PHYSICAL REVIEW A VOLUME 56, NUMBER 6 DECEMBER 1997

Predictions for laser-cooled Rb clocks

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(Received 28 May 1997)

Using information from a recent ^{85}Rb two-color photoassociation experiment, we evaluate the merits of fountain clocks based on ^{87}Rb and ^{85}Rb isotopes as alternatives to ^{133}Cs and find that they offer significant advantages. In the case of ^{87}Rb the collisionally induced fractional frequency shift is 15 times smaller than for ^{133}Cs. This small shift is associated with a small difference in the triplet and singlet scattering lengths for ^{87}Rb. For ^{85}Rb, the shift produced by the two $m_f=0$ clock states may have opposite signs allowing the shift to be eliminated by controlling the relative populations of these states. We also present collision quantities relevant to atomic fountain clocks containing multiply launched groups of atoms, and for evaporative cooling of ^{85}Rb atoms. [S1050-2947(97)50312-X]

PACS number(s): 32.80.Pj, 42.50.Vk

Techniques developed in recent years to produce and manipulate cold atoms are expected to lead to rapid improvements in atomic clocks. The development of an atomic fountain based on laser-cooled atoms [1,2] has created prospects for a considerably improved accuracy and stability of the cesium frequency standard. In a fountain clock, a cloud of atoms is cooled to μK temperatures and launched upwards through a microwave cavity. The cloud is slowed by gravity and then returns through the cavity. The combination of slow atoms and a long interrogation time between the two cavity traversals can potentially lead to a 100- to 1000-fold improvement of accuracy and stability [3]. Soon after the first demonstration of a Cs fountain clock [2] it was suggested that elastic collisions between the atoms during their ballistic flight between the two cavity passages shift the phase of the atomic coherence and produce an apparent frequency shift [4]. A subsequent experiment by Gibble and Chu observed this effect, measuring a large shift $\delta\nu=-16$ mHz for a cold Cs density $n=10^9$ cm^{-3} and a temperature $T=1$ μK [3]. As a consequence of the fundamentally quantum character of the collisions, the collisional shift has a nonzero $T\rightarrow 0$ limit [4], and at 1 μK, the shift is nearly the $T\rightarrow 0$ value. While the real world performance of an atomic clock certainly depends on a complicated balance of many factors, the cold-collision shift is one of the largest and most difficult systematic errors to accurately measure.

Reviewing possibilities to eliminate the cold-collision shift, Gibble and Verhaar [5] noted that clocks based on other atomic species may give a better performance and pointed out that cold-collision shifts could, in favorable circumstances, even be eliminated. Two of the alternative species, ^{87}Rb and ^{85}Rb, are considered in this Rapid Communication. As we will show, ^{87}Rb is a very promising isotope for cold-clock applications because its collisional shift is small. ^{85}Rb turns out to be promising because the cold-collision shift can probably be eliminated by adjusting the atomic populations in the fountain [5].

To assess the merits of these isotopes as clock species, we need reliable information on the cold-atom interaction properties. The last few months have seen a breakthrough in the knowledge of such interactions, mainly because of the importance of these to Bose-Einstein condensation. Three one-color photoassociation (PA) experiments [6–8] led to a determination of parameters in the triplet sector. A first indication for the singlet sector came from the observation of two overlapping Bose condensates [9], pointing to nearly equal node structures of the singlet and triplet radial wave functions at long range (i.e., nearly equal singlet and triplet scattering lengths [10]). The determination of the energies of 12 close-to-dissociation vibrational levels of $^{85}Rb_2$ in a recent two-color PA experiment, has led to the most systematic and accurate knowledge of cold rubidium atom-atom interactions so far, including the singlet sector [11].

A prediction made possible by this development consisted of a number of magnetic field values where field-induced resonances in ^{87}Rb+^{87}Rb and ^{85}Rb+^{85}Rb scattering should occur [12]. As another prediction, here we calculate the collisional frequency shifts for cold rubidium atomic clocks.

