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Nature of spinor Bose-Einstein condensates in rubidium

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We perform detailed close-coupling calculations for the rubidium isotopes ^{85}Rb and ^{87}Rb to ascertain the nature of their spinor Bose-Einstein condensates. These calculations predict that the spinor condensate for the spin-1 boson ^{87}Rb has a ferromagnetic nature. The spinor condensates for the spin-2 bosons ^{85}Rb and ^{87}Rb, however, are both predicted to be polar. The nature of a spin-1 condensate hinges critically on the sign of the difference between the *s*-wave scattering lengths for total spins 0 and 2 while the nature of a spin-2 condensate depends on the values of the differences between *s*-wave scattering lengths for the total spins 0, 2, and 4. These scattering lengths were extracted previously and found to have overlapping uncertainties for all three cases, thus leaving the nature of the spinor condensates ambiguous. The present study exploits a refined uncertainty analysis of the scattering lengths based on recently improved result from experimental work by Roberts *et al.*, which permits us to extract an unambiguous result for the nature of the ground state spinor condensates.

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In a conventional magnetic trap for ultracold alkali-metal atoms the spin degrees of freedom are "frozen out" since the atom must be in a weak-field seeking Zeeman state to be trapped. In an optical trap, however, the spins of the alkali-metal atoms are essentially free, and all magnetic substates $|f,m\rangle$ for a given spin f can be populated. Since the atom-atom interaction depends on spin, these magnetic substates can be changed in a scattering event. Accordingly, it is of interest to see how the spins are organized in the ground state and to explore the nature of the spin-mixing dynamics in an optically trapped Bose-Einstein condensate (BEC).

Multicomponent condensates have been formed in magnetic traps. For instance, Ref. [1] used a double magneto-optical trap and a magnetic trap to create condensates in either the $|f=2,m=2\rangle$ or the $|f=1,m=-1\rangle$ spin state of ^{87}Rb, and in a mixture of both by cooling $|1,-1\rangle$ evaporatively and $|2,2\rangle$ via thermal contact with the $|1,-1\rangle$ atoms. In this case the spin projections are approximately frozen out because the spin-flip cross sections in ^{87}Rb are anomalously small [2–4]. By contrast, Ref. [5] made a sodium condensate consisting simultaneously of all three magnetic substates of the $f=1$ atomic state, by cooling the atoms in a magnetic trap and then transferring them into an optical trap. This experimental technique produces what is referred to as a spinor condensate, because it can explore its full range of spin degrees of freedom. See also Refs. [6–8]. In the theoretical description of Refs. [9,10], the spinor condensates are classified according to the relative values of certain characteristic scattering lengths. Note that alternative theoretical treatments [11,12] differ in their detailed predictions concerning the nature of the spinor BEC ground state. Nevertheless, in this paper we determine the interaction parameters for spinor condensates of ^{85}Rb and ^{87}Rb which, based on Refs. [9,10,13] fall into the two following categories.

Spin-1 atoms (^{87}Rb). Let F be the total spin of two bosonic spin $f=1$ atoms, and let a_F be the *s*-wave scattering length for the total spin F symmetry. Since $f=1$, only $F=0,2$ are allowed by Bose symmetry for an *s*-wave collision. The nature of the spin-1 BEC ground state depends critically on the relative values of a_0 and a_2. According to Ho [9] a spinor Bose condensate composed of spin-1 bosons in an optical trap can be either "ferromagnetic" or "antiferromagnetic" in nature [9,10]. The antiferromagnetic state has alternatively been termed "polar," and we use this terminology here. The difference between the scattering lengths a_0 and a_2 determines the nature of the spin-1 condensate: the ferromagnetic state emerges when $a_0>a_2$, whereas the polar state emerges when $a_0<a_2$ [9]. In the ferromagnetic state virtually all atoms reside in the same spin substate (either $m=1$ or $m=-1$); in the polar state the spin projections are mixed.

