Collective Excitations, Metastability, and Nonlinear Response of a Trapped Two-Species Bose-Einstein Condensate

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We present a new theoretical treatment of the collective excitation spectrum of a two-species Bose-Einstein condensate confined in a magnetic trap. We show that the interspecies interaction significantly modifies the excitation spectrum and gives rise to a rich set of new phenomena. We identify a novel metastable state of the double condensate and show that under external perturbation there can be a macroscopic quantum transition between this metastable state and the true ground state of the double condensate system. [S0031-9007(97)05175-2]

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Since the first observation of Bose-Einstein condensation (BEC) in a dilute alkali vapor [1], substantial effort has been made to study the properties of these weakly interacting trapped degenerate Bose gases. As theory and experiment have advanced, a new rich phenomenology has appeared in which new conditions arise, conditions which are not accessible in other BEC systems. One of the most stunning of these has been the recent experimental demonstration of a condensate mixture composed of two spin states of ^{87}Rb [2]. This observation has prompted significant interest in the physics of a new class of quantum fluids: the two-species Bose Einstein condensate (TBEC). Fundamental issues distinguish the trapped TBEC from the single species BEC, and at the heart of many of these issues is the presence of interspecies interactions and the resulting coupling of the two condensates. Previous theoretical treatments have shown that due to interspecies interactions, the ground state density distribution of a TBEC can display novel structures that do not exist in a one-species condensate [3,4]. In support of this, in the recent ^{87}Rb experiments, the measured density profiles of the two-spin state condensates indicated that there were observable consequences of the interactions between the two condensates. However, due to gravitational effects, the trap centers of each of the condensates were separated and a detailed theoretical analysis of the data was needed before the condensate coupling effect could be placed on firm grounds [5].

To better understand the properties of the TBEC, important questions remain to be answered. For example: How do the interactions affect the excitation spectra and stability of the condensates? How will the condensates evolve under external perturbations? These questions are the subject of the present Letter.

One of the fundamental properties of the confined condensate lies in the nature of the collective excitations. For single species alkali BEC, two research groups have experimentally measured some of the excitation frequencies [6], and theoretical calculations based on the Bogoliubov-Hartree theory [7,8] have shown excellent agreement with many of the experimental results. As a natural starting point to our TBEC investigation, we have numerically calculated the excitation spectra of a TBEC confined in an isotropic harmonic trap. We find that the spectra are significantly modified by the coupling between different species: the mode frequencies of the individual condensates are shifted and imaginary frequency (i.e., unstable) modes are found to exist for large repulsive interspecies interactions. Next we have carried out a nonlinear response analysis and discovered that the interspecies interaction gives rise to excitation modes of different symmetry analogous to the modes of two coupled pendulums and that harmonic generation can occur. Our analysis allows us to demonstrate the existence of novel metastable states of the TBEC. We show that under sufficiently strong external perturbation this metastable state will jump to a different more stable state, a phenomenon that may be regarded as a macroscopic quantum transition.

At zero temperature, the self-consistent nonlinear Schrödinger equations, known as Gross-Pitaevskii equations (GPE's), for a TBEC may be written as [3–5]

$$i\hbar \frac{\partial \psi_1(r,t)}{\partial t} = [T_1 + V_1 + N_1 U_1 |\psi_1|^2 + N_2 U_{12} |\psi_2|^2]\psi_1 , \quad (1a)$$

$$i\hbar \frac{\partial \psi_2(r,t)}{\partial t} = [T_2 + V_2 + N_2 U_2 |\psi_2|^2 + N_1 U_{12} |\psi_1|^2]\psi_2 , \quad (1b)$$

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. $T_i = -\hbar^2\nabla^2/2m_i$ and $V_i = m_i\omega_i^2 r^2/2$ are the respective kinetic and potential energy operators. The interaction between particles is 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

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species $U_{12} = 2\pi\hbar^2 a_{12}/[m_1 m_2/(m_1 + m_2)]$, where a_i is the scattering length of species i and a_{12} that between species 1 and 2. The time-independent GPE's are obtained by replacing the left-hand sides of Eqs. (1) with $\mu_i \psi_i(r)$ $(i = 1,2)$, with μ_i being the chemical potential.