For both isotopes we consider an atomic clock operating on the transition at frequency ω between the lower and upper $m_f=0$ states at a field of order 1 mG. We indicate the possible Zeeman and hyperfine f,m_f substates of the Rb ground state by the index j, singling out the lower and upper clock states as $j=1$ and 2, respectively. A derivation on the basis of the quantum Boltzmann equation [13] shows the collisional shift $\delta\omega$ and line broadening Γ of the clock transition to have the form of a sum over all atomic states j:

$$i\,\delta\omega-\Gamma\equiv\sum_j n_j\langle v(i\lambda_j-\sigma_j)\rangle, \tag{1}$$

with $\langle\ \rangle$ a thermal average, n_j the density of atoms in state j, v the relative velocity, and λ_j and σ_j the so-called shift and width cross sections. The sum over j includes all populated substates, including the two clock states $j=1$ and 2. The shift due to states other than $j=1$ and 2 is absent if the fountain contains only the two clock states. The shift and width cross sections are obtained from S-matrix elements for the elastic scattering processes $1+j\rightarrow 1+j$ and $2+j\rightarrow 2+j$, in which the two clock states participate:

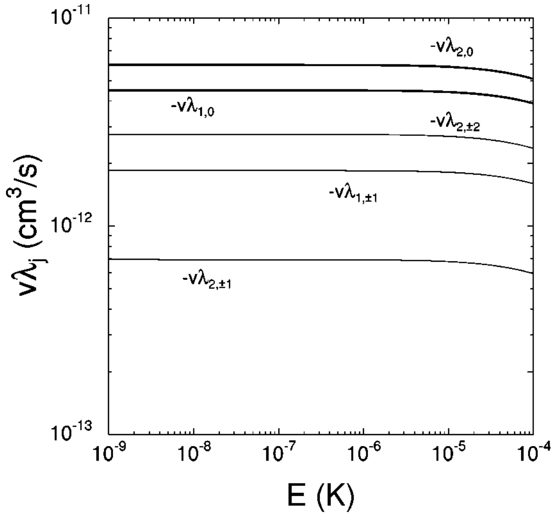

FIG. 1. Predicted s-wave frequency shift rate constants $v\lambda_j$ for ^{87}Rb as a function of collision energy.

$$i\lambda_j-\sigma_j=(1+\delta_{1j})(1+\delta_{2j})\frac{\pi}{k^2}\sum_l (2l+1)$$
$$\times[S^l_{\{1j\},\{1j\}}S^{l*}_{\{2j\},\{2j\}}-1], \quad (2)$$

with m the atomic mass, l the partial wave index, and $\hbar k=\sqrt{mE}=\frac{1}{2}mv$. In our case temperatures are low enough to restrict ourselves to s-wave ($l=0$) collisions. For $T\to 0$ we can apply the effective-range approximation and express the low-energy S-matrix elements in (complex) scattering lengths: $S_{\{nj\},\{nj\}}\approx 1-2ika_{nj}$. We then obtain

$$\delta\omega=-\frac{4\pi\hbar}{m}\sum_j n_j(1+\delta_{1j})(1+\delta_{2j})\mathrm{Re}(a_{1j}-a_{2j}), \quad (3)$$

$$\Gamma=-\frac{4\pi\hbar}{m}\sum_j n_j(1+\delta_{1j})(1+\delta_{2j})\mathrm{Im}(a_{1j}+a_{2j}). \quad (4)$$

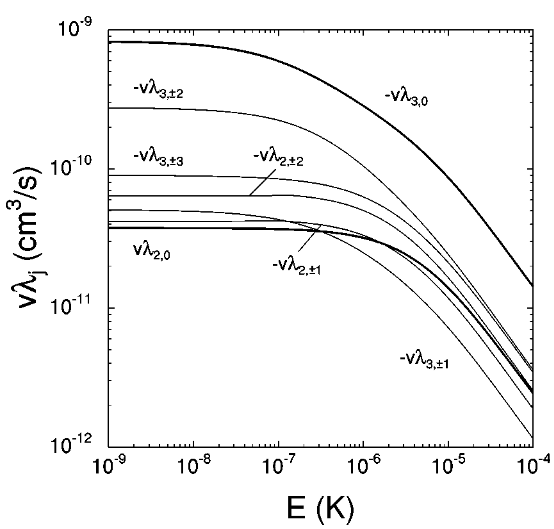

FIG. 2. Same as Fig. 1 for ^{85}Rb.

TABLE I. Predicted collision shifts $(nv\lambda)_j/2\pi$ and broadening rates $(nv\sigma)_j$ for ^{87}Rb at $E/k_B=1$ μK and $n_j=10^9$ cm^{-3}. For a total density 10^9 cm^{-3}, an ^{87}Rb clock has a cold-collision shift $\delta\nu/\nu=-1.2\times10^{-13}$ vs -17×10^{-13} for ^{133}Cs. ^{87}Rb has a hyperfine frequency $\nu=\omega/(2\pi)=6.835$ GHz.

