Spontaneous spatial symmetry breaking in two-component Bose-Einstein condensates

B. D. Esry
Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138

Chris H. Greene
Department of Physics and JILA, University of Colorado, Boulder, Colorado 80309-0440
(Received 22 June 1998)

We discuss the general features of spontaneous spatial symmetry breaking in trapped two-component alkali-metal–atom Bose-Einstein condensates, and give qualitative guidelines for when it will occur. We further show that the Hartree-Fock equations admit symmetry-broken solutions for as few as two trapped atoms, discussing the particular system of one ^{85}Rb atom and one ^{87}Rb atom. It is also shown that the critical value of the interspecies scattering length for a mixture of Na and Rb in an isotropic trap depends strongly on the number of atoms in a manner not described by the standard Thomas-Fermi phase separation condition.
[S1050-2947(99)00101-8]

PACS number(s): 03.75.Fi, 05.30.Jp

Spontaneous symmetry breaking (SSB) has striking manifestations when it occurs in mean-field descriptions of the quantum many-body problem. Macroscopic implications of SSB are dramatic and immediate, as in the case of ferromagnetism. But symmetry breaking in a microscopic quantum system, a small molecule for instance [1], is far more surprising. At first glance it even seems to contradict familiar theorems of quantum mechanics on the expected nature of eigensolutions when a symmetry operator $\hat{P}$ commutes with the Hamiltonian of the system $\hat{H}$. Of course, no true contradiction exists when mean-field theory predicts that the ground state of a system is not an eigenstate of a commuting symmetry operator $\hat{P}$. In fact, two possible explanations can be invoked when this is observed: (i) if the eigenstates of $\hat{H}$ are degenerate (not normally expected for the ground state), they need not be eigenstates of $\hat{P}$, although it is always possible to form linear combinations of the degenerate energy eigenstates which *are* simultaneous eigenstates of $\hat{P}$ and $\hat{H}$; or (ii) the symmetric mean-field ground state is simply a poor approximation to the lowest-energy eigenstate of the full many-body Hamiltonian.

The phenomenon of SSB could become important for an interpretation of current generation experiments on two-component dilute alkali-metal–atom Bose-Einstein condensates (BEC's) [2–4]. It has recently been demonstrated theoretically that, in certain regimes of the interaction parameters, the Hartree-Fock (or Gross-Pitaevskii) ground-state solution does not possess the symmetries of the magnetic trap used to contain the condensate [5,6]. In some cases this symmetry breaking was made explicit, as in the work of Refs. [5,6], whereas in other cases this effect was only indirectly suggested by the occurrence of complex excitation frequencies in solutions of the Bogoliubov (or random-phase approximation) equations [7].

Here, we address spatial SSB in trapped BEC's from a more general perspective. In particular, we point out that spatial SSB in microscopic systems is purely a result of the independent-particle approximation, and that a ''symmetry-restored'' wave function should be used for calculating physical observables. In addition, we present a qualitative framework within which the necessary conditions for spatial SSB can be understood. We then discuss the manner in which symmetry breaking is expected to manifest itself in the solutions of the Hartree-Fock equations for a wide range of trap geometries, and study the Na-Rb system in detail. We conclude with a few remarks on the observable consequences of spatial SSB.

The occurrence of symmetry breaking is of particular interest for dilute alkali-metal–atom BEC's, since they lie in some sense on the border between macroscopic and microscopic quantum systems. In fact the most common theoretical description adopted in BEC's is ''macroscopic'' in outlook, in anticipation of eventually taking a thermodynamic limit. Yet the two-component BEC under discussion in this work can be described equally well in simple Schrödinger theory [8,9], with strict conservation of particle number, more akin to the approach used to describe the microscopic quantum-mechanical ground state of a molecule or cluster. The ground state of such a microscopic system retains the symmetries of the Hamiltonian.

