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Impact of spontaneous spatial symmetry breaking on the critical atom number for two-component Bose-Einstein condensates

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The consequences of spatial symmetry breaking in two-component Bose-Einstein condensates are explored for the ^{85}Rb$+$^{87}Rb system. It is shown that the mean-field critical number of ^{85}Rb atoms depends strongly on whether the single-particle wave function is symmetry preserving or symmetry breaking. This system thus provides a uniquely straightforward experimental means of observing spatial symmetry breaking.
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Two-component atomic Bose-Einstein condensates display a wide variety of interesting ground-state structures. In large part, the sheer number of parameters available—three trapping frequencies for each species, three scattering lengths, and the number of atoms of each species—renders this multiplicity possible. Add to this list the effects of external fields, including gravity, and the possible combinations are virtually endless. The description of the system by mean fields plays a large role also, since the reduction of the linear many-body Schrödinger equation to a system of effective single-particle equations yields nonlinear equations. Nonlinear equations can display a quite complicated dependence on the parameters involved.

Only a few small regions of this parameter space have been explored either theoretically or experimentally, however. Nevertheless, interesting phenomena such as gravitational separation [1], phase separation [2,3], and spontaneous spatial symmetry breaking [4–6] have been predicted. Of these, only the first—the effect of gravity—has been observed experimentally [7]. The second is merely a matter of finding and condensing a system with appropriate scattering lengths. But, the third effect, spontaneous spatial symmetry breaking, generally requires a somewhat subtle measurement in order to be seen [6]. I present in this paper a special case for which the consequences of spontaneous spatial symmetry breaking can be experimentally observed by relatively straightforward means.

A single condensate with a negative scattering length whose number exceeds a critical value is unstable with respect to recombination processes that eject atoms from the trap [8]. The same instability persists for two-component condensates when one of the intraspecies scattering lengths is negative. The combination of ^{85}Rb and ^{87}Rb in their $|F=3, M_F=3\rangle$ and $|2,2\rangle$ hyperfine states, respectively, is one such system. I will show below that the critical number of ^{85}Rb atoms depends strongly on whether or not the mean-field solution is symmetry preserving. Thus, an experimental measurement of the critical number of ^{85}Rb atoms will be a clear indicator of spatial symmetry breaking. The caveat is that a condensate of ^{85}Rb and ^{87}Rb has yet to be successfully created experimentally. On the other hand, any two-species system that shares the same characteristics as the ^{85}Rb$+$^{87}Rb system (one negative intraspecies scattering length, the other positive, and a positive interspecies scattering length) will presumably be a candidate for experimentally observing spatial symmetry breaking.

Spontaneous spatial symmetry breaking occurs only for particular combinations of the parameters listed above and is characterized by the fact that the solutions of the mean-field (or Hartree-Fock) equations do not possess the spatial symmetries of the original many-body Hamiltonian. The exact ground state of the system must, of course, retain these spatial symmetries and so a symmetry-restored wave function should be constructed from the symmetry-broken mean-field solution in order to calculate physical observables. In an isotropic trap or a pancakelike cylindrically symmetric trap, symmetry breaking means that the rotational symmetry is broken. In a cigarlike cylindrically symmetric trap or a completely anisotropic trap, the parity in the weakest trap direction is broken. By forcing the trap symmetry onto the Hartree-Fock solution, a symmetry-preserving solution can also be found. In symmetry-breaking regimes, however, it has a higher total energy than the symmetry-breaking solution, and is rejected in favor of the latter in accord with the variational principle.

The trap considered in this paper is the cigarlike trap from the experiment of Myatt *et al.* [7] and thus will display a broken parity symmetry. Since the mean-field critical number for a single condensate with a negative scattering length increases with decreasing ω ($N_c \propto \omega^{-1/2}$ in an isotropic trap of frequency ω), I will use frequencies near the lowest possible ones in that experiment [9], $\nu_\rho = 12$ Hz and $\nu_z = 6$ Hz. Even for these frequencies, the critical number for a single condensate of ^{85}Rb atoms is only about 90 because the ^{85}Rb scattering length is large and negative. Reliably and accurately measuring the number of atoms in such a small sample is a nontrivial technical task that would only be exacerbated by reducing the critical number. It might even be hoped that the critical number could be increased under the stabilizing influence of the second species in a double condensate. This is not the case, however, as will be shown below.

The $|3,3\rangle$ and $|2,2\rangle$ spin states have been chosen for two reasons: (i) the spin-flip decay rate is sufficiently small for mixed species collisions, and (ii) the magnetic moment is the same for both species so that gravity does not break the symmetry of the trap. I have used 109.1, -400, and 210 a.u.

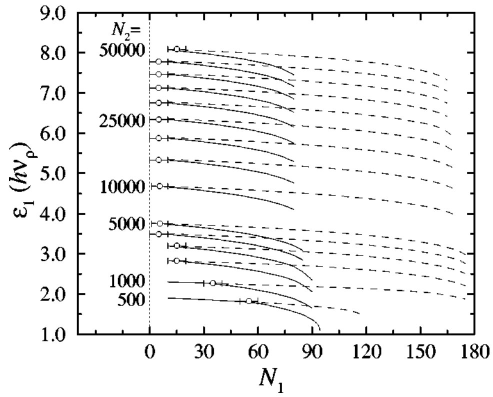

FIG. 1. ^{85}Rb orbital energy ε_1 as a function of the number N_1 of ^{85}Rb atoms. Various values of the number of ^{87}Rb atoms N_2 are shown—500, 1000–5000 in steps of 1000, and 10000–50000 in steps of 5000—a few of which are labeled for clarity. The solid lines denote the mean-field ground-state solution; and the dashed lines, the symmetry-preserving solution. The circles mark the point at which the energies for the two types of solutions begin to deviate. Also, each curve terminates at the critical number of N_1.

for the ^{87}Rb intraspecies scattering length, the ^{85}Rb intraspecies scattering length, and the interspecies scattering length, respectively [10,11]. Two parameters remain—the numbers of atoms N_1 and N_2 (here and below, the label 1 refers to ^{85}Rb and 2 to ^{87}Rb).

Figure 1 shows the orbital energy ε_1 of ^{85}Rb as a function of N_1 for various values of N_2. The solid lines are for the ground-state solution of the Hartree-Fock equations whether they are symmetry preserving or symmetry breaking. The dashed lines indicate the orbital energy for solutions forced to maintain the z-parity symmetry. Thus, where the solid and dashed curves overlap, the Hartree-Fock ground state is symmetry preserving, but is otherwise symmetry breaking, so that the transition from symmetry preserving to symmetry breaking as a function of N_1 can also be seen in the figure. This transition point is indicated in the figure by circles, and the error bars simply indicate the coarseness of the grid in N_1. It is interesting to note that for $N_1=1$ the mean-field ground state is symmetry preserving in all cases.

For reference, the Hartree-Fock equations for the orbital wave functions ψ_i are [1–5]

$$[h_1+(N_1-1)U_{11}|\psi_1|^2+N_2U_{12}|\psi_2|^2]\psi_1=\varepsilon_1\psi_1,$$

$$[h_2+N_1U_{21}|\psi_1|^2+(N_2-1)U_{22}|\psi_2|^2]\psi_2=\varepsilon_2\psi_2. \quad (1)$$

The one-body operators h_i in these equations include the kinetic energy and trapping potential contributions. The atom-atom interaction potentials have been approximated in these equations by a Dirac δ function pseudopotential [12]. 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 single condensates with a negative scattering length, the orbital energy acquires an infinite slope at the critical value of the number of atoms [8]. Beyond this critical value, the system is said to be unstable against collapse. It can be expected that the Hartree-Fock equations for a double condensate show a similar behavior. It can be seen in Fig. 1 that the ^{85}Rb orbital energy does indeed repeat the single condensate behavior near the critical value. Since numerically solving Eq. (1) is increasingly resource intensive as the critical value is approached, I have only extended the lowest curve ($N_2=500$) to values near the critical value. This curve illustrates the general behavior each curve would display if it were continued to its respective critical number. In all cases, the critical value occurs within ten atoms of the final point shown.