f,m_f	$(nv\lambda)_{f,m_f}/2\pi$ in mHz	$(nv\sigma)_{f,m_f}$ in s^{-1}
1,0	$-0.7^{+0.2}_{-0.2}$	$(1.7^{+1}_{-0.9})\times10^{-5}$
2,0	$-0.9^{+0.2}_{-0.2}$	$(1.3^{+2}_{-0.7})\times10^{-4}$
1,±1	$-0.29^{+0.02}_{-0.02}$	$(3^{+3}_{-2})\times10^{-5}$
2,±1	$-0.110^{+0.007}_{-0.009}$	$(3^{+2}_{-1})\times10^{-5}$
2,±2	$-0.44^{+0.03}_{-0.04}$	$(1.2^{+0.9}_{-0.3})\times10^{-4}$

The above expressions for $\delta\omega$ and Γ can be interpreted in terms of a Hartree-Fock mean field [14], leading to shifts and imaginary parts of the energies of the individual clock states 1 and 2.

On the basis of the above-mentioned explanation for the reduced intercondensate decay rate, one would also expect a near coincidence of all other scattering lengths, and this implies, by Eq. (3), a small collisional shift. This is indeed borne out by coupled-channel calculations. In Figs. 1 and 2 we present the predicted partial collisional shift rate constants $v\lambda_j$ for ^{87}Rb and ^{85}Rb, respectively. Besides the important results for the clock states $j=1$ and 2, we also present results for the other m_f states. (Values for opposite m_f are equal for $B\approx 0$ [4,13].)

In Tables I and II we give the partial collision shifts $(nv\lambda)_j/2\pi$ and partial broadenings $(nv\sigma)_j$ for the Rb isotopes for a partial density of 10^9 cm^{-3}. For atomic clocks, we expect that broadening rates are sufficiently small to not limit the accuracy or stability, although they may play an important role in other experiments [15]. The error limits are intended to provide a conservative estimate of the range of possible values.

In a laser-cooled ^{133}Cs clock, the cold-collision shift can be reduced by reducing the atomic density. This, however, lowers the shot-noise-limited signal-to-noise ratio (S/N) and hence increases the short-term instability of the clock. Therefore, to appropriately compare the potential performance of

TABLE II. Same as Table I for ^{85}Rb. For a population ratio $n_{3,0}/n_{2,0}=-\lambda_{2,0}/\lambda_{3,0}\approx\frac{1}{9}$ the collision shifts produced by the populations in the two clock states cancel. For ^{85}Rb, $\nu=3.0357$ GHz.

f,m_f	$(nv\lambda)_{f,m_f}/2\pi$ in mHz	$(nv\sigma)_{f,m_f}$ in s^{-1}
2,0	5^{+10}_{-8}	$(1^{+9}_{-1})\times10^{-3}$
3,0	-45^{+11}_{-3}	$(2.2^{+2}_{-0.9})\times10^{-1}$
2,±1	-5^{+2}_{-3}	$(6^{+10}_{-4})\times10^{-3}$
3,±1	-4^{+1}_{-1}	$(2^{+3}_{-1})\times10^{-2}$
2,±2	-8^{+3}_{-4}	$(1.1^{+2}_{-0.6})\times10^{-2}$
3,±2	-17^{+5}_{-3}	$(9^{+11}_{-5})\times10^{-2}$
3,±3	-10^{+3}_{-5}	$(3^{+4}_{-2})\times10^{-2}$

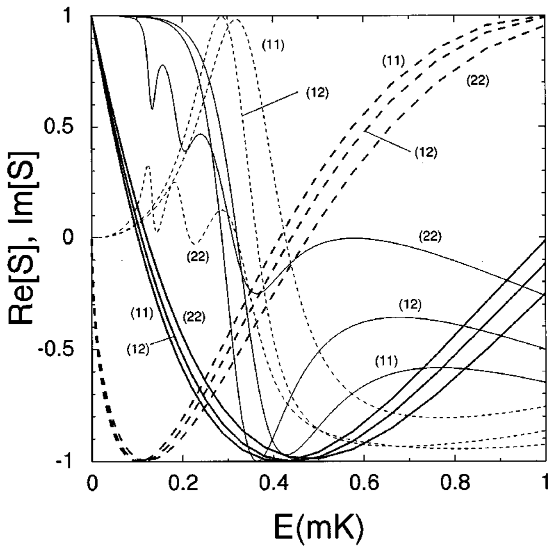

FIG. 3. Real (solid) and imaginary (dashed) part of the $l=0$ (bold) and $l=2$ (normal) S-matrix elements for elastic collisions between the clock states of ^{87}Rb, indicated by 1 and 2.

