibit novel features that do not exist for a pure system [2–4]. Recently it has been shown that the spatial regions occupied by different components can be "tuned" by changing the number of atoms in each species [4]. Although previous studies have provided detailed descriptions of ground state density distributions within the mean-field theory, general properties of a two-species condensate are still open topics. In particular, problems involving quantum fluctuations would require theories that go beyond the mean-field description.

A main question of two-species condensates is how to identify the stability properties of the mixtures [5]. In the case of one-species condensates of dilute gas, the sign of atom-atom interactions (i.e., repulsive or attractive) determines the intrinsic stability of the system against runaway collapse. For example, a single condensate with repulsive interactions is never unstable, but a condensate with attractive interactions may be [6–8]. Hence for a one-species system, the sign of the particle-particle interaction can be treated as a *stability signature*. Now the problem is whether a two-species condensate has a similar stability signature which distinguishes the stability nature of the system. The answer is not obvious because of the presence of interspecies interactions. In fact Goldstein and Meystre have shown that instability may occur even if all the interactions (intraspecies and interspecies) are repulsive [9]. Therefore the sign of the interactions alone does not determine the stability of the system.

In this paper we describe a method to find the *stability signature* of a dilute two-species condensate mixture. The main idea of our method is to represent the quantum fluctuations around the mean-field ground state in a suitable basis, and then show that the sign of an eigenvalue provides the same key as the sign of the scattering length in the one-species case. With this method, we can provide a uniform treatment for the characterization of the stability properties of both one-component and multicomponent condensates. There are several advantages of our approach. First, a stability test of the system can be performed efficiently because only the sign of one eigenvalue needs to be computed. Second, a connection between stability and particle number fluctuations can be established. Such a connection has not been found in previous time-dependent mean-field approaches [9–11]. In this paper, we shall also examine the case of a sodium-rubidium mixture in a harmonic trap, and we show that there is a finite range of interspecies interaction strengths within which the mixture can be stable.

To begin, we consider a second-quantized grand canonical Hamiltonian of two interacting trapped species

$$K = \sum_{j=1}^{2} \left[\int d^3x \, \Psi_j^\dagger h_j \Psi_j + \frac{g_j}{2} \int d^3x \, \Psi_j^\dagger \Psi_j^\dagger \Psi_j \Psi_j \right] + g_{12} \int d^3x \, \Psi_1^\dagger \Psi_2^\dagger \Psi_1 \Psi_2 , \qquad (1)$$

where Ψ_j $(j = 1, 2)$ is the atomic field annihilation operator for the jth species, and the single particle operator h_j is defined by

$$h_j = -\frac{\hbar^2}{2M_j} \nabla^2 + U_j - \mu_j \qquad j = 1, 2 . \qquad (2)$$

Here U_j is the trapping potential, M_j is the atomic mass of the species j, and μ_j is the chemical potential which preserves average particle numbers. For weakly interacting dilute gases, the interactions between atoms are modelled by δ potentials [12,13]. We have used g_j to describe the interaction strength within the same species, and g_{12} for the interaction strength between species 1 and 2. In this paper, we neglect the effects due to spin-exchange collisions.

At the temperature $T = 0$ K, we linearize the Hamiltonian (1) by assuming [14]

$$\Psi_j = \sqrt{N_j}\,\phi_{j0} + \psi_j\,. \tag{3}$$

Here N_j is the average atom number of species j, and the condensate (c number) wave functions ϕ_{j0} are the ground states of the self-consistent Hartree-Fock nonlinear equations [3,4], defined by,

$$(h_1 + g_1 N_1 \phi_{10}^2 + g_{12} N_2 \phi_{20}^2)\phi_{10} = 0\,, \tag{4}$$

$$(h_2 + g_2 N_2 \phi_{20}^2 + g_{12} N_1 \phi_{10}^2)\phi_{20} = 0\,. \tag{5}$$

Notice that ϕ_{j0} are taken to be real because any (constant) phases that may appear in ϕ_{j0} can be removed by redefining Ψ_j. The fluctuations part of Ψ_j is described by ψ_j which obeys the usual equal-time commutation relations $[\psi_j(\vec{x}), \psi_k(\vec{x}')] = 0$, $[\psi_j(\vec{x}), \psi_k^\dagger(\vec{x}')] = \delta_{jk}\delta(\vec{x} - \vec{x}')$.