To calculate the excitation frequencies within the Bogoliubov approximation [9], we first derive the Bogoliubov equations using the linear response method described by Ruprecht *et al.* [10]. Let the time-dependent wave functions $\psi_i(r,t)$ take the following form:

$$\sqrt{N_i}\,\psi_i(r,t) = e^{-i\mu_i t/\hbar}[\sqrt{N_i}\,\psi_i(r) + u_i(r)e^{-i\omega t} + v_i^*(r)e^{i\omega t}]. \tag{2}$$

After inserting Eq. (2) into Eqs. (1), retaining only terms up to first order in $u_i(r)$ and $v_i(r)$, and equating like powers of $e^{\pm i\omega t}$, we derive the equations for $u_i(r)$ and $v_i(r)$ which can be cast into a matrix form:

$$M\phi_\lambda = \omega_\lambda\,\eta\,\phi_\lambda, \tag{3}$$

where $\phi_\lambda = (u_{1\lambda}, u_{2\lambda}, v_{1\lambda}, v_{2\lambda})^T$ is the mode function of the TBEC with mode frequency ω_λ. The matrices M and η have the following forms:

$$M = \begin{pmatrix} H^{(1)} & \tilde{U} & N_1U_1\psi_1^2 & \tilde{U} \\ \tilde{U} & H^{(2)} & \tilde{U} & N_2U_2\psi_2^2 \\ N_1U_1\psi_1^2 & \tilde{U} & H^{(1)} & \tilde{U} \\ \tilde{U} & N_2U_2\psi_2^2 & \tilde{U} & H^{(2)} \end{pmatrix},$$
$$\eta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{4}$$

where $\tilde{U} = \sqrt{N_1N_2}\,U_{12}\psi_1\psi_2$, and $H^{(i)} = T_i + V_i - \mu_i + 2N_iU_i\psi_i^2 + N_jU_{12}\psi_j^2$ $(i,j = 1,2;\ i \neq j)$. Here $\psi_1(r)$ and $\psi_2(r)$ are ground state wave functions which, without loss of generality, are assumed to be real. Applying the finite difference approximation [4], the problem of computing the normal modes is cast in the form of a generalized-eigenvalue problem, which can be solved using standard numerical software packages. A distinguishing feature of our approach is that we include the full coupled Hamiltonian [see Eqs. (1)] in our solution without making the Thomas-Fermi approximation (TFA) (i.e., without neglecting the kinetic terms). This fact is important since the widely used TFA [3–5,11] has been shown to be quantitatively unreliable in the treatment of the TBEC [5].

As in the case of a one-species condensate, the mode frequencies occur in equal magnitude pairs of opposite sign in our solutions. This can be understood because if $\omega_\lambda \to -\omega_\lambda$ and if $u_{i\lambda}$ and $v_{i\lambda}$ are exchanged, then Eq. (3) remains unchanged. The zero mode is twofold degenerate, with mode function $(u_{10}, u_{20}, v_{10}, v_{20}) = (\psi_1, 0, -\psi_1, 0)$ or $(0, \psi_2, 0, -\psi_2)$, and a corresponding frequency $\omega_0 = 0$.

In a 3D spherical potential, the excitation frequencies ω_λ depend on the radial and angular momentum quantum numbers n and l [7]. A sufficient condition for ω_λ to be real is that matrix M is semipositive [12]. Our numerical studies show that, if all the other parameters are fixed, M is semipositive for a finite range of interspecies scattering length a_{12}. This range characterizes the stable region of the TBEC [13]. Figure 1 shows the first two mode frequencies for $l = 1$ (for convenience, assuming both species have the same angular momentum) as functions of a_{12}. In our calculations, we take Rb as species 1 and Na as species 2, with scattering lengths taken as 6 and 3 nm, respectively. For the trap, we assume $\omega_1 = 2\pi \times 160$ Hz and $\omega_2 = 2\pi \times 310$ Hz. At $a_{12} = 0$ (for two uncoupled condensates), the values of these two mode frequencies do not depend on particle numbers. In fact, they are exactly equal to the respective trap frequencies for Rb and Na (in our dimensionless units, they are 1 and 1.945, respectively). In these modes, the atoms in each condensate slosh back and forth as a whole, such that the motion is not affected by the interactions between the atoms. Interspecies interactions significantly alter the mode spectra. For negative a_{12}—which means there exists an attractive interaction between Rb and Na—both frequencies shift upward. This can be understood as each condensate sees a somewhat tighter trap due to the extra attractive potential imposed by the other condensate. For positive a_{12}, the opposite is true: mode frequencies decrease as a_{12} increases. At a critical value of a_{12}, the $n = 0$ mode frequency reaches zero. Beyond that critical value, the frequency becomes imaginary (in this region, matrix M has negative eigenvalues). Imaginary excitation frequencies mean that fluctuations above the condensate can grow exponentially in time. Thus, a large repulsive interaction between the two species can induce instability in the system [14].