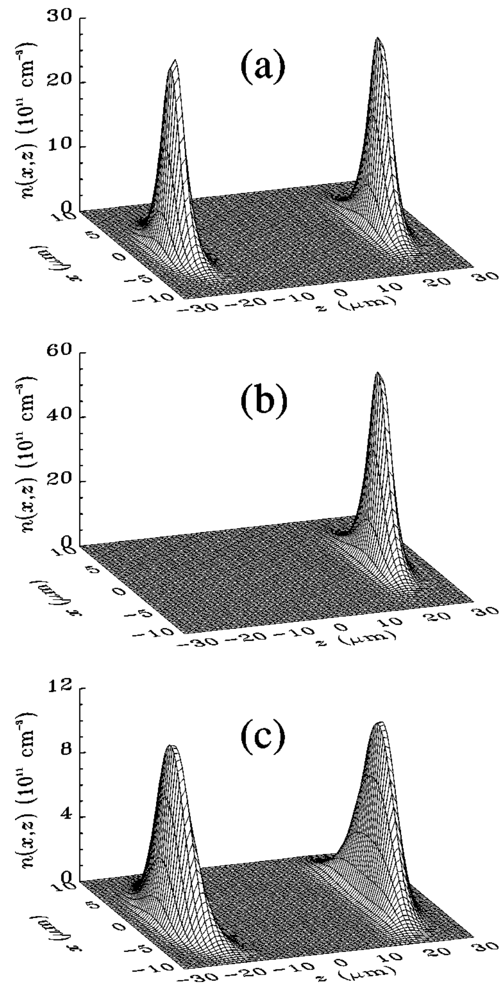

FIG. 2. ^{85}Rb number densities $n_1(x,y=0,z)$ for (a) the symmetry-restored wave function Eq. (2), (b) the symmetry-broken solution, and (c) the symmetry-preserving solution for $N_1=80$ ^{85}Rb atoms and $N_2=50\,000$ ^{87}Rb atoms. Since $N_2\gg N_1$, the ^{87}Rb number density forms a relatively imperturbable cloud near $z=0$. In (a) and (c), for instance, it fills the region between the ^{85}Rb peaks.

The main result of this paper is embodied by Fig. 1, namely, that the critical number for the symmetry-broken solution is approximately half that of the symmetry-preserving solution for any given value of N_2. The origin of this difference is relatively straightforward to understand, as can be seen in Fig. 2. The ^{85}Rb number densities are shown for both symmetry-preserving and symmetry-breaking cases, with the numbers of atoms fixed at $N_1=80$ and $N_2=50\,000$. Since $N_2\gg N_1$, the ^{87}Rb in all cases forms an essentially inert cloud around $z=0$ and is thus not shown. When Eq. (1) is scaled by the harmonic-oscillator length and energy for ^{87}Rb, the effective trapping frequency for ^{85}Rb is a factor of m_1/m_2 smaller. Combined with the repulsive interspecies interaction this weaker trap explains why the ^{85}Rb rests at the edge of the ^{87}Rb. The ^{85}Rb lies at the ends because the trap frequency in the z direction is smaller. In the symmetry-preserving solution, the ^{87}Rb is seen to separate the ^{85}Rb into essentially two condensates, each of which can sustain approximately the single condensate critical number of atoms. For the symmetry-breaking solution the ^{85}Rb atoms cluster at one end of the trap, behaving roughly as would a single condensate of ^{85}Rb atoms in the sense that it can only sustain about the single condensate critical number of atoms.

The variation in the critical number of atoms in Fig. 1 as a function of N_2 is due to the variation in the effective frequency ''seen'' by the ^{85}Rb atoms. That is, the ^{85}Rb atoms lie at the minima of an effective potential comprised of the trap plus ^{87}Rb mean field. Near these minima, the effective potential is approximately harmonic with some effective frequency. As the number of ^{87}Rb atoms increases, the effective frequency in the z direction also increases. And, since the single condensate critical number is proportional to $\omega^{-1/2}$, it follows that the critical number decreases as a function of N_2.

A physical wave function possessing definite z-parity symmetry can now be constructed from the symmetry-broken Hartree-Fock solutions. Although the general method of constructing symmetric wave functions from symmetry-broken ones for either continuous or discrete symmetries is well known [13], this procedure is greatly simplified by the fact that the symmetry-broken one is a discrete symmetry. Writing the many-body Hartree-Fock wave function as

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

the symmetry-restored wave function is

$$\Phi_{\pm}=\mathcal{N}_{\pm}[\Phi_{\mathrm{HF}}\pm\Pi_z\Phi_{\mathrm{HF}}]. \tag{2}$$

The normalization constant $\mathcal{N}_{\pm}$ is given by

$$\mathcal{N}_{\pm}^{-2}=2[1\pm\langle\Pi_z\Phi_{\mathrm{HF}}|\Phi_{\mathrm{HF}}\rangle],$$

and Π_z is the total z-parity operator that changes all z_i to $-z_i$. In terms of the orbitals ψ_i and their reflections $\pi_z\psi_i$, the remaining matrix element in $\mathcal{N}_{\pm}$ is given by

$$\langle\Pi_z\Phi_{\mathrm{HF}}|\Phi_{\mathrm{HF}}\rangle=\langle\pi_z\psi_1|\psi_1\rangle^{N_1}\langle\pi_z\psi_2|\psi_2\rangle^{N_2}.$$

Because the overlap of each orbital with its reflected counterpart is raised to the N_ith power, this matrix element is essentially zero except for small numbers of atoms. The same argument holds for the cross term arising in the expectation value of nearly any observable. For instance, while restoring the symmetry in principle lifts the degeneracy of the symmetry-broken state, in practice the splitting is negligible since the cross term in the total energy,

$$E_{\pm}=2\mathcal{N}_{\pm}^2[E_{\mathrm{HF}}\pm\langle\Pi_z\Phi_{\mathrm{HF}}|H|\Phi_{\mathrm{HF}}\rangle],$$

is vanishingly small. When a continuous symmetry is broken, however, the cross terms in expectation values of observables likely remain non-negligible for a larger range of atom number. Nevertheless, for either discrete or continuous broken symmetries, the degenerate symmetry-broken states decouple completely in the limit of large atom number. Of course, these degenerate states can still be combined to form symmetry eigenstates.

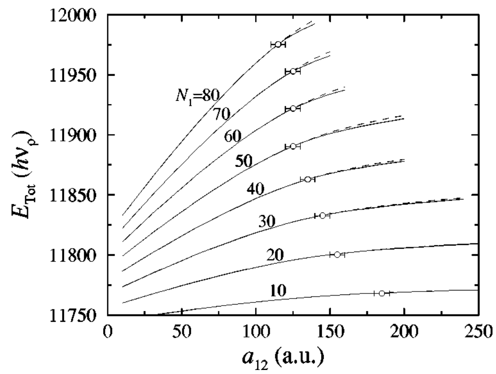

FIG. 3. Total energy as a function of a_{12} for 5000 ^{87}Rb atoms and different numbers of ^{85}Rb atoms as indicated. The solid lines denote the mean-field ground-state solution; and the dashed lines, the symmetry-preserving solution. The circles mark the critical value of a_{12} for symmetry breaking.

A more suitable observable for studying the impact of restoring the symmetry is the number density. Assuming real orbital wave functions, the ^{85}Rb number density for the symmetry-restored wave function is

$$n_1^{\pm}(\mathbf{x})=N_1\mathcal{N}_{\pm}^2[|\psi_1(\mathbf{x})|^2+|\pi_z\psi_1(\mathbf{x})|^2\pm2\psi_1(\mathbf{x})\pi_z\psi_1(\mathbf{x}) \times\langle\pi_z\psi_1|\psi_1\rangle^{N_1-1}\langle\pi_z\psi_2|\psi_2\rangle^{N_2}].$$

(The ^{87}Rb number density can be written similarly.) The cross term remains negligibly small, but as Fig. 2(a) shows, the density is symmetric with respect to reflections through the $z=0$ plane unlike the symmetry-broken number density shown in Fig. 2(b). For comparison, the number density for the symmetry-preserving solution is shown in Fig. 2(c). The symmetry-broken number density also differs from the symmetry-preserving and symmetry-restored densities by being localized at one end of the trap rather than at both ends. This configuration is representative of all choices of N_1 and N_2 consistent with Fig. 1, except for the smallest values of N_2 for which the symmetry-preserving ^{85}Rb number density remains localized near $z=0$. The number density thus provides a means for distinguishing the symmetry-broken solution.

Since two-component condensates with one negative intraspecies scattering length have not yet been studied and the Thomas-Fermi approximation is not applicable, the dependence of their ground-state properties on the system's parameters is essentially unknown. Some of this parameter space was explored above for the physical scattering lengths of the ^{85}Rb+^{87}Rb system. To gain additional insight for systems with one negative intraspecies scattering length, I have studied the ^{85}Rb+^{87}Rb system treating a_{12} as unknown. That is, I have solved the Hartree-Fock equations with ^{85}Rb+^{87}Rb parameters as a function of a_{12}. The total energies are shown in Fig. 3 for various values of N_1 and fixed N_2 (N_2N_2 ($N_2=5000$). The total energy of the ground

Hartree-Fock solution is given by the solid lines; and the symmetry-preserving solution, by the dashed lines. As in Fig. 1, where the solid and dashed curves overlap, the ground Hartree-Fock solution is symmetry preserving. The dependence on N_1 of the critical value of a_{12} above which the Hartree-Fock solution is symmetry broken can thus be seen. The circles again indicate the critical value, and the error bars reflect the coarseness of the grid used in a_{12}. The general trend of the critical value of $a_{12}(N_1)$—large for small N_1 and decreasing with increasing N_1—is in qualitative agreement with previous studies [6].

I have shown that a mixed isotope condensate of ^{85}Rb and ^{87}Rb is an excellent candidate for experimentally observing the effects of spontaneous spatial symmetry breaking. Using the combination of a critical number measurement and a number density measurement, the three possible ground-state wave functions based on solutions of Eq. (1)—symmetry preserving, symmetry breaking, and symmetry restored—can be distinguished. This statement, however, assumes that the z parity of the trapping potentials is perfect. The rotational symmetry assumed in this paper need not be perfect. Indeed, it need not be present at all. But, if the z parity is broken (by the separation of the trap centers for each species, for instance), the critical number for ^{85}Rb will again be roughly that of an isolated condensate. Moreover, the number density will closely resemble the symmetry-broken density shown in Fig. 2(b). Test calculations show that this is already the case by the time the trap centers are separated by 0.25 μm.

In the course of this study of the $^{85}\mathrm{Rb}+^{87}\mathrm{Rb}$ system, I have also mapped out the ground state properties for a two-component condensate with a negative intraspecies scattering over a wide range of parameters. Such studies begin to provide a framework for the qualitative understanding of the ground-state properties of other similar systems.

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