The experimental observation of interacting BEC's by Myatt *et al.* [2] (see also Refs. [3,4]) has sparked great theoretical interest in two-component BEC's [5–7,9–15] . The subject of two-component BEC's was addressed in the past [16], but most relevant to the present discussion are the more recent papers by Öhberg and Stenholm [5], by Timmermans [12], by Gordon and Savage [6], and by Pu and Bigelow [7]. Öhberg and Stenholm suggested the possibility of symmetry breaking based upon some numerical results in two dimensions, and Timmermans discussed the thermodynamic properties of the boundary between phase separated species. Gordon and Savage investigated the particular case of the $|F=1,M_F=-1\rangle$ and $|2,1\rangle$ hyperfine states of ^{87}Rb in a time-orbiting potential trap. They demonstrated that the cylindrical symmetry is broken, and that the conditions for symmetry breaking in this case depend upon both the number of atoms and the interspecies scattering length a_{12}. Finally, Pu and Bigelow investigated the ground-state configuration of a mixed Na-Rb condensate in an isotropic trap. Since the

Na-Rb scattering length a_{12} is not known, they considered a range of values, finding phase separation for a_{12} larger than some critical value (similar results have been presented by Bashkin and Vagov [13]). They explicitly assumed isotropic solutions, however, and thus saw no symmetry breaking, although it is suggested by the fact that they found an imaginary frequency $l=1$ excitation.

At this point, a clear statement of the phenomenon is in order. Spontaneous symmetry breaking is said to occur if the mean-field solutions do not possess the symmetry of the underlying many-body Hamiltonian for values of some parameter beyond a critical value [17]. When compared to solutions obtained with symmetric orbitals, the symmetry-broken states better approximate the true ground state, as judged by the variational principle. That is, the mean-field solutions can be viewed as the result of a variational analysis in the Hartree-Fock approximation, and the total energy calculated with the symmetry-broken state is lower than that obtained using the symmetry-preserving state. One theoretical signature of symmetry breaking (and of instabilities of the Hartree-Fock solution in general) is the appearance of vanishing or imaginary excitation frequencies in a random-phase approximation or Bogoliubov quasiparticle analysis. The zero-frequency excitation first occurs at exactly the transition from symmetry preserving to symmetry breaking, and signals the Goldstone mode typically associated with SSB.

For fixed numbers N_1 and N_2 of two types of distinguishable bosonic atoms, the Hartree-Fock approximation to the ground state takes the form

$$\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_{N_1+N_2})=\psi_1(\mathbf{x}_1)\cdots\psi_1(\mathbf{x}_{N_1})\times\psi_2(\mathbf{x}_{N_1+1})\cdots\psi_2(\mathbf{x}_{N_1+N_2}),$$

where the orbitals ψ_1 and ψ_2 satisfy the Hartree-Fock equations

$$\begin{aligned}[h_1+(N_1-1)U_{11}|\psi_1|^2+N_2U_{12}|\psi_2|^2]\psi_1&=\varepsilon_1\psi_1,\\ [h_2+N_1U_{21}|\psi_1|^2+(N_2-1)U_{22}|\psi_2|^2]\psi_2&=\varepsilon_2\psi_2.\end{aligned}\tag{1}$$

The one-body operators h_i in these equations include the kinetic energy and trapping potential contributions. Note that the interaction potentials have been approximated in these equations by a Dirac δ function pseudopotential [18]. The coefficient U_{ij} of the δ function is $2\pi\hbar^2a_{ij}/\mu_{ij}$, where $\mu_{ij}=m_im_j/(m_i+m_j)$ is the reduced mass of atoms i and j, with a_{ij} their s-wave scattering length. For a large repulsive interaction a_{12} between the different atoms (compared to a_{11} and a_{22}), the mean-field interaction energy will clearly be minimized if the orbitals do not overlap. This energy reduction is the origin of the phase separation discussed by many authors. The critical value of a_{12}, beyond which separation occurs in the Thomas-Fermi approximation, can be shown to be

$$a_{12}^c=\left(\frac{4\mu_{12}}{m_1+m_2}a_{11}a_{22}\right)^{1/2}.\tag{2}$$

In some cases, the total energy can be further lowered if the species separate in an asymmetrical manner; for this to happen, Eq. (2) is a necessary but not sufficient condition—a point discussed in greater detail below. In the case of a TOP trap, symmetry breaking has been shown [6] to hinge on the number of atoms, in contrast to Eq. (2). Similarly, we show below that, for a Na-Rb mixture, the condition for symmetry breaking has an even more interesting atom number dependence. Thus, in accord with conventional views of SSB, there is a critical value of some parameter related to the symmetry breaking. The specific dependence of this parameter on the numbers of atoms, scattering lengths, and trap frequencies is, however, nontrivial and not readily obtainable except by direct solution of the Hartree-Fock equations.

