Low-velocity elastic scattering of Rb-Rb

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With reference to recent progress in preparing slow and intense Rb beams (*rubidium atomic funnel* and *low-velocity intense source of atoms from a magneto-optical trap*) we have calculated total and differential elastic scattering cross sections and scattering lengths for ground-state collisions of ^{85}Rb as well as ^{87}Rb. Our results are based on the state of the art $X^1\Sigma_g^+$ and $a\ ^3\Sigma_u^+$ potentials. Pronounced resonances in the total scattering cross sections occur for collision velocities below 15 m/s. We propose scattering experiments with slow Rb beams in order to check the currently known singlet and triplet potential-energy curves. [S1050-2947(97)02508-0]

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The effective ground-state energy curves of homonuclear alkali-metal diatoms—usually determined by *ab initio* calculations—are necessary to understand ultracold collisions and frequency shifts in atomic clocks following from such collisions [1]. Furthermore, a scattering length, the most important parameter for Bose-Einstein condensation (BEC), can be deduced from every ground-state potential curve. For comparatively simple atoms, like H and Li, the potentials are accurate enough to predict valid scattering lengths [2,3]. For Na the uncertainties in the potentials are a bit greater, especially for the triplet state. In a previous work we have calculated cross sections and the triplet scattering length for Na-Na [4]. Regarding heavier alkali metals the uncertainties further increase due to the more complex electronic structure.

To calculate scattering cross sections complete potential-energy curves, from the repulsive part up to a few hundred Å of the interatomic distance, are needed. Neglecting hyperfine interactions the diatoms of both rubidium isotopes, ^{85}Rb (84.911 794 amu) and ^{87}Rb (86.909 187 amu), can be described by the same ground-state Coulomb potentials which follows from the Born-Oppenheimer approximation.

Almost complete short-range potential curves for Rb_2 (singlet and triplet) have been calculated by Krauss and Stevens [5]. They present two sets of energy points, obtained by *ab initio* calculations, which are suitable to determine the potentials up to 10.6 Å. The repulsive part of the singlet potential has been extended by data from Ref. [6]. The long-range part can be described by an analytic equation with three dispersion coefficients. We choose the coefficients calculated by Marinescu, Sadeghpour, and Dalgarno [7].

Due to the lack of other short-range potential curves, or more accurate dispersion coefficients, we can assume to get state-of-the-art potential curves for Rb_2. From these potentials scattering cross sections (and scattering lengths) can be deduced.

We found pronounced resonance structures in the total cross sections, which can be regarded as detailed fingerprints of the interaction potentials. Low-velocity scattering experiments are the ideal way to directly check the validity of the best available *ab initio* potentials.

With the recent development of a rubidium atomic funnel by Swanson *et al.* [8] it should be possible to perform scattering experiments in the most interesting velocity range. The funnel produces a flux of 10^{10} ^{85}Rb atoms/s with a temperature of 500 μK in all three dimensions, which is quite near to the Doppler cooling limit. According to the authors the mean velocity is stable to 2 cm/s and controllable in the range of 3–10 m/s. Another interesting setup has recently been reported by Lu *et al.* [9] where a slow atomic ^{87}Rb beam has been extracted from a three-dimensional magneto-optical trap. This technique is admittedly quite simpler to perform than a funnel, but the obtained mean velocity (14 m/s) and velocity width (FWHM=2.7 m/s) demand further cooling to get a suitable projectile beam.

In this paper we present total and differential scattering cross sections in order to point out at which collision velocities one has to search for significant structures in a scattering experiment.

The total scattering cross section (TCS) is determined by

$$\sigma_{\text{tot}}^{+}=\frac{4\pi}{k^2}\sum_{\text{even }\ell}(2\ell+1)\sin^2\delta_\ell^{S/T}=\frac{2\pi}{4}\int_0^\pi|f_{S/T}^{+}(\theta)|^2d\theta. \tag{1}$$

Due to the boson character of both Rb isotopes (the hyperfine coupling is assumed to be conserved during low-velocity collisions) only even partial waves contribute to the cross sections. Alternatively the usual scattering amplitude

$$f_{S/T}(\theta)=\frac{1}{k}\sum_{\ell=0}^{\ell_{\max}}(2\ell+1)(e^{2i\delta_\ell^{S/T}}-1)P_\ell(\cos\theta), \tag{2}$$

TABLE I. Energy points added to the Krauss-Stevens potentials.