The linearized Hamiltonian is obtained by discarding fluctuations beyond the second order. We can also drop the c-number terms, and we obtain a compact expression for the quadratic Hamiltonian,

$$K' = \frac{1}{2}\sum_{i,j=1}^{4}\int d^3x\, V_i^\dagger M_{ij} V_j\,. \tag{6}$$

Here $(V_1, V_2, V_3, V_4) \equiv (\psi_1, \psi_2, \psi_1^\dagger, \psi_2^\dagger)$ and the matrix M is Hermitian and its diagonal elements are $M_{11} = M_{33} = h_1 + g_{12} N_2 \phi_{20}^2 + 2 g_1 N_1 \phi_{10}^2$, $M_{22} = M_{44} = h_2 + g_{12} N_1 \phi_{10}^2 + 2 g_2 N_2 \phi_{20}^2$ and the off-diagonal elements are $M_{12} = M_{23} = M_{34} = M_{41} = g_{12}\sqrt{N_1 N_2}\,\phi_{10}\phi_{20}$, $M_{13} = g_1 N_1 \phi_{10}^2$, and $M_{24} = g_2 N_2 \phi_{20}^2$.

We define the two-species system to be stable if all eigenvalues of M are non-negative (i.e., M is semipositive). We define the system to be unstable if the lowest eigenvalue of M is negative. These criteria are justified by the fact that arbitrary nonzero small fluctuations ψ_j *do not decrease the energy* of the system if the system meets our definition of stability. Here the energy refers to the expectation value of K' associated with the fluctuations. We emphasize that our criteria are general enough to account for all possible fluctuations ψ_j, including the fluctuations of particle numbers. As we shall see later, the consideration of stability against changes of particle numbers would provide a way to "probe" the effective interactions between particles, and hence the stability signature of the system.

It is important that the lowest eigenvalue of M also determines the stability of the mean fields. Since the evolution of the mean fields is governed by the coupled time-dependent nonlinear Schrödinger equations [9–11], small perturbations of the mean fields will remain bounded if all the normal mode frequencies (or the collective excitation frequencies [15]) of the linearized system are real. Indeed, a semipositive M guarantees real normal mode frequencies, and hence ensures stability of the mean fields. A necessary but not sufficient condition for mean fields to be unstable, i.e., to have complex normal mode frequencies, is for the lowest eigenvalue of M to be negative [16].

To simplify the eigenvalue problem of M, we make a unitary transformation so that

$$U^\dagger M U = \begin{pmatrix} L_1 & 0 \\ 0 & L_2 \end{pmatrix}, \tag{7}$$

where L_1 and L_2 are given by

$$L_1 = \begin{pmatrix} M_{11} - g_1 N_1 \phi_{10}^2 & 0 \\ 0 & M_{22} - g_2 N_2 \phi_{20}^2 \end{pmatrix}, \tag{8}$$

$$L_2 = \begin{pmatrix} M_{11} + g_1 N_1 \phi_{10}^2 & 2M_{12} \\ 2M_{21} & M_{22} + g_2 N_2 \phi_{20}^2 \end{pmatrix}. \tag{9}$$

Notice that $M_{11} - g_1 N_1 \phi_{10}^2$ and $M_{22} - g_2 N_2 \phi_{20}^2$ are the same as the self-consistent Hartree-Fock Hamiltonians that appear in the brackets on the left sides of Eqs. (4) and (5). Therefore the eigenvalues of L_1 must be non-negative because ϕ_{j0} were already defined as ground states. The branch of eigenvalues associated with L_2 can be negative. Therefore the system is stable if L_2 has a non-negative lowest eigenvalue, and the system is unstable if L_2 has a negative lowest eigenvalue. Thus the lowest eigenvalue of L_2 can be treated as a *stability signature* of the system. This generalizes the case of one-species systems in which the corresponding lowest eigenvalue is negative (positive) if the atom-atom interaction is attractive (repulsive).