In Fig. 2, we illustrate the first three isotropic breathing modes (corresponding to $l = 0$, excluding the zero mode) as functions of a_{12}. Unlike the $l = 1$ modes shown in Fig. 1, these modes are not monotonic functions of a_{12}. Instead, they reach minima at a positive value of a_{12} and never become imaginary. As indicated in Fig. 2, for positive a_{12}, the lowest lying mode is an out-of-phase mode in which the Rb and Na density distributions oscillate with a 180° phase difference. This can be intuitively understood by realizing that for a repulsive interaction, the excitation

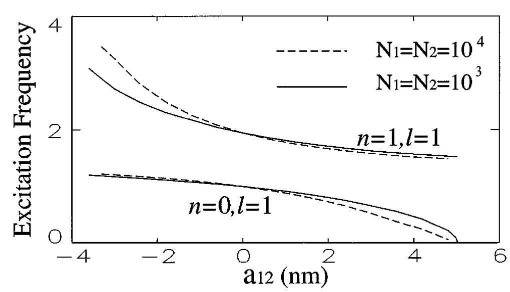

FIG. 1. Spectra for the first two $l = 1$ modes as functions of a_{12}. The units for frequency is ω_1.

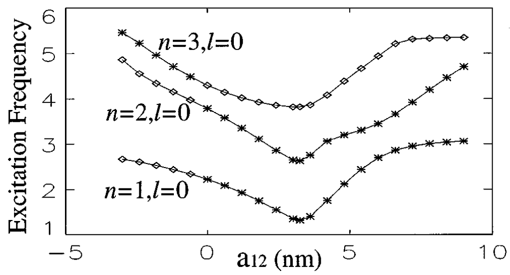

FIG. 2. First three nonzero isotropic ($l = 0$) modes as functions of a_{12}. Diamonds: in-phase mode; Stars: out-of-phase mode. Solid lines are guides to eyes. Here $N_1 = N_2 = 10^4$.

mode energy is lowered when the time averaged overlap of the condensates is minimized. Naturally, higher lying modes include in-phase motion. Similarly, we find that an in-phase mode becomes the lowest lying mode if a_{12} is negative since the time averaged overlap of the condensates is maximized in this mode.

The values of the isotropic mode frequencies and the mode type (whether it is an out-of-phase or in-phase mode) are verified by a nonlinear response analysis [10]. We introduce a small sinusoidal modulation to the trapping potential with modulation frequency Ω, and let the initial wave functions be the solutions to the time-independent GPE's. The wave functions at a later time t are obtained by direct integration of the time-dependent GPE's [Eqs. (1)] using the Crank-Nicholson method. Figures 3(a)–3(c) show the density for both species at the center of the trap as a function of time. Figure 3(a) represents an off-resonant modulation. The fluctuations remain small as compared to Figs. 3(b) and 3(c) where the modulation frequency Ω equals to an out-of-phase mode and in-phase mode frequency, respectively. Figures 3(a′)–3(c′) display the respective Fourier spectra of the Rb density fluctuations depicted in 3(a)–3(c). For an off-resonance perturbation [Fig. 3(a′), the intensity of the spectrum is increased by a factor of 5 in this plot], we see a weak response at the driving frequency Ω and the first few normal mode frequencies. For the on-resonance perturbation [Figs. 3(b′) and 3(c′)], not only is the response at Ω much stronger, but the oscillation spectrum also shows higher harmonics [15]. The marked difference between the off- and on-resonance, as well as the in-phase and out-of-phase response allows us to identify the resonance frequencies and the mode types.