Spin-2 atoms (^{85}Rb, ^{87}Rb). Two bosonic spin $f=2$ atoms possess $F=0,2,4$ total spin states exhibiting the appropriate Bose symmetry for an *s*-wave collision. For spin-2 ^{87}Rb the scattering lengths a_0, a_2, and a_4 are determined by the real part of the phase shift since the inelastic scattering processes are also allowed. According to Ciobanu *et al.* [13], a spinor condensate of spin-2 bosons in an optical trap can be one of the three types "ferromagnetic," "polar," or "cyclic" in nature, which we abbreviate as *F*, *P*, or *C*, respectively. Ferromagnetic and polar condensates are similar to those above. The name "cyclic" arises from a close analogy with *d*-wave BCS superfluids. The nature of the spin-2 BEC ground state depends critically on the relative values of a_0-a_2 and a_2-a_4 [13].

The three states emerge under the following conditions.

$$P: \quad a_0-a_4<0, \ \tfrac{2}{7}(a_2-a_4)<\tfrac{1}{5}|a_0-a_4|,$$

$$F: \quad a_2-a_4>0, \ \tfrac{1}{5}(a_0-a_4)+\tfrac{2}{7}(a_2-a_4)>0,$$

$$C: \quad a_2-a_4<0, \ \tfrac{1}{5}|a_0-a_4|-\tfrac{2}{7}(a_2-a_4)>0.$$

For spin-1 ^{87}Rb the total spin $F=0$ and $F=2$ scattering lengths a_0 and a_2 are almost equal. They have been calculated before [9] based on the analysis of Ref. [14], but the uncertainties determined still overlap for a_0 and a_2, so that the sign of the difference has remained uncertain. In particular, the scattering lengths have been interpreted rather conservatively in Ref. [14]. For spin-2 ^{85}Rb and ^{87}Rb the uncertainties for the total spin F scattering lengths a_0, a_2, and a_4 have been too large to uniquely identify the nature of the spinor condensates [10]. The uncertainty region for ^{85}Rb was large enough to overlap all three regions P, F and C, while the uncertainty region for ^{87}Rb overlapped both the polar and the cyclic regions. In the present study we determine the scattering lengths a_0 and a_2 and their uncertainties for spin-1 ^{87}Rb, and a_0, a_2, and a_4 and their uncertainties for spin-2 ^{85}Rb and ^{87}Rb. We concentrate on an accurate determination of the difference a_0-a_2 for spin-1 ^{87}Rb and the pair (a_0-a_4, a_2-a_4) for spin-2 ^{85}Rb and ^{87}Rb. If one accepts the spinor condensate treatment of Refs. [9,10] this analysis gives an unambiguous determination of the nature of the BEC ground states.

Uncertainties in the scattering lengths arise primarily from imperfect knowledge of three parameters: the long-range van der Waals coefficient C_6, and the singlet and triplet *s*-wave scattering lengths a_s and a_t, respectively. In addition, when using potential curves determined for one isotope to predict scattering for another isotope, the results can depend on the precise number of bound states in the triplet potential, N_b, as well as the precise number of bound states in the singlet potential. Roberts *et al.* analyzed a magnetic-field Feshbach resonance to determine "state of the art" potentials for ^{85}Rb [14]. Recently they have reevaluated some of the rethermalization measurements in Ref. [14] and improved the uncertainties for the long-range van der Waals coefficient and the singlet and triplet *s*-wave scattering lengths for ^{85}Rb [15].

Using these new values of C_6, a_s, and a_t we show below unambiguously that $a_0 > a_2$ for spin-1 ^{87}Rb. This result in turn implies that the spinor condensate is definitely ferromagnetic, as was previously suspected [9]. By contrast, the spin-1 ^{23}Na scattering lengths, recently determined in Ref. [16], imply that a ^{23}Na $f=1$ spinor BEC is polar, as has been suggested before [9]. By extracting the scattering length from a spectroscopic experiment, Crubellier *et al.* found that, for ^{23}Na, $a_0=50.0\pm1.6$ a.u. and $a_2=55.0\pm1.7$ a.u. [16]. They calculated the scattering lengths for two values of the C_6 coefficient for ^{23}Na and found that the influence of the C_6 value is very small (a 4% change in C_6 results in a variation in the scattering length of the order of 0.1%). Consequently, the analysis for ^{23}Na [16], in conjunction with the present analysis for ^{87}Rb, implies that both types of spin-1 condensate can be realized with the atoms used most frequently in BEC experiments (^{23}Na and ^{87}Rb).