An obvious application of our method is to the recent realization of rubidium condensates in two different spin states [1], and our analysis predicts stability in such a case even in the absence of gravity. However, a much more interesting case is presented by a true two-species situation, for example, the mixture of sodium and rubidium condensates. In Fig. 1 we plot λ, the lowest eigenvalue of L_2, as a function of interspecies scattering length a_{12} (which is proportional to g_{12}) for this case. Here we have considered a mixture of sodium and rubidium atoms of equal numbers in a spherical harmonic trap. We see that the system is stable only for a finite range of a_{12}. The onset of instability occurs when λ is zero, and λ drops rapidly for a sufficiently large negative a_{12} which indicates a highly unstable system. This should be expected because large attractive interactions can collapse the system as in the single-species case. However, we see that there is still a finite range of negative a_{12} where the system can be stable. It is interesting to note that a large positive a_{12} can also introduce instability. We remark that the stability of the system depends on the number of atoms in the condensates. We have made several calculations for $N_1 \approx N_2$ in a range of 10^3–10^4, but we find that the stable region in Fig. 1 changes only slightly (within 10%). Our numerical calculations also verify that the collective excitation frequencies are real in the stable regime, and some of the excitation frequencies become complex in the unstable regime defined by the λ curve.

The nature of the instability near the critical point $\lambda = 0$ is related to fluctuations of particle numbers in the condensates. To explain this, let us calculate how

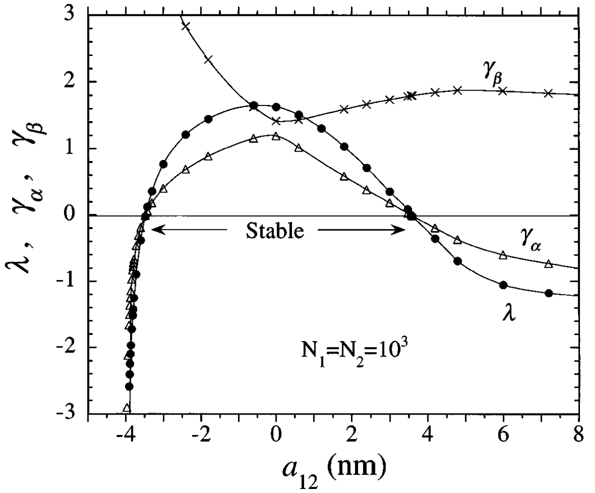

FIG. 1. Plots of λ, the lowest eigenvalue of the matrix L_2 (circles), the coefficient γ_α (triangles), and the coefficient γ_β (crosses) as functions of a_{12}, the scattering length between species 1 and 2. Here $g_{12} = 2\pi\hbar^2 a_{12}/m$, with m being the reduced mass of the two species. In our calculations, we take Rb $|F = 2, m_F = 2\rangle$ as species 1 and Na $|F = 1, m_F = -1\rangle$ as species 2, with scattering lengths taken as 6 and 3 nm, respectively. The respective trapping frequencies are: $\omega_1 = 2\pi \times 160$ Hz and $\omega_2 = 2\pi \times 310$ Hz, assuming the magnetic moments are the same for the two species. λ, γ_α, and γ_β are presented in units of $\hbar\omega_1$. In this calculation, the condensate wave functions are assumed to be spherically symmetric [17].

much energy δK is required in order to push the system to a new condensate state where the particle numbers are shifted by δn_j, while keeping the chemical potentials fixed. The δK is defined by

$$\delta K = \langle K \rangle_{\phi'} - \langle K \rangle_{\phi} \,. \tag{10}$$

Here $\langle K \rangle_\phi$ is the value of K obtained by substituting $\Psi_j = \sqrt{N_j}\, \phi_{j0}$ in Eq. (1), and $\langle K \rangle_{\phi'}$ is obtained by substituting $\Psi_j = \sqrt{N_j + \delta n_j}\, \phi'_{j0}$ in Eq. (1), where ϕ'_{j0} are new condensate wave functions with respect to the new particle numbers $N_j + \delta n_j$. After some tedious calculations [18], we find that for $N_j \gg \delta n_j$

$$\delta K \approx \frac{\gamma_\alpha}{2} (\delta\tilde{n}_1 \cos\theta - \delta\tilde{n}_2 \sin\theta)^2 + \frac{\gamma_\beta}{2} (\delta\tilde{n}_1 \sin\theta + \delta\tilde{n}_2 \cos\theta)^2, \tag{11}$$

where $\delta\tilde{n}_j \equiv \delta n_j / N_j^{1/2}$, and the constants γ_α and γ_β are determined from the coupled equations,

$$L_2 \begin{bmatrix} A_\alpha \\ B_\alpha \end{bmatrix} = \gamma_\alpha \begin{bmatrix} \phi_{10} \cos\theta \\ -\phi_{20} \sin\theta \end{bmatrix}, \qquad L_2 \begin{bmatrix} A_\beta \\ B_\beta \end{bmatrix} = \gamma_\beta \begin{bmatrix} \phi_{10} \sin\theta \\ \phi_{20} \cos\theta \end{bmatrix} \tag{12}$$

with the normalization,

$$\int d^3x\, A_\alpha \phi_{10} = \int d^3x\, B_\beta \phi_{20} = \frac{1}{2} \cos\theta \,, \tag{13}$$

$$\int d^3x\, A_\beta \phi_{10} = -\int d^3x\, B_\alpha \phi_{20} = \frac{1}{2} \sin\theta \,. \tag{14}$$

It can be shown that Eqs. (12)–(14) uniquely determine the functions A_α, A_β, B_α, B_β, the angle θ, and the γ's.

The connection between our stability criterion and δK becomes clear as the same L_2 appears in Eq. (12). It is easy to show that γ_α and γ_β must be non-negative when $\lambda \geq 0$, and γ_α (or γ_β) is negative only when $\lambda < 0$. In fact we can show that one of the γ's always has the same sign as λ in the vicinity of critical points $\lambda = 0$. This is an important result because the onset of instability is always accompanied by a sign change of one of the γ's. In Fig. 1, we plot the values of γ_α and γ_β corresponding to the values of λ. We see that γ_α indeed behaves like λ, which turns negative in the unstable regimes.

Since an increase of particle numbers δn_j adds an energy δK to the system with respect to fixed chemical potentials, the instability arising from negative γ_α signals a tendency of increasing $\delta\tilde{n}_1 \cos\theta - \delta\tilde{n}_2 \sin\theta$. This means that an unstable system cannot maintain the given particle numbers N_1 and N_2. In Fig. 1, we find that $\theta \approx \pi/4$ for positive g_{12} and $\theta \approx -\pi/4$ for negative g_{12}, near the critical points ($\lambda = 0$). Therefore an unstable system with a repulsive interspecies interaction tends to increase the *difference* of particle numbers in order to attain a lower energy. Similarly, an attractive interaction tends to increase the *sum* of particle numbers.

It is helpful to compare Eq. (11) with the corresponding equation for the one-species case: $\delta K \approx \gamma(\delta\tilde{n})^2/2$, where γ has the same sign as the scattering length. Therefore Eq. (11) suggests that the two-species system can be considered as two decoupled *quasispecies* associated with γ_α and γ_β, and the parameter θ can be interpreted as the quasispecies *mixing angle*. The effective change of particle numbers for the two quasispecies are $(\delta\tilde{n}_1 \cos\theta - \delta\tilde{n}_2 \sin\theta)$ and $(\delta\tilde{n}_1 \sin\theta + \delta\tilde{n}_2 \cos\theta)$, respectively. In this way a quasispecies with a negative γ_α is like a one-species condensate with an attractive self-interaction. The new feature here is that the particle numbers for the quasispecies are mixed in a linear combination of particle numbers of the original species. We point out that the decoupled quasispecies picture appears more naturally in the diagonalized Hamiltonian at low temperature where collective excitations can be ignored. In that case we find that the diagonalized Hamiltonian contains only two independent degrees of freedom,

$$K' = \frac{\gamma_\alpha P_\alpha^2}{2} + \frac{\gamma_\beta P_\beta^2}{2} + (\cdots)\,, \tag{15}$$

where $(\cdots)$ are collective excitation modes, and $P_\alpha \equiv P_1 \cos\theta - P_2 \sin\theta$ and $P_\beta \equiv P_1 \sin\theta + P_2 \cos\theta$, with

$$P_j = \int d^3x\, \phi_{j0} (\psi_j + \psi_j^\dagger) \qquad j = 1, 2\,. \tag{16}$$

Since P_α and P_β commute with each other, we may interpret these two decoupled degrees of freedom as two quasispecies.

As an interesting remark, expression (15) can be used to study the fluctuations of quantum phases of the condensate wave functions. Lewenstein and You [19] have derived an expression equivalent to (15) for a one-species system, and they indicated that the corresponding γ determines the quantum phase-diffusion rate. Such a diffusive behavior is due to the fluctuations of particle numbers and the nonlinearity of particle-particle interactions [19,20]. Their result can be generalized to our two-species system as given in (15). We have found that γ_α and γ_β indeed determine the diffusion rates of quantum phases associated with the condensate wave functions. At the critical point $\gamma_\alpha = 0$ the diffusion rate is zero, which implies a perfect phase locking effect. This interesting effect will be discussed elsewhere [21].

