Differential scattering of Na-Na in the subthermal energy range

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We have calculated total and differential cross sections for the Na_2 scattering complex in the triplet ground state, using the state-of-the-art triplet Coulomb potential. Resonances in the cross section appear in the projectile velocity range 0–50 m/s for the even partial waves $\ell=2,6,8,12,16$. The most significant resonance occurs at 10.48 m/s due to $\ell=6$ with a total cross section of 7145 Å^2. Pronounced structures in the differential cross sections can be resolved for projectile velocity widths of about 1 m/s which are typical for laser Doppler cooling. In order to check and improve the currently used triplet potential curve we have evaluated the feasibility of a scattering experiment. [S1050-2947(96)04711-7]

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Sophisticated thermal atomic beam differential scattering experiments have been carried out until the end of the 1960s in the interatomic velocity range of hundreds of m/s [1,2]. The primary aim of most of these experiments was the determination of interatomic potentials and the verification of spectroscopic and theoretical methods for their determination [3]. The deceleration of atoms by laser light [4–7] and the trapping of neutral atoms in various traps [8–10] have revived the interest—now in cold atom collisions, i.e., at considerably lower interatomic velocities [11]. The rapid development of atom traps led to extensive investigations of the collisions between trapped Na atoms [12,13] in order to understand the loss mechanisms in these traps. Bose-Einstein condensation (BEC) of neutral atoms is being considered as the most spectacular goal at extremely low interatomic velocities in such traps. The first successful observation of this Bose-Einstein condensation has been reported recently with ^{87}Rb [14], ^{7}Li [15], and ^{23}Na [16]. As mentioned in Ref. [17] there are insufficient experimental data to improve the Na triplet potential which is of particular interest for predictions concerning resonance properties of ultracold collisions [17] and BEC with Na atoms [18].

In this paper we want to evaluate the feasibility of a scattering experiment with a slow (laser decelerated) atomic Na beam and (magnetically trapped) Na target atoms nearly at rest. For projectile velocities below 50 m/s such an experiment would produce valuable information about the interatomic Coulomb potentials. The singlet potential $X\ ^1\Sigma_g^+$ is very well known already, for this reason we shall concentrate on the insufficiently known triplet potential $a\ ^3\Sigma_u^+$. In general both ground-state potentials affect the scattering process and spin exchange can occur during the collision. Fortunately one can prepare the atoms in such a way that only triplet scattering occurs and that (even hyperfine) spin exchange is impossible. For this purpose both projectile and target atoms have to be polarized in the $|F=2,\ m_F=2\rangle$ hyperfine state. In this case the scattering is expected to be elastic since magnetic dipolar relaxation [19] can be neglected in an atomic beam experiment.

I. CALCULATION METHOD

Subthermal Na-Na scattering at collision energies of about 10^{-6} eV corresponds to de Broglie wavelengths of the Na atoms of about $\lambda_{dB}\approx$ 10–40 Å, whereas the effective potential range will be $R_{max}\approx$ 50–150 Å. The partial wave method without any approximations is thus appropriate for the calculation of the scattering amplitudes. The radial part of Schrödinger's equation in the CM system

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2}+\frac{\ell(\ell+1)\hbar^2}{2\mu R^2}+V_T(R)-E_{CM}\right]\Psi_\ell(R)=0 \tag{1.1}$$

can be solved by the Numerow algorithm. From the computation of the phase shifts δ_ℓ^T the scattering amplitude

$$f_T(\theta)=\frac{1}{k}\sum_{\ell=0}^{\ell_{max}}(2\ell+1)(e^{2i\delta_\ell^T}-1)P_\ell(\cos\theta) \tag{1.2}$$

with $k=\sqrt{2\mu E_{CM}/\hbar^2}$ and the Legendre polynomials $P_\ell(\cos\theta)$ is obtained in the usual way [20].

In order to obtain valid results the effective potential range R_{max} has to be chosen. The scattering amplitudes as well as the total cross sections are scarcely modified (<0.1%) when R_{max} is extended to values greater than 150 Å, therefore we set $V_T(R>150\ \text{Å})=0$. Furthermore, the condition $\ell_{max}=\text{Integer}(0.6kR_{max})+5$ always leads to a sufficient number of partial waves.

The differential scattering cross section (DCS) concerning doubly spin polarized Na atoms is given by

$$d\sigma^+(\theta)=|f_T(\theta)+f_T(\pi-\theta)|^2=|f_T^+(\theta)|^2. \tag{1.3}$$

The symmetrization of the scattering amplitude follows from the integer hyperfine quantum number $F=2$ and the identity of the colliding atoms. Although the total angular momentum is composed of the half integer electron and nuclear spins the Na atoms clearly behave like bosons as has been impressively demonstrated by the BEC formation described in Ref. [16]. The total scattering cross section (TCS) is then

$$\sigma_{tot}^+=\frac{4\pi}{k^2}\sum_{\text{even}\,\ell}(2\ell+1)\sin^2\delta_\ell^T=\frac{2\pi}{4}\int_0^\pi|f_T^+(\theta)|^2d\theta \tag{1.4}$$