Here we present a qualitative framework in which the conditions for symmetry breaking can be understood. Observe first that phase separation adds, in effect, a boundary to the unseparated density distributions, and places all atoms of one species on one side of the boundary and all atoms of the other species on the other side. Moreover, near the critical value the total number density is roughly the same for both separated and unseparated systems. The interspecies interaction energy of the separated state is clearly lower, but this loss is partially offset by the kinetic energy gained in forming the interphase boundary and the energy gained from the intraspecies interactions. The impact of the additional kinetic energy is largest for small numbers of atoms, however, since the interaction energies contain an additional factor of particle number(s) relative to the kinetic energy. These same energy considerations hold for SSB as well. To achieve an even lower total energy than the phase-separated state, the symmetry-broken state seeks a simpler interphase boundary. For example, in an isotropic trap with equal numbers of atoms of each species that differ only in their respective scattering lengths, the symmetry-preserving, phase-separated state has a spherical interphase boundary with one species forming a spherical shell around the other. The symmetry-broken state acquires a roughly planar boundary between the two hemispheres of each species. The kinetic energy associated with the boundary curvature is reduced, as is the interface volume.

We illustrate these points with a two-body example. Two atoms in the ground state of a trap do not constitute a condensate, but the above development—i.e., Eq. (1)—holds equally well for two atoms as for two million. A two-body system is also physically intuitive and ''exactly solvable.'' For one ^{85}Rb atom and one ^{87}Rb atom in a trap with frequencies $\nu_\rho=4\nu_z=1$ MHz, Eq. (1) indeed yields a symmetry-breaking solution with a total energy of 2.4949 $\hbar\omega_\rho$ compared to 2.5676$\hbar\omega_\rho$ for the symmetry-preserving solution. The relevant symmetry operator Π_z represents reflection through the $z=0$ plane. The symmetry-preserving solution is partially phase separated due to a repulsive scattering length—$a_{12}=210$ a.u. for a $|3,3\rangle$ ^{85}Rb atom colliding with a $|2,2\rangle$ ^{87}Rb atom [19]—with interphase boundaries above and below the xy plane and parallel to it. (There are two boundaries in order to preserve the symmetry.) The symmetry-broken solution has only one boundary at $z=0$; based on the above energy considerations, it has lower energy since it has one fewer interphase boundary. The exact two-body ground-state wave function has a definite symmetry with respect to reflections about $z=0$, and can be approximated as a linear combination of the degenerate symmetry-

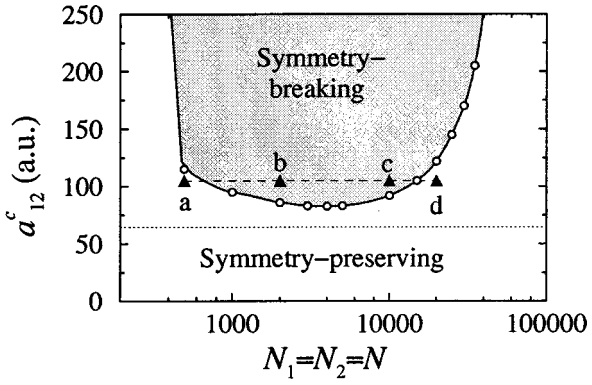

FIG. 1. ''Phase diagram'' for the Na-Rb condensate. In the shaded region, the symmetry-breaking solution is the lowest-energy Hartree-Fock state, while the symmetry-preserving solution has the lowest energy elsewhere. The thick solid line and circles denote the calculated a_{12}^c; the dotted line represents the Thomas-Fermi critical value of a_{12} from Eq. (2). The triangles and labels refer to Fig. 2.

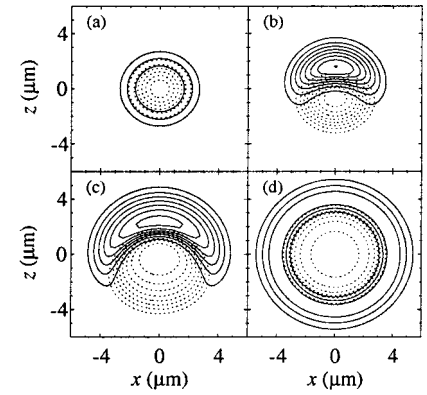

FIG. 2. The number densities in the $y=0$ plane corresponding to the triangles in Fig. 1, $N_1=N_2=N$ and $a_{12}=105$ a.u.: (a) $N=500$, (b) $N=2000$, (c) $N=10\,000$, and (d) $N=20\,000$. The dotted lines mark the contours of Rb and the solid lines those of Na.

broken Hartree-Fock states $\Psi(\mathbf{x}_1,\mathbf{x}_2)$ and $\Pi_z\Psi(\mathbf{x}_1,\mathbf{x}_2)$. Specifically, the symmetry-restored states $(1\pm\Pi_z)\Psi(\mathbf{x}_1,\mathbf{x}_2)$ are eigenstates of Π_z, with energy expectations $2.4750\hbar\omega$ $(+)$ and $2.5256\hbar\omega$ $(-)$. The first of these gives a clear improvement over the simple product solutions, both symmetry preserving and symmetry broken. It is the best ''independent-particle'' ground state of this system of the various possibilities considered here. Note that these linear combinations of Hartree-Fock states are not themselves solutions of Eq. (1) and cannot be represented as a simple product of single-particle states. This two-body example illustrates the general fact that spatial SSB in a microscopic quantum system is purely a result of the Hartree-Fock approximation.

When a system is in the symmetry-breaking regime, the solution of the Hartree-Fock equations will break the symmetry in the direction corresponding to the weakest trap frequency. For a cylindrically symmetric trap in which the stronger trapping frequency is in the axial direction, the rotational symmetry L_z will be broken. The solution, however, retains a plane of symmetry that includes the z axis, but whose orientation is random. In a cigarlike cylindrically symmetric trap, the z-parity symmetry is broken. In a completely anisotropic trap, the parity in the weakest trap direction will be broken. The rotational symmetry $\mathbf{L}^2$ in an isotropic trap can also be broken, but the system will retain an axis of symmetry whose orientation is random. When a continuous symmetry is broken, constructing a many-body state with the correct symmetry is more complicated than in the discrete case considered in the two-atom example above. Nevertheless, a general prescription for constructing the symmetry-restored many-body state is simply to project the symmetry-broken state onto an eigenstate of the desired symmetry [17]. Equivalently, the Hamiltonian can be diagonalized in the subspace of degenerate states related by the symmetry transformation under consideration.

To gain further insight into the nature of spatial SSB in double-condensate systems, we investigate a particular example: a mixture of Na and Rb in an isotropic trap. This system was studied by Pu and Bigelow in a series of papers [7] in which they focused on its stability and on a predicted metastable state stabilized by the phase separation. In their work, the solutions of Eq. (1) were constrained to be isotropic. Here we allow for symmetry-broken solutions and focus on the criteria for symmetry breaking. Specifically, we solve the Hartree-Fock equations for the isotropic trap in cylindrical coordinates, thus choosing the axis of symmetry *a priori*. The solution, however, is not forced to be either symmetry broken or symmetry preserving. Rather, the numerical method forces the solution to converge to the lowest-energy solution regardless of its symmetry. This is accomplished by propagating Eq. (1) as a diffusion equation with $\tau=it$, while constraining the orbitals ψ_i to be normalized to unity. Starting from random initial orbitals, ψ_1 and ψ_2 will converge to the state of lowest energy in the limit of $\tau\rightarrow\infty$ whether it is symmetry breaking or preserving. The symmetry-preserving solution is readily found by imposing an additional symmetry constraint.

Choosing the Rb parameters as a reference, we write the Hartree-Fock equations using $\hbar\omega_1$ as the energy unit and $\sqrt{\hbar/m_1\omega_1}$ as the length unit. In order to match previous studies, we use trap frequencies $\nu_1=160$ Hz for the Rb atoms and $\nu_2=310$ Hz for the Na atoms. The effective trapping frequencies are thus 1 and $m_2\omega_2/m_1\omega_1\approx 0.5$ for the Rb and Na atoms, respectively. The difference in trapping frequencies causes the Na atoms to form a spherical shell around the Rb atoms in the phase-separated regime, as suggested in Refs. [7,13]. While the intraspecies scattering lengths a_{11} and a_{22} are relatively well known, the interspecies scattering length a_{12} is not. We use the slightly inaccurate values of $a_{11}=113.38$ a.u. (6 nm) and $a_{22}=56.692$ a.u. (3 nm), however, in order to match Ref. [7]. There remain three parameters in the problem: a_{12}, N_1, and N_2. Setting $N_1=N_2=N$, we solved the Hartree-Fock equations as a function of N and a_{12}.

Figure 1 summarizes the results for the Na-Rb mixture. The critical value of a_{12} is just the curve separating the two regions, and it depends strongly on the number of atoms. For small N_1, a_{12}^c is roughly proportional to N^{-1}, reflecting the ratio of kinetic to mean-field energy. For large N, the N dependence of a_{12}^c is a result of the relatively large difference in effective trapping frequencies each species experiences combined with the disparity between a_{11} and a_{22}. These

differences lead to a shell-filling effect for the Na atoms where the shell is the spatial region between the mean field of the Rb atoms in the tighter trap and the weaker trap experienced by the Na atoms.

At a fixed interspecies scattering length greater than about 80 a.u., the system starts in a symmetric configuration for small N. since the kinetic energy barrier of forming an interphase boundary is too high [see Fig. 2(a)]. As N is increased, the symmetry-broken state becomes energetically favorable when the energy lost in the mean-field interaction energy offsets the kinetic-energy gain [see Fig. 2(b)]. With N increased further (but still within the symmetry-broken regime) the Na atoms wrap further around the Rb core [see Fig. 2(c)]. The Rb core is pushed slightly off center, but the trap is too tight to make large displacements energetically favorable. The number of atoms eventually grows large enough that the Na atoms wrap all of the way around the Rb core, filling the spatial shell available to them. Thus, the symmetric configuration is again reached [see Fig. 2(d)].

We conclude with the remark that it is difficult to envision an experimental realization of the conditions necessary to see spontaneous spatial symmetry breaking. Any stray field or fluctuation in trapping fields that favors a direction in space will likely destroy the symmetry of the trap in a manner catastrophic for the effect. Should such technical difficulties be overcome, however, the symmetry properties of the ground state should be reflected in measurable observables. For instance, in the z-parity symmetry-breaking case, a straightforward species specific absorption image, or, e.g., a light diffraction experiment, can quickly distinguish a symmetry-broken state from either the symmetry-preserving or the symmetry-restored state. The latter two types of states could then be differentiated in an experiment that measures the two-body correlation function.

The work of C.H.G. was supported in part by the U.S. Department of Energy, Office of Basic Energy Sciences. B.D.E. is now supported by the National Science Foundation through the Institute for Theoretical Atomic and Molecular Physics.

[1] P. Y. Ayala and H. B. Schlegel, J. Chem. Phys. **108**, 7560 (1998).
[2] C. J. Myatt, E. A. Burt, R. W. Ghrist, E. A. Cornell, and C. E. Wieman, Phys. Rev. Lett. **78**, 586 (1997).
[3] D. S. Hall, M. R. Matthews, J. R. Ensher, C. E. Wieman, and E. A. Cornell, e-print cond-mat/9804138.
[4] D. M. Stamper-Kurn, M. R. Andrews, A. P. Chikkatur, S. Inouye, H. J. Miesner, J. Stenger, and W. Ketterle, Phys. Rev. Lett. **80**, 2027 (1998).
[5] P. Öhberg and S. Stenholm, Phys. Rev. A **57**, 1272 (1998).
[6] D. Gordon and C. M. Savage, Phys. Rev. A **58**, 1440 (1998).
[7] C. K. Law, H. Pu, N. P. Bigelow, and J. H. Eberly, Phys. Rev. Lett. **79**, 3105 (1997); H. Pu and N. P. Bigelow, *ibid.* **80**, 1130 (1998); H. Pu and N. P. Bigelow, *ibid.* **80**, 1134 (1998).
[8] B. D. Esry, Phys. Rev. A **55**, 1147 (1997).
[9] B. D. Esry, C. H. Greene, J. P. Burke, Jr., and J. L. Bohn, Phys. Rev. Lett. **78**, 3594 (1997); B. D. Esry and C. H. Greene, Phys. Rev. A **57**, 1265 (1998).
[10] T. L. Ho and V. B. Shenoy, Phys. Rev. Lett. **77**, 3276 (1996).
[11] R. Graham and D. Walls, Phys. Rev. A **57**, 484 (1998).
[12] E. Timmermans, e-print cond-mat/9709301.
[13] E. P. Bashkin and A. V. Vagov, Phys. Rev. B **56**, 6207 (1997).
[14] Th. Busch, J. I. Cirac, V. M. Perez-Garcia, and P. Zoller, Phys. Rev. A **56**, 2978 (1997).
[15] T. L. Ho, Phys. Rev. Lett. **81**, 742 (1998).
[16] W. B. Colson and A. L. Fetter, J. Low Temp. Phys. **33**, 231 (1978).
[17] P. Ring and P. Shuck, *The Nuclear Many-Body Problem* (Springer, New York, 1980).
[18] K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).
[19] J. P. Burke, Jr., J. L. Bohn, B. D. Esry, and C. H. Greene, Phys. Rev. Lett. **80**, 2097 (1998).