In conclusion, we have departed from the mean-field equations to develop an efficient method to test the stability of a trapped two-species dilute condensate near zero temperature. The method provides a uniform way to identify the "stability signature" relevant for multicomponent dilute condensates, including the one-species case. We found that the stability signature is not determined by the sign of interactions, but by the lowest eigenvalue of L_2. As the sign of the eigenvalue changes to negative, the system behaves as if it has attractive self-interactions. We have applied our model to study a sodium-rubidium mixture in a harmonic trap. Our calculations predict that there is a finite range of interspecies interaction strength in which the mixture is stable. There are many open questions regarding the behavior of unstable condensates, for example, the nature of the dynamics in unstable regimes and whether or not a true ground state exists there. These questions may require a more sophisticated analysis beyond linear approximations, and details of interaction potentials between particles may become important. Further investigations would be necessary.

We thank Professor W. Reinhardt for discussions. This research was supported by NSF Grants No. PHY-9415583 and No. PHY-9457897, and the David and Lucile Packard Foundation.

---

[1] C. J. Myatt *et al.,* Phys. Rev. Lett. **78**, 586 (1997).

[2] Tin-Lun Ho and V. B. Shenoy, Phys. Rev. Lett. **77**, 3276 (1996).

[3] B. D. Esry *et al.,* Phys. Rev. Lett. **78**, 3594 (1997).

[4] H. Pu and N. Bigelow (to be published).

[5] For an early study in the stability of a multicomponent superfluid system, see A. F. Andreev and E. P. Bashkin, Sov. Phys. JETP **42**, 164 (1976).

[6] One-species homogeneous systems with attractive particle-particle interactions were predicted to be unstable. See L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, London, 1958), 1st ed.

[7] The issue of stability for inhomogenous one-species systems with attractive interactions was discussed, for example, by P. A. Ruprecht *et al.,* Phys. Rev. A **51**, 4704 (1995); Y. Kagan, G. V. Shlyanikov, and J. T. M. Walraven, Phys. Rev. Lett. **76**, 2670 (1996); R. J. Dodd *et al.,* Phys. Rev. A **54**, 661 (1996); E. V. Shuryak, Phys. Rev. A **54**, 3151 (1996); M. Houbiers and H. T. C. Stoof, Phys. Rev. A **54**, 5055 (1996).

[8] C. C. Bradley *et al.,* Phys. Rev. Lett. **75**, 1687 (1995); C. C. Bradley, C. A. Sackett, and R. G. Hulet, Phys. Rev. Lett. **78**, 985 (1997).

[9] E. V. Goldstein and P. Meystre, Phys. Rev. A **55**, 2935 (1997).

[10] R. Graham and D. Walls, cond-mat/9611111.

[11] Th. Busch, J. I. Cirac, V. M. Perez-Garcia, and P. Zoller, cond-mat/9705008.

[12] K. Huang, *Statistical Mechanics* (Wiley, New York, 1987).

[13] M. Lewenstein and L. You, Phys. Rev. A **53**, 909 (1996).

[14] This is the same strategy as in one-species systems. See A. L. Fetter, Ann. Phys. (N.Y.) **70**, 67 (1972).

[15] The collective excitation frequencies are defined by

$$\eta M \begin{bmatrix} u_{1k} \\ u_{2k} \\ v_{1k} \\ v_{2k} \end{bmatrix} = \omega_k \begin{bmatrix} u_{1k} \\ u_{2k} \\ v_{1k} \\ v_{2k} \end{bmatrix},$$

$$\eta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix},$$

with $(u_{1k}, u_{2k}, v_{1k}, v_{2k})$ being the mode functions.

[16] For properties of M for general systems, see J. P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (MIT Press, Cambridge, MA, 1986).

[17] For calculations of an asymmetric condensate wave function in a two-dimensional trap, see P. Öhberg and S. Stenholm, cond-mat/9708110.

[18] To derive Eq. (11), we calculate the new condensate wave functions ϕ'_{j0}. This is done by expanding ψ_j in terms of collective excitation modes, including two "zero modes" [defined in Eq. (12)]. The procedure is based on the method given in Ref. [19] for one-species problems. We find that the zero-mode functions are in fact the corrections of the condensate wave functions when the particle number is slightly shifted.

[19] M. Lewenstein and L. You, Phys. Rev. Lett. **77**, 3489 (1996).

[20] A. Imamoglu, M. Lewenstein, and L. You, Phys. Rev. Lett. **78**, 2511 (1997).

[21] C. K. Law *et al.* (unpublished).