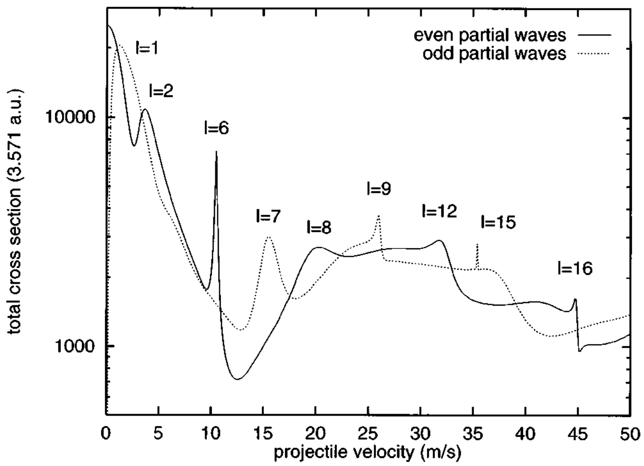

FIG. 1. Total scattering cross sections of Na-Na in the triplet ground state (3.571 a.u.$=1$ Å$^2=10^{-16}$ cm^2).

where the ℓ selection is due to the parity of the scattering wave function for bosons. Nevertheless there may be a smooth decoupling of electron and nuclear spins if the collision energy is well above the ground-state hyperfine splitting energy of $h\times1772$ MHz. Such a *loss of bosonity* has been measured in nuclear physics for ^{12}C-^{12}C differential scattering [21]. Therefore we have also calculated the sum over the odd partial waves (see dotted line in Fig. 1). Measured resonances due to odd partial waves would be a signature for a spin decoupling.

For our calculations we used essentially the ground-state potential curve presented by Zemke and Stwalley [22], which may be called the state-of-the-art triplet potential for Na_2. Twenty-three energy points are listed in [22] for $V_T(R)$ due to spectroscopically resolved rovibrational levels. As recommended by Zemke and Stwalley we eliminated the point $V_T(11.046\,804$ Å). For large interatomic distances we adopted the analytic equation [23]

$$V_T(R)=-\frac{C_6}{R^6}-\frac{C_8}{R^8}-\frac{C_{10}}{R^{10}}+Ae^{-aR}, \tag{1.5}$$

where the last term is the exchange energy. In order to obtain continuous $V(R)$ and dV/dR we extended the data sets by $V_T(11.046\,804$ Å$)=6017.359$ cm^{-1}, and $V_T(13.229\,431$ Å$)=6020.523$ cm^{-1}, calculated by Eq. (1.5). The repulsive region of the potential is extended by energy points from Konowalow *et al.* [24], but we omitted the point $V_T(8.0a_0)$ since it is not suited to the points from Zemke and Stwalley. The resulting data set was then fitted by cubic splines, setting $V''(R)$ to zero at the end points. At $R<2$ Å the potential curve is strongly repulsive and does not have any influence on low-energy scattering which allows us to set $V_T(R<2$ Å) to $V_T(2$ Å).

Figure 1 shows triplet TCS's in dependence on the collision velocity which is assumed to be identical to the projectile velocity. For ultracold collisions and BEC formation, i.e., in the zero energy limit, the $\ell=0$ partial wave is of crucial importance. The corresponding s-wave TCS is directly correlated with the triplet scattering length a_T via $\sigma_{tot}(E_{CM}\rightarrow0)=4\pi a_T{}^2$. Three calculated values for the scattering length are listed in Table I where the first and third values are also calculated with the triplet potential of Ref. [22], but in both cases the potential has been modified in some details. By use of the original potential curve our value lies between the other ones. This indicates that new experimental data are necessary to really improve the triplet potential curve.

TABLE I. Triplet scattering length.

a_T (units of a_0)	(Å)	Source
$77.3^{+107.7}_{-32.3}$	$40.9^{+57.0}_{-17.1}$	Ref. [11]
84.7	44.8	This work
106^{+79}_{-30}	$56.1^{+41.8}_{-15.9}$	Ref. [30]

For higher collision energies partial waves with $\ell>0$ become important. If the hyperfine coupling remains conserved during the collision the odd partial waves (dotted curve) can be ignored. In this case we have pure boson scattering described by the solid line (even ℓ). The peaks in both lines are dominated by particular partial waves. We have listed all occurring TCS resonances in Table II.

In Ref. [11] the collision energy of the $\ell=6$ resonance corresponds to a collision velocity of 10.0 m/s whereas our value is 10.48 m/s. This significant discrepancy follows again from the uncertainty within the triplet Coulomb potential. A scattering experiment with projectile velocities around 10 m/s may be a good test for the currently known potential data.

To determine in an experiment the dominant partial wave and the symmetry of the scattering amplitude, measurements of the DCS's are recommended. We calculated DCS's in the laboratory frame for all even partial wave resonances which are listed in Table II (see Fig. 2). Assuming a laser-cooled atomic Na beam the longitudinal projectile velocