On the 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 spin 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 spin 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 ultra-cold alkali 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 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.

Multi-component 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, 3, 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. In the theoretical description of Ref. [6, 7], the spinor condensates are classified according to the relative values of certain characteristic scattering lengths. Note that alternative theoretical treatments [8, 9] 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 Ref. [6, 7, 8] fall into the 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 [6] a spinor Bose condensate composed of spin-1 bosons in an optical trap can be either “ferromagnetic” or “antiferromagnetic” in nature [6, 7]. 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 $a_0 < a_2$. 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. [10], 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 $a_2 - a_4$ [11].
The three states emerge under following conditions:

P: \( a_0 - a_s < 0, \frac{1}{5} |a_2 - a_4| < \frac{1}{5} |a_0 - a_4| \),
F: \( a_2 - a_4 > 0, \frac{1}{5} |a_0 - a_4| + \frac{2}{5} |a_2 - a_4| > 0 \),
C: \( a_2 - a_4 < 0, \frac{1}{5} |a_0 - a_4| - \frac{2}{5} |a_2 - a_4| > 0 \).

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 \([8]\) based on the analysis of Ref. \([13]\), 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. \([8]\). 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 \([8]\). 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 region. 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 \( (a_0 - a_2, a_2 - a_4) \) for spin-2 \(^{85}\)Rb and \(^{87}\)Rb. If one accepts the spinor condensate treatment of Ref. \([8, 9]\) 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 the 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 resonant to determine “state of the art” potentials for \(^{85}\)Rb \([1]\). Recently they have revisited some of the re-orthonormalization measurements in Ref. \([1]\) and improved the uncertainties for the long-range van der Waals coefficient and the singlet end triplet s-wave scattering lengths for \(^{85}\)Rb \([1]\).

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 \([8]\). By contrast the spin-1 \(^{23}\)Na scattering lengths, recently determined in Ref. \([3]\), imply that a \(^{23}\)Na \( f = 1 \) spinor BEC is polar, as has been suggested before \([3]\). By extracting the scattering length from a spectroscopic experiment, Crubellier et al. found that, for \(^{23}\)Na, \( a_0 = 50.0 \pm 1.6 \) a.u. and \( a_2 = 55.0 \pm 1.7 \) a.u. \([3]\). 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 \([3]\), in conjunction with the present analysis for \(^{87}\)Rb, implies that both types of spin-1 condensates 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 \( a_0 - a_4 < 0, \frac{1}{5} |a_2 - a_4| < \frac{1}{5} |a_0 - a_4| \), 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 polar, but that \(^{87}\)Rb would be cyclic \([10]\). 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 \([10]\). The results for spin-1 \(^{87}\)Rb and for spin-2 \(^{85}\)Rb and \(^{87}\)Rb are summarized in Figs. \([1, 2, 3]\) respectively.

Our calculations start from the singlet and triplet Born-Oppenheimer potentials between two rubidium atoms that were calculated in Ref. \([4]\), where the singlet potential is adjusted to have 125 bound states \([5]\). These potentials are matched smoothly at \( r = 22.0 \) 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. \([1]\) and reanalyzed according to Ref. \([5]\) and using the \( C_4 \) and \( C_{10} \) coefficients from the calculations of Ref. \([5]\). The potentials are adjusted to match the scattering length by including short-range inner-wall corrections that are parameterized 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, \( a_s \) and \( a_t \) for \(^{85}\)Rb are: \( C_6 = 4660 \pm 20 \) a.u., \( a_s = 3650^{+1500}_{-670} \) a.u. and \( a_t = -332 \pm 18 \) a.u. \([12]\), while the calculations of Ref. \([10]\) determined that \( C_6 = 550600 \) a.u.. These are the values we adopt in the present calculations. Our calculations here do not allow for variance in \( C_6 \). This is reasonable because the dependence of \( C_6 \) 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 \( 39 \pm 1 \) \([14, 15]\), but more refined experimental analysis suggests that it is instead \( 40 \leq N_b \leq 42 \) \([13, 15]\). 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
The single-channel triplet scattering lengths are found to fall within the range of previous measured values. These single-channel calculations have been repeated for two relevant differences (singlet and triplet scattering length in our empirical range. This permits us to check whether the single-channel triplet scattering lengths are found to be:

\[
N_b \quad a_t \\
39 \quad 107 \pm 1 \text{ a.u.} \\
40 \quad 103 \pm 1 \text{ a.u.} \\
41 \quad 100 \pm 1 \text{ a.u.} \\
42 \quad 97 \pm 1 \text{ a.u.}
\]

and the single-channel singlet scattering length is found to be: \(a_s = 91 \pm 1 \text{ a.u.}\). The \(a_s\) and \(a_t\) values for \(N_b = 39\) are in good agreement with previous work \[13, 14\]. As another confirmation, and since \(N_b\) is unknown we have also calculated the \(^{87}\text{Rb}\) scattering length for \(f = 2, m = -2\) at various magnetic fields to compare the obtained values with the values from Roberts \textit{et al.}: \[13\]. This comparison shows good agreement. For each of the \(N_b\) the scattering lengths obtained for the specific magnetic fields exhibits an uncertainty greater than the one given by \[13\].

The values for \(a_0\) and \(a_2\) for spin-1 \(^{87}\text{Rb}\), 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 \(^{87}\text{Rb}\) 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
FIG. 3: 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 spin-2 \(^{85}\text{Rb}\). 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 \(^{85}\text{Rb}\) 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 phase of the spinor condensate: \( (a_2 - a_4) = \frac{1}{2}(a_0 - a_t) \) and the close-up shows the average values for the four different \( N_b \).

\( C_6 \), as was the case for \(^{23}\text{Na} \) [13].

The results of \( a_0 - a_4 \) and \( a_2 - a_4 \) with uncertainties for \(^{87}\text{Rb}\) 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 \(^{87}\text{Rb}\) spin-2 condensate unambiguously determined. The pair \( (a_0 - a_4, a_2 - a_4) \) moves closer to the boundary between the polar and the cyclic regions as \( N_b \) is increased but never reaches the boundary, within the present uncertainties. For a fixed value of \( N_b \), \( a_0 - a_4 \) 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 \( a_s \) 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 \( a_0 + a_t \).

The results for \(^{85}\text{Rb}\) spin-2 are shown on Fig. 3. In contrast to the case of \(^{87}\text{Rb}\), 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 \(^{85}\text{Rb}\) 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 \( a_o \).

Since the graphs for spin-2 \(^{85}\text{Rb}\) and \(^{87}\text{Rb}\) show only scattering lengths differences rather than scattering lengths, we summarize \( a_0, a_2 \) and \( a_4 \) in the following table. The scattering lengths for \(^{85}\text{Rb}\) 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 \(^{85}\text{Rb}\) are (in a.u.):

\[
\begin{align*}
\begin{array}{ccc}
\text{a} & \text{b} & \text{c} \\
0 & 680 & 870 \\
2 & -540 & 50 \\
4 & -390 & 30
\end{array}
\end{align*}
\]

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

\[
\begin{align*}
\begin{array}{cccc}
\text{N} & \text{a} & \text{b} & \text{c} \\
0 & 90.5 & 77.5 & 106.8 \\
2 & 89.0 & 94.8 & 103.6 \\
4 & 87.7 & 92.4 & 100.5 \\
6 & 86.4 & 90.2 & 97.4
\end{array}
\end{align*}
\]

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 and 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 pico Kelvin 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 only changed the calculated scattering lengths by about 0.1%.

The present values of \( a_0, a_2, a_4 \) for spin-1 \(^{87}\text{Rb}\) and \( a_0, a_2, a_4 \) for spin-2 \(^{85}\text{Rb}\) and \(^{87}\text{Rb}\) are consistent with values obtained from Ref. [11]. 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 \( a_0, a_2, a_4 \) for spin-1 \(^{87}\text{Rb}\) and \( a_0, a_2, a_4 \) for spin-2 \(^{85}\text{Rb}\) and \(^{87}\text{Rb}\) form \( a_s, a_t \) for \(^{85}\text{Rb}\) and \( C_6 \) as given in Ref. [11], and find that they support our classifications of the spinor condensates as presented in this paper. The new values from Ref. [14] 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 \(^{85}\text{Rb}\) and \(^{87}\text{Rb}\) spin-2 condensates should be polar. In addition, the ground state of the \(^{87}\text{Rb}\) spin-1 condensate should be ferromagnetic. Therefore, in view of the known scattering parameters for \(^{23}\text{Na}\), both ferromagnetic and polar spin-1 condensates are experimental accessible whereas no cyclic or ferromagnetic spin-2 condensate appears to exist for the most common rubidium isotopes.

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