R (Å)	Singlet (eV)	Triplet (eV)	Source
2.501	1.190 679		Ref. [6]
2.801	0.431 934		Ref. [6]
3.121	$-4.333\,773\times10^{-3}$		Ref. [6]
12.001	$-1.157\,223\times10^{-3}$	$-1.157\,223\times10^{-3}$	Ref. [7]
13.001	$-6.864\,978\times10^{-4}$	$-6.864\,978\times10^{-4}$	Ref. [7]
14.001	$-4.258\,460\times10^{-4}$	$-4.258\,460\times10^{-4}$	Ref. [7]

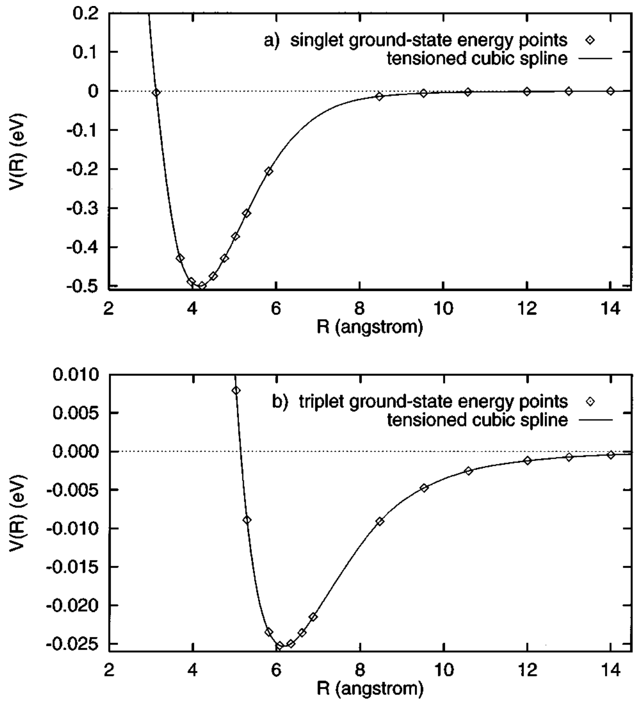

FIG. 1. Ground-state singlet and triplet energy curves of Rb-Rb.

with $k=\sqrt{2\mu E_{CM}/\hbar^2}$ and the Legendre polynoms $P_{\ell}(\cos\theta)$ can be symmetrized. The differential scattering cross section (DCS) is then

$$d\sigma^{+}(\theta)=|f_{S/T}(\theta)+f_{S/T}(\pi-\theta)|^2=|f_{S/T}^{+}|^2. \qquad (3)$$

For easier comparison with experimental results we have transformed all DCSs to the laboratory frame. To obtain the singlet and triplet phase shifts $\delta_{\ell}^{S/T}$ we solved Schrödinger's equation by the Numerow algorithm using a potential range of $R_{\max}=250$ Å.

The Rb potential data sets by Krauss and Stevens [5] have been extended by a couple of energy points (Table I) and connected by tensioned cubic splines (see Fig. 1). The additional points at 12 Å, 13 Å, and 14 Å listed in Table I are neccessary to get a continuous transition from the short-range part to the long-range part of the potentials, i.e., $V(R)$ and $dV(R)/dR$ have to be continual at the junction point. We have joined the analytical long-range part

$$V_{S/T}(R)=-\frac{C_6}{R^6}-\frac{C_8}{R^8}-\frac{C_{10}}{R^{10}} \qquad (4)$$

with the dispersion coefficients (in a.u.) $C_6=4.426\times10^3$, $C_8=5.506\times10^5$, and $C_{10}=7.665\times10^7$ to the cubic spline curves at $R=13$ Å. The difference between the singlet and triplet potential is negligible for $R>13$ Å, so we do not need an analytical expression for the exchange interaction in Eq. (4). Retardation effects [10] have been neglected since they are much smaller than the discrepancy to alternative sets of dispersion coefficients (see Table VI in Ref. [7]).