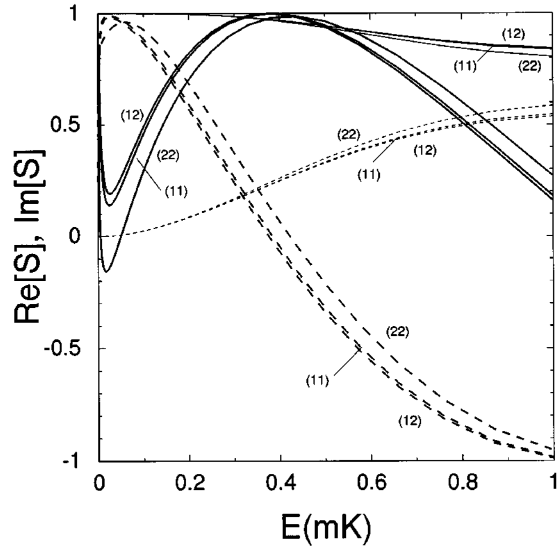

FIG. 4. Same as Fig. 3 for ^{85}Rb.

two clocks, we compare the fractional collision shift $n v \lambda_j/(2\pi\nu)$ at the same fractional short-term instability. The latter is given by $\delta\nu/\nu = \Delta\nu/(\pi\nu\ \mathrm{S/N})$ for a single launch in a fountain, where $\Delta\nu$ is the transition line width. Since Rb and Cs fountains are expected to have the same fountain height, $\Delta\nu$ will be the same for both. Therefore, the instability will be generally independent of the transition frequency because the shot-noise-limited S/N scales as ν^{-1}. This occurs because, given the same atomic density and temperature in the two clocks, a lower transition frequency allows for a larger hole in the microwave cavity, implying that the number of detected atoms scales as ν^{-2}, so that $\mathrm{S/N} = N^{1/2} \propto \nu^{-1}$. Of course, this is only true if there are no technical obstacles to achieving the shot-noise limit. This may be particularly important for ^{85}Rb fountains where the S/N must be three times higher than that for ^{133}Cs to achieve the same stability, due to its lower transition frequency. Therefore, the appropriate comparison is the fractional collision shift at the same density, since the fractional instability only depends on the density (and not on the transition frequency), if the shot-noise limit is realized.

The cold-collision fractional frequency shift for ^{87}Rb is $\delta\nu/\nu = -1.2\times 10^{-13}$ at $E=1$ μK and a density of 10^9 cm^{-3}; this is 15 times smaller than that for ^{133}Cs. Besides this factor of 15 improvement, ^{87}Rb and ^{133}Cs are remarkably similar, as both clock states produce negative collision shifts of similar size, and therefore we anticipate that the systematic errors associated with the cold-collision shift in both clocks will scale accordingly.

The cold-collision shifts for ^{85}Rb in Table II are also interesting for future atomic clocks. Near the central values of the predicted $(n v \lambda)_j$ intervals, the two clock-state populations produce opposite collision shifts so that the cold-collision shift can be canceled by adjusting the population ratio of these two states in the fountain [5]. By driving a $\pi/5$ pulse on the first pass through the microwave cavity, there will be 10% of the atoms in the $|f=3,m_f=0\rangle$ state and 90% in $|f=2,m_f=0\rangle$. In this way, an ^{85}Rb clock has no cold-collision shift. The principal advantage of eliminating the shift is that an extrapolation to zero density no longer requires accurate density measurements [5]. This may allow the clock to operate at much higher densities and therefore obtain higher stabilities. Driving a $\pi/5$ pulse reduces the Ramsey fringe contrast by 40% [5]. Therefore, to achieve the same stability, an ^{85}Rb clock will have to operate at a density 2.75 times higher than a ^{133}Cs or ^{87}Rb clock. Thus, for $n=2.75\times 10^9$ cm^{-3}, the collision shifts produced by the individual clock states are $\pm 4\times 10^{-12}$. These are twice as large as the shift of a ^{133}Cs clock and 30 times larger than the shift of an ^{87}Rb clock. In addition, because the transition frequency for ^{85}Rb is half that of ^{87}Rb, this will require a potentially technically challenging S/N. For these reasons, a clock based on ^{85}Rb may be best suited for microgravity applications where the long interrogation times require a smaller S/N to achieve the same stability. Investigation of

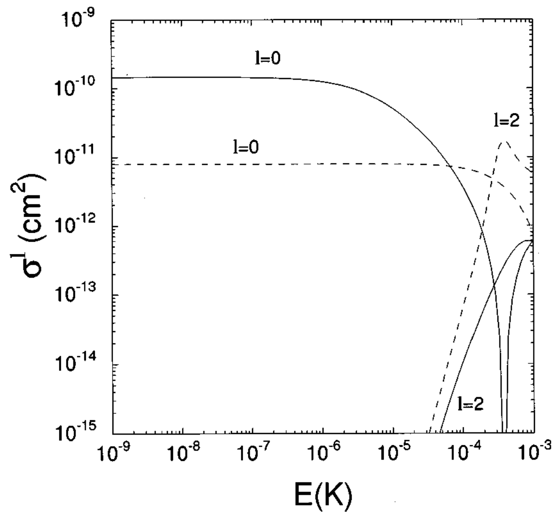

FIG. 5. S-wave $(l=0)$ and d-wave $(l=2)$ contributions to the elastic cross section of the $m_f=-f$ state of the lower hyperfine manifold, as a function of collision energy, i.e., $\sigma_{f=2,m_f=-2}$ for ^{85}Rb (solid) and $\sigma_{f=1,m_f=-1}$ for ^{87}Rb (dashed).

the cancellation technique and its systematic errors is needed to show whether the advantages in the density extrapolation offset the larger cross section and 40% smaller S/N. Note that the error bar for $(nv\lambda)_{2,0}$ does not guarantee the opposite sign for the (2,0) and (3,0) collision shifts that is needed for the above cancellation method. With the current interaction uncertainties, we find that the collision shifts can be canceled in about 75% of the multiparameter volume.

Figure 2 shows that the partial collision shifts are nearly energy independent below 1 μK for ^{85}Rb. For ^{87}Rb (see Fig. 1), the partial collision shifts are almost constant to much higher energies $E\sim 100$ μK. At nK energies, the rates will be important for experiments, including clocks, using Bose condensed samples [16].

The s-wave results mentioned previously are sufficient to describe the effects of low-energy collisions ($E<10$ μK). Future fountain clocks may juggle atoms to achieve higher short-term stabilities [17]. For the scattering between two successively launched balls of atoms in a juggling fountain [18], d-wave effects are potentially important. In the case of ^{87}Rb we expect a sizable effect from the d-wave triplet shape resonance [7], which will also influence mixed singlet-triplet channels. For ^{85}Rb we expect to see effects associated with a Ramsauer-Townsend s-wave minimum in the elastic cross section σ_{2-2}, which appears to obstruct evaporative cooling in a cloud of $|2-2\rangle$ atoms at energies of a few hundred μK [19]. In that connection it is of interest to know whether the d-wave elastic amplitude, with its rapid increase with collision energy, might fill the s-wave minimum of σ_{2-2} and also dominate the s-wave collision shifts.

In Figs. 3 and 4 we present a selection of elastic d-wave S-matrix elements, of importance for the clock collision shifts at higher collision energies, and compare them with the corresponding s-wave S-matrix elements for the same range of energies. Clearly for ^{85}Rb, close to 400 μK the latter elements have their unscattered value 1, while the d-wave values are still small. Calculating the elastic s- and d-wave elements for the $(2-2)+(2-2)$ channel, we find a similar result (solid lines in Fig. 5): A pronounced Ramsauer-Townsend minimum in $\sigma^{l=0}_{2-2}\sim|S^{l=0}_{\{(2-2)(2-2)\},\{(2-2)(2-2)\}}-1|^2$, only partially filled by the d-wave cross section (this holds to fields of at least 750 G).

Figure 4 for ^{85}Rb shows some remarkable differences with Fig. 3 for ^{87}Rb. A first point is the rapid energy dependence of the s-wave curves close to $E=0$, similar to that in Fig. 2. It is probably related to the close proximity of a pole in the complex energy plane, corresponding to a virtual triplet state and a large negative scattering length. A second point of difference is the complexity of the d-wave curves for ^{87}Rb. Apparently the (1,2) channel, which is pure triplet, displays the above-mentioned d-wave shape resonance behavior. A similar behavior arises also in the two remaining mixed-S channels, due to the same approximate equality of singlet and triplet node structures that gave rise to the small collisional frequency shifts in the foregoing. This and other similarities between channels are easily understood using a simple three-parameter long-range collision model proposed in Ref. [20]. The d-wave shape resonance also shows up in the σ_{1-1} elastic cross section of ^{87}Rb (dashed curves in Fig. 5).

K.G. acknowledges support from the National Science Foundation, a NIST Precision Measurement grant, the NASA Microgravity Research Division, and Yale University. D. J. H. acknowledges support from the R. A. Welch Foundation, the National Science Foundation, and the NASA Microgravity Research Division.

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