The improved results for C_6, a_s, and a_t also predict that $a_0-a_4<0$, $\frac{2}{7}|a_2-a_4|<\frac{1}{5}|a_0-a_4|$, for both spin-2 ^{85}Rb and ^{87}Rb. This result implies that both spin-2 ^{85}Rb and ^{87}Rb will be polar. Previously, it was estimated that ^{87}Rb would be

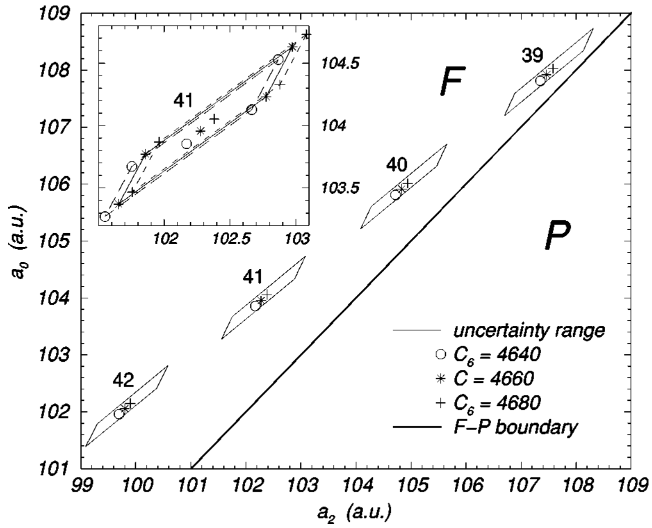

FIG. 1. ^{87}Rb spin 1. Total spin $F=0$ scattering length versus total spin $F=2$ scattering length. The uncertainties of a_0 and a_2 are determined by the uncertainties on a_s, a_t, C_6, and N_b, the number of bound states in the ^{85}Rb triplet potential. The symbols in the middle of the"diamonds" are the mean scattering length for each C_6 and the diamonds encircle the uncertainties arising from uncertainties on a_s and a_t for all C_6. The thick black line shows the boundary between the ferromagnetic and polar phases of the spinor condensate $a_0=a_2$, and the number next to each diamond is N_b.

polar, but that ^{85}Rb would be cyclic [13]. This implies that the ground state for spin-2 ^{85}Rb and ^{87}Rb will have the same nature as spin-2 ^{23}Na. Spin-2 ^{23}Na was already unambiguously classified since the uncertainties on differences between the relevant scattering lengths place a_0-a_4 and a_2-a_4 within the polar region [13]. The results for spin-1 ^{87}Rb and for spin-2 ^{85}Rb and ^{87}Rb are summarized in Figs. 1, 2, and 3, respectively.

Our calculations start from the singlet and triplet Born-Oppenheimer potentials between two rubidium atoms that were calculated in Ref. [17], where the singlet potential is adjusted to have 125 bound states [18]. These potentials are matched smoothly at $r=20.0$ a.u. to the standard long-range van der Waals potentials using the new value of the long-range coefficient C_6 inferred from the experiment in Ref. [14] and reanalyzed according to Ref. [15], and using the C_8 and C_{10} coefficients from the calculations of Ref. [19]. The potentials are adjusted to match the scattering length by including short-range inner-wall corrections that are parametrized for each spin by $c\arctan[(r-r_{\min})^2/(c_r)]$ for $r<r_{\min}$. c_r is a constant (the same order of magnitude as $r_{\min}$; slightly different for the singlet and the triplet), the inner-wall parameters c are of the order of 10^{-5} to 10^{-4} a.u., r is the separation between the two Rb atoms, and $r_{\min}$ is the separation for which the potential is minimal. The inner-wall parameters c are varied over a range that reproduces the recently improved values of a_s and a_t. The improved values of C_6 for rubidium and a_s and a_t for ^{85}Rb are $C_6=4660\pm20$ a.u., $a_s=3650^{+1500}_{-670}$ a.u., and $a_t=-332\pm18$ a.u. [15], while the calculations of Ref. [19] determined