Figure 2 shows TCSs for both isotopes and both electronic ground states. Due to the integer hyperfine quantum numbers F the atoms are bosons and only even partial waves should contribute to the cross sections (solid lines). Odd partial waves are shown for completeness (dotted lines). As it is

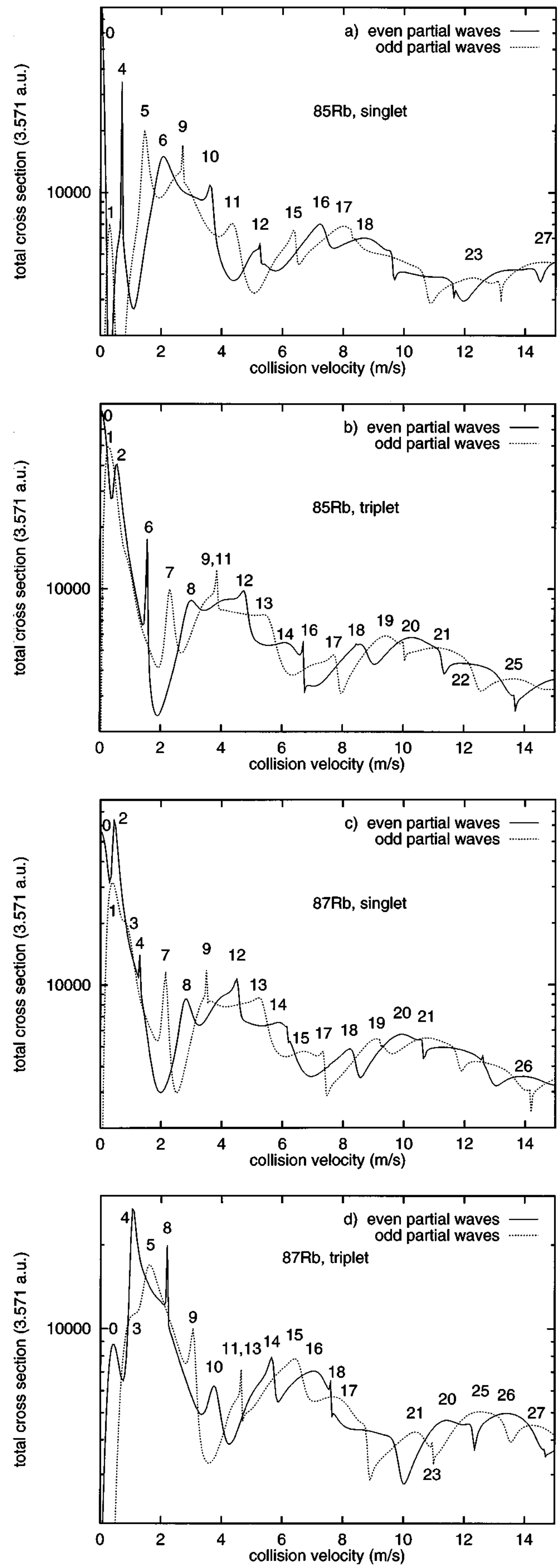

FIG. 2. Total scattering cross sections of Rb-Rb (identical collision partners) in the ground state. The numbers indicate the dominant partial wave (ℓ) of the resonances. (3.571 a.u.$=1$ Å$^2=10^{-16}$ cm^2).