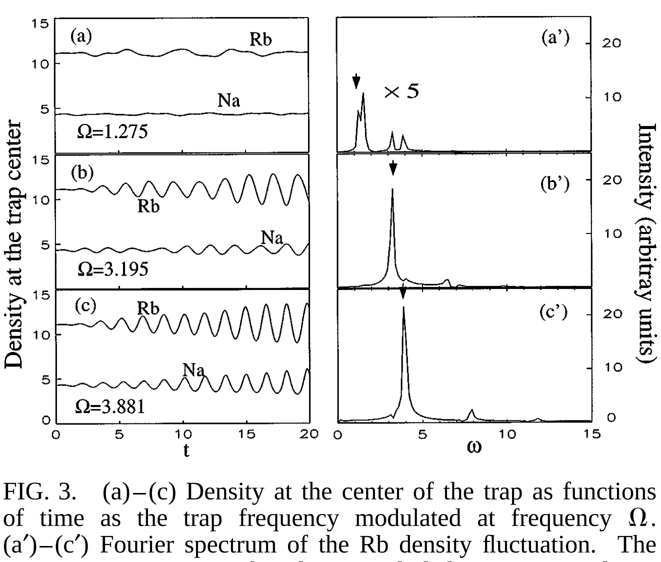

FIG. 3. (a)–(c) Density at the center of the trap as functions of time as the trap frequency modulated at frequency Ω. (a′)–(c′) Fourier spectrum of the Rb density fluctuation. The component at $\omega = 0$ has been excluded. Arrows indicate the positions of the driving frequency Ω. The units for density and time are $(2m_1\omega_1/\hbar)^{3/2}$ and $1/\omega_1$, respectively. Here $N_1 = N_2 = 10^3$, $a_{12} = 3.6$ nm. The first three nonzero isotropic excitation frequencies are 1.575, 3.195, and 3.881.

Another feature of this nonlinear response analysis is that it can be used to investigate the mechanical stability of the wave functions. Figures 4(a) and 4(b) display two possible solutions to the time-independent GPE's. In both solutions the two condensates have become segregated into a central core dominated by one species with an outer shell of the second species, the difference between the two being which atom comprises the core and which comprises the shell. In Figs. 4(a′) and 4(b′) we illustrate the respective time evolution of the initial wave functions plotted in 4(a) and 4(b) under external drive. In both cases the trapping potentials are modulated with the same frequency and amplitude. Figure 4(a′) shows a typical off-resonance response expected for a stable ground state—the condensates oscillate around their equilibrium state. On the other hand, as can be seen in 4(b′), the state represented by 4(b) is not unconditionally stable: under a sufficiently strong external perturbation the initial state (b) makes a sudden jump to the other state (a). A calculation of the expectation value of Hamiltonian confirms that the energy of state (a) is, in fact, lower than that of (b). We point out that the jump from state (b) to (a) will not occur if the perturbation is not strong enough. Hence, state (b) represents a metastable state of the TBEC. These macroscopic metastable states arise from the interspecies interactions and hence are unique for the multicomponent condensates. We suggest that the jump between such metastable and stable states may be regarded as a macroscopic quantum transition, a novel phenomenon whose detailed dynamics is currently under investigation. Our calculations confirm that it is possible to generate such a metastable state experimentally. For example, if the Na condensate is formed prior to the Rb condensate such that the Rb atoms condense in the presence of the preexisting, repulsive Na condensate core, then the Rb will condense into the metastable shell.

In summary, we have used a nonlinear response analysis and an extended Bogoliubov-Hartree theory to investigate the collective excitation spectra for a trapped TBEC. We have shown that the coupling between the condensates has a dramatic effect on the excitation spectrum and can give rise to a novel metastable state. Finally, we have found that imaginary frequencies exist in nonisotropic modes for strong repulsive interspecies

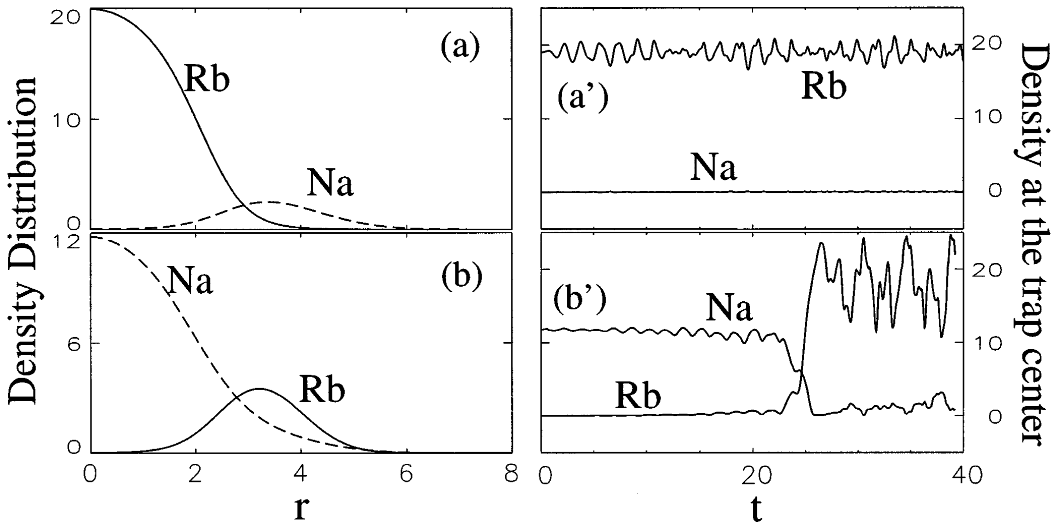

FIG. 4. (a),(b) Two sets of solutions to the time-independent GPE's. (a) Represents the ground state; (b) represents a metastable state. (a′),(b′) Density at the center of the trap as functions of time under an off-resonance modulation of the trapping potential. The unit for length is $(\hbar/2m_1\omega_1)^{1/2}$. Parameters: $N_1 = N_2 = 10^3$, $a_{12} = 9.6$ nm.

interactions. We note that although we have not taken gravity into account, even when gravity is included the essence of our results remain intact for realistic choices of atomic species, spin states, and trapping potentials. The main effect of including gravity is to break the perfect spherical symmetry of the condensates. This change will quantitatively but not qualitatively modify our results.

Goldstein and Meystre have shown that a homogeneous (untrapped) TBEC also possesses imaginary excitation frequencies, an effect which is reminiscent of the cross-phase modulation (XPM) instability in nonlinear optics [14,16], where such modulation instability can lead to the breakup of intense cw radiation into ultrashort pulses and the formation of solitons. In fact, the homogeneous GPE's for BEC are very similar to the nonlinear Schrödinger equations describing wave propagation inside optical fibers. We believe that the extensive work in the field of nonlinear optics may help us understand the dynamics of condensates; however, how the TBEC will evolve under the influence of these instabilities remains to be studied.

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[1] M. H. Anderson *et al.*, Science **269**, 198 (1995); C. C. Bradley *et al.*, Phys. Rev. Lett. **75**, 1687 (1995); K. B. Davis *et al.*, Phys. Rev. Lett. **75**, 3969 (1995).
[2] C. J. Myatt *et al.*, Phys. Rev. Lett. **78**, 586 (1997).
[3] Tin-Lun Ho and V. B. Shenoy, Phys. Rev. Lett. **77**, 3276 (1996).
[4] H. Pu and N. P. Bigelow, Phys. Rev. Lett. **80**, 1130 (1998).
[5] B. D. Esry *et al.*, Phys. Rev. Lett. **78**, 3594 (1997).
[6] D. S. Jin *et al.*, Phys. Rev. Lett. **77**, 420 (1996); M.-O. Mewes *et al.*, Phys. Rev. Lett. **77**, 988 (1996); D. S. Jin *et al.*, Phys. Rev. Lett. **78**, 764 (1997).
[7] S. Stringari, Phys. Rev. Lett. **77**, 2360 (1996).
[8] Mark Edwards *et al.*, Phys. Rev. Lett. **77**, 1671 (1996); Y. Castin and R. Dum, Phys. Rev. Lett. **77**, 5315 (1996); V. M. Pérez-García *et al.*, Phys. Rev. Lett. **77**, 5320 (1996); B. D. Esry, Phys. Rev. A **55**, 1147 (1997); L. You *et al.*, Phys. Rev. A **55**, R1581 (1997).
[9] A. L. Fetter, Ann. Phys. (N.Y.) **70**, 67 (1972); A. Griffin, Phys. Rev. B **53**, 9341 (1996).
[10] P. A. Ruprecht *et al.*, Phys. Rev. A **54**, 4178 (1996); see also Mark Edwards *et al.*, J. Res. Natl. Inst. Stand. Technol. **101**, 553 (1996).
[11] R. Graham and D. Walls, Report No. cond-mat/9611111.
[12] J.-P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (MIT Press, Cambridge, MA, 1986).
[13] A more detailed analysis of the stability character of the TBEC is reported elsewhere: C. K. Law, H. Pu, N. P. Bigelow, and J. H. Eberly, Phys. Rev. Lett. **79**, 3105 (1997).
[14] E. Goldstein and P. Meystre, Phys. Rev. A **55**, 2935 (1997).
[15] Harmonic generation has also been studied in the case of a one-species condensate: M. Brewczyk, K. Rzążewsk, and Charles W. Clark, QELS'97, OSA Tech. Digest **12**, 104 (1997). See also Ref. [10].
[16] G. P. Agrawal, *Nonlinear Fiber Optics* (Academic Press, Inc., New York, 1989).