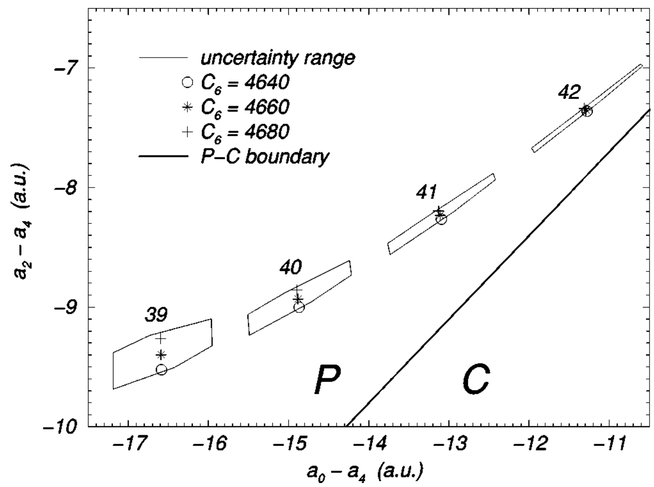

FIG. 2. ^{87}Rb spin 2. Difference between total spin $F=2$ and $F=4$ scattering lengths versus the difference between total spin $F=0$ and $F=4$ scattering lengths. The uncertainties of a_0, a_2, and a_4 are determined by the uncertainties of a_s, a_t, C_6, and N_b, the number of bound states in the ^{85}Rb triplet potential. The symbols in the middle of the "diamonds" are the mean scattering length for each C_6 and the diamonds encircle the uncertainties arising from uncertainties on a_s and a_t for all C_6. The thick black line shows the boundary between the polar and the cyclic phase of the spinor condensate $(a_0-a_4)=(7/10)(a_2-a_4)$, and the number next to each diamond is N_b.

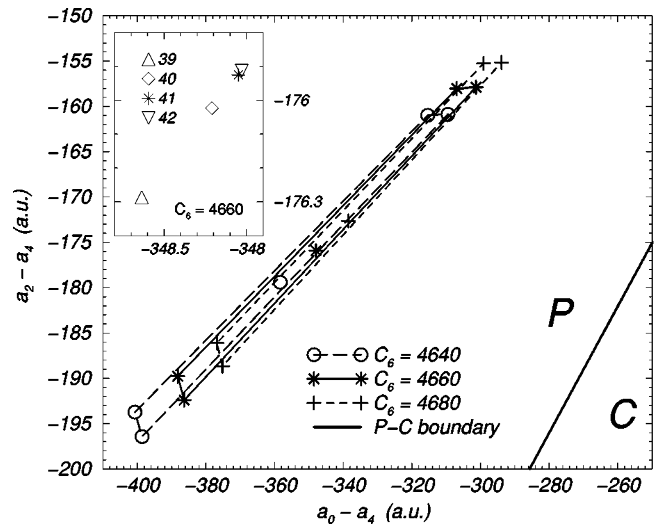

FIG. 3. ^{85}Rb spin 2. Difference between total spin $F=2$ and $F=4$ scattering lengths versus the difference between total spin $F=0$ and $F=4$ scattering lengths for. The uncertainties of a_0, a_2, and a_4 are determined by the uncertainties of a_s, a_t, C_6, and N_b, the number of bound states in the ^{85}Rb triplet potential. The symbols in the middle of the "diamonds" are the mean scattering length for $N_b=41$ and each C_6 and the diamonds encircle the uncertainties arising from uncertainties on a_s and a_t for each C_6. The thick black line shows the boundary between the polar and the cyclic phases of the spinor condensate $(a_0-a_4)=(7/10)(a_2-a_4)$, and the closeup shows the nominal values for the four different N_b.

that $\overline{C_8}=550\,600$ a.u.. These are the values we adopt in the present calculations. Our calculations here do not allow for variance in C_8. This is reasonable because the dependence of C_8 is one order of magnitude smaller than the dependence of C_6. Furthermore, the number of bound states in the triplet potential was previously believed to be 39 ± 1 [18,20], but more refined experimental analysis suggests that it is instead $40\leqslant N_b\leqslant42$ [18,21]. The present calculations are done for $N_b=39,40,41,42$. The number of bound states in the singlet potential is not changed.