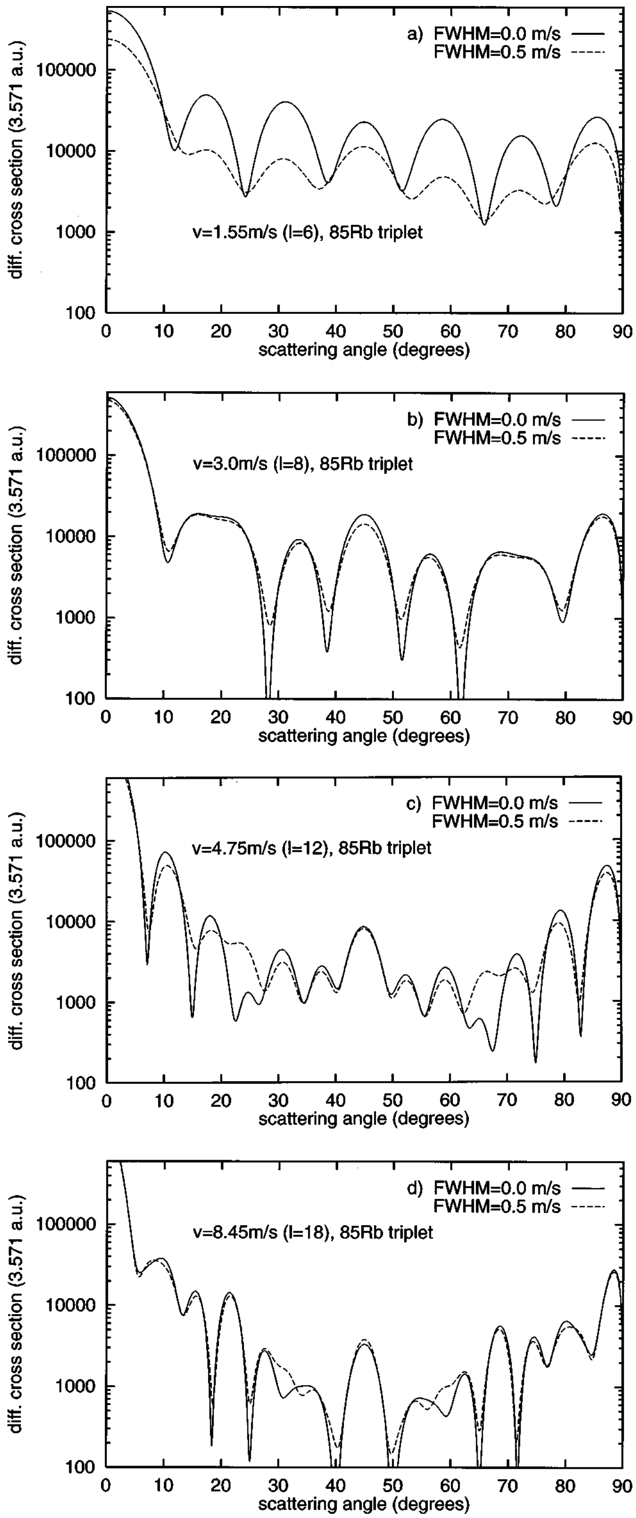

FIG. 3. Differential scattering cross sections (laboratory frame) of ^{85}Rb-^{85}Rb in the ground state for several longitudinal projectile velocities. The target atoms are assumed to be at rest. Solid lines: sharp projectile velocity, dashed lines: projectile velocity width is 0.5 m/s (full width half maximum).

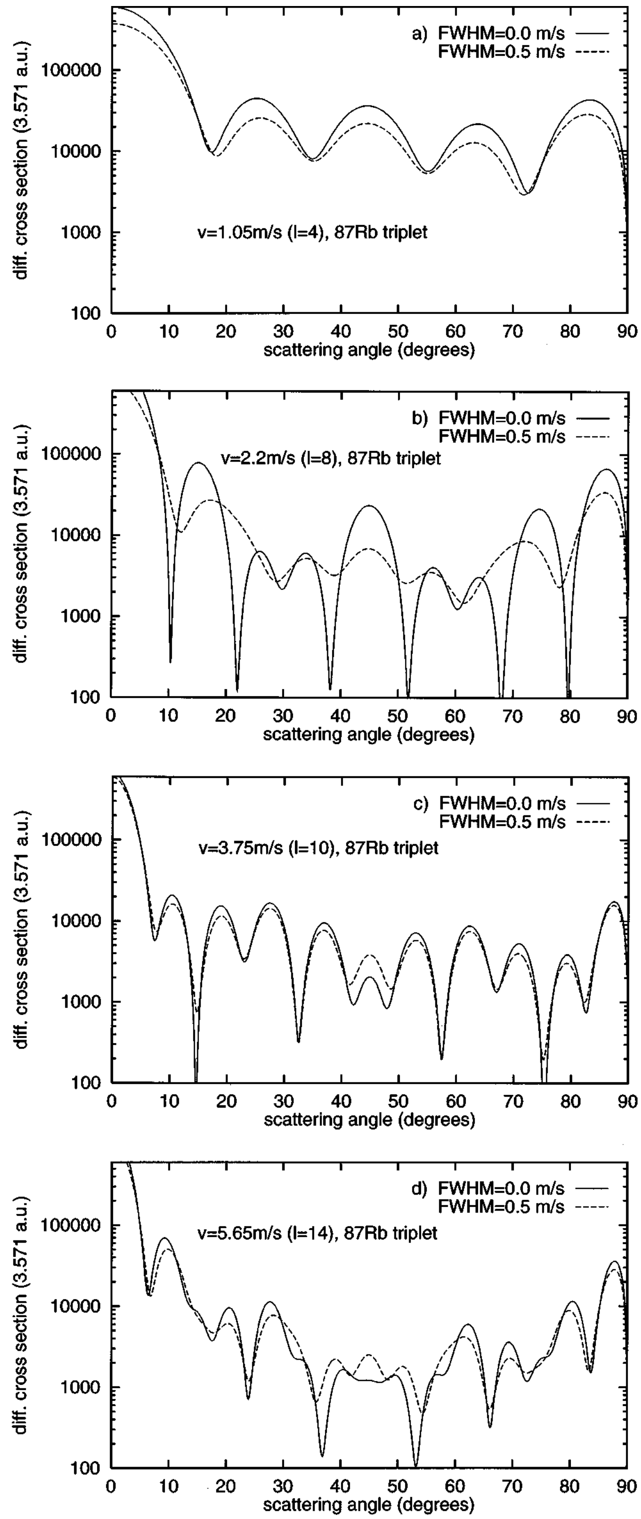

FIG. 4. Differential scattering cross sections of ^{87}Rb-^{87}Rb (same conditions as in Fig. 3).

impossible to measure pure singlet scattering cross sections, we recommend to first look for pure triplet cross sections. In this case projectile and target atoms have to be in the hyperfine states $|F=3,m_F=3\rangle$ for ^{85}Rb and $|F=2,m_F=2\rangle$ for ^{87}Rb. Then measured TCSs can be directly compared with the solid lines in Figs. 2(b) and 2(d). The peaks in Fig. 2 are usually caused by single partial waves, so every peak (or resonance) corresponds to a characteristic differential scattering distribution because the ℓ-dependent Legendre polynoms in Eq. (2) shape the DCSs.

To identify in an experiment the number of the dominant partial wave, the only reliable method consists in the measurement of the differential scattering distribution. We have

TABLE II. Scattering lengths following from the used potential curves ($1a_0 = 0.529\,177$ Å$=5.29\,177\times10^{-11}$ m).

Isotope	State	a (a_0)	a (Å)
^{85}Rb	Singlet	−171.4	−90.7
^{85}Rb	Triplet	146.3	77.4
^{87}Rb	Singlet	126.4	66.9
^{87}Rb	Triplet	18.0	9.52

selected the four most significant TCS resonances of every Rb isotope and calculated the corresponding DCSs, shown in Figs. 3 and 4. The selection gives typical scattering distributions for the dominant partial waves $\ell = 4$, 6, 8, 10, 12, 14, and 18. Five of the eight projectile velocities are directly available by use of the mentioned rubidium funnel, assuming that the funnel also works with ^{87}Rb. A longitudinal velocity width of FWHM=0.5 m/s changes most of the DCSs marginally as exhibited by the dashed lines.

We have also calculated the s-wave scattering lengths, $a = -\lim_{k\to 0} \tan\delta_0^{S/T}/k$, although it is not expected that the used *ab initio* potentials are good enough for zero energy limit calculations. The results are listed in Table II. In Ref. [11] a photoassociation experiment has been exploited to limit the triplet scattering lengths to $85 < a_T < 200$ for ^{85}Rb and $99 < a_T < 119$ for ^{87}Rb (units of a_0). Our value for the triplet scattering length of ^{85}Rb is in agreement with these limits, whereas our value for ^{87}Rb is much smaller than the lower limit. In Ref. [12] a scattering length of $|a| = 46 \pm 11$ Å has been found for ^{87}Rb in the $|F=1, m_F=-1\rangle$ ground state, deduced from elastic scattering cross section measurements of magnetically trapped atoms. This measured value, a mixture of singlet and triplet scattering lengths, lies between our calculated triplet and singlet values.

Since the scattering lengths deduced from the used potential curves roughly agree with other calculated and measured values, it can be assumed that the accuracy of TCSs and DCSs computed at considerable higher collision energies is good enough for a valid prediction of cross-section resonances. This assumption follows from the fact that the importance of the details of the potential curves decreases with increasing collision energy.

In our calculations perfect collimation of the projectile beam and target atoms at rest are assumed. The latter requirement should not be a practical problem, since Rb atom clouds have been cooled down to temperatures where BEC occurs [13]. It may also be an interesting experiment to look for differences between scattering of slow atomic beams at ‘‘normal’’ target atoms (which is the subject of this paper) and Bose-Einstein condensated atoms.

In conclusion, we are convinced that scattering experiments with very slow atomic Rb beams—recently experimentally reached—will yield valuable new data concerning the interaction of two Rb atoms.

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