Our calculations have been carried out for three values of C_6 that span the empirical range (4640–4680 a.u.). These values are adequate since the quantities of interest vary smoothly with C_6 over the range of interest. We also tested the triplet potential for each one of the four relevant N_b (39,40,41,42). For each value of N_b we determine the values of the inner-wall corrections that correspond to the uncertainty range of ^{85}Rb a_s and a_t for each of the three values of C_6. These calculations are carried out at zero magnetic field and 130 nK since the given values of C_6, a_s, and a_t are determined from collisions at this temperature [15]. The same potentials optimized for ^{85}Rb have been used in our ^{87}Rb calculations, except for an appropriate change in the reduced mass. Since N_b in rubidium is unknown at present, and since we utilize the same potentials determined by the ^{85}Rb singlet and triplet scattering length in our ^{87}Rb calculations, we incorporate N_b in our analysis of the uncertainties for ^{87}Rb. The singlet and triplet potentials are used in multichannel calculations to compute a_0 and a_2 for spin-1 ^{87}Rb and a_0, a_2, and a_4 for spin-2 ^{85}Rb and ^{87}Rb (again at zero magnetic field and at 130 nK), with fixed C_6 and N_b. The calculations are then repeated for each value of C_6 and N_b with the corresponding new values of the inner-wall corrections. These calculations span the empirical C_6, N_b, a_s, and a_t range, which permits us to extract the overall uncertainty in the difference between the relevant scattering lengths, a_0-a_2 for spin 1 and the two relevant differences (a_0-a_4, a_2-a_4) for spin 2. As a confirmation, the same rubidium potentials have also been used to calculate the singlet and triplet s-wave scattering lengths a_s and a_t for ^{87}Rb (at 130 nK energy). These single-channel calculations have been repeated for the three values of C_6 and four values of N_b that span the empirical range. This permits us to check whether a_s and a_t fall within the range of previous measured values. The single-channel triplet scattering lengths are found to be as follows

N_b	a_t
39	107 ± 1 a.u.
40	104 ± 1 a.u.
41	100 ± 1 a.u.
42	97 ± 1 a.u.

and the single-channel singlet scattering length is found to be $a_s=91\pm1$ a.u. The a_s and a_t values for $N_b=39$ are in good agreement with previous work [14,22]. As another confirmation and since N_b is unknown we have also calculated the ^{85}Rb scattering length for $f=2$, $m=-2$ at various magnetic fields to compare the values obtained with the values from

Roberts *et al.* [15]. This comparison shows good agreement. For each of the N_b, the scattering lengths obtained for the specific magnetic fields exhibit an uncertainty greater than the one given by [16].

The values for a_0 and a_2 for spin-1 ^{87}Rb, along with their uncertainties, are shown in Fig. 1. a_0 is always greater than a_2 in the multichannel calculations, which unambiguously determine the nature of spin-1 ^{87}Rb to be ferromagnetic. The global difference lies between 0.3 and 2.7 a.u. over the uncertainty range. The difference is an increasing function of N_b, while a_0 and a_2 themselves are decreasing functions of N_b. For a given N_b, the range of possible values of a_0 and a_2 varies only weakly with C_6, as was the case for ^{23}Na [16].

The results of a_0-a_4 and a_2-a_4 with uncertainties for ^{87}Rb spin 2 are shown in Fig. 2. For all four values of N_b and all three values of C_6 the uncertainty region is within the "polar" region, making the nature of ^{87}Rb spin-2 condensate unambiguously determined. The pair (a_0-a_4,a_2-a_4) moves closer to the boundary between the polar and cyclic regions as N_b is increased but never reaches the boundary, within the present uncertainties. For a fixed value of N_b a_2-a_4 is increasing as a function of C_6, while a_0-a_4 is almost independent of C_6. The uncertainty region for a fixed value of N_b is very narrow (especially for higher N_b). The long axis of this region corresponds to the difference a_s-a_t, whereas the narrow axis corresponds to the sum a_s+a_t. The results for ^{85}Rb spin 2 are shown on Fig. 3. In contrast to the case of ^{87}Rb, here a_2-a_4 and a_0-a_4 are more dependent on the value of C_6 than on N_b, but only very little. a_2-a_4 and a_0-a_4 are slowly increasing functions of C_6 as well as of N_b. The uncertainties for all N_b and values of C_6 unambiguously determine the nature of ^{85}Rb spin 2 to be polar. The uncertainty region is again very narrow. The long axis of this region corresponds to a_t, whereas the narrow axis corresponds to a_s.

Since the graphs for spin-2 ^{85}Rb and ^{87}Rb show only scattering length differences rather than scattering lengths, we summarize a_0, a_2, and a_4 in the following table. The scattering lengths for ^{85}Rb show only very little dependence of N_b. Over the entire range of a_s, a_t, C_6, and N_b the estimated scattering lengths for ^{85}Rb are (in a.u.) $a_0=-740\pm60$, $a_2=-570\pm50$, $a_4=-390\pm20$.

The scattering lengths for spin-2 ^{87}Rb over the entire range of a_s, a_t, and C_6 are estimated as follows (in a.u.).

N_b	a_0	a_2	a_4
39	90.3 ± 1	97.5 ± 1	106.8 ± 1
40	88.8 ± 1	94.8 ± 1	103.6 ± 1
41	87.4 ± 1	92.4 ± 1	100.5 ± 1
42	86.2 ± 1	90.2 ± 1	97.4 ± 1

These numbers conservatively give the global uncertainties for each N_b. In the context of spinor condensates it is necessary to consider the actual allowed regions of the parameters, as we have done above, which permit us to draw meaningful conclusions.

To see how the results change when the multichannel and single-channel energy changes, we calculated the scattering lengths at various energies (with 1 pK in the single and multichannel as the lowest value) to cover the relevant temperature for some experiments. This did not change our conclusions about the nature of the spinor Bose-Einstein condensates in rubidium.

Since the shape of the inner-wall potential is not known exactly and since we change it to have potentials with the four different values of N_b, we also performed the calculations with a quadratic inner-wall correction $[c(r-r_{\min})^2$ for $r<r_{\min}]$ instead of the arctan form. This did not change the conclusions and changed the calculated scattering lengths by only about 0.1%.

The present values of a_0,a_2 for spin-1 ^{87}Rb and a_0,a_2,a_4 for spin-2 ^{85}Rb and ^{87}Rb are consistent with values obtained from Ref. [14]. Note that, to carry out the calculations based on Ref. [14], the correlations among a_s, a_t, and C_6 must be taken into account. We have separately calculated the values of a_0,a_2 for spin-1 ^{87}Rb and a_0,a_2,a_4 for spin-2 ^{85}Rb and ^{87}Rb from a_s and a_t for ^{85}Rb and C_6 as given in Ref. [14], and find that they support our classifications of the spinor condensates as presented in this paper. The new values from Ref. [15] allow us to determine a smaller uncertainty on the calculated scattering lengths, but they do not change our conclusions.

In summary, our analysis based on the new results for the values of C_6, a_s, a_t, and the number of bound states in the triplet potential demonstrate that the nature of the ground states of ^{85}Rb and ^{87}Rb spin-2 condensates should be polar. In addition, the ground state of the ^{87}Rb spin-1 condensate should be ferromagnetic. Therefore, in view of the known scattering parameters for ^{23}Na, both ferromagnetic and polar spin-1 condensates are experimentally accessible, whereas no cyclic or ferromagnetic spin-2 condensate appears to exist for the most common rubidium isotopes.

Note added in proof. Recently, it has come to our attention that Verhaar *et al.*.[24] have investigated the singlet and triplet scattering lengths for ^{85}Rb and ^{87}Rb. They have also determined the nature of spin-1 ^{87}Rb BEC and agree with our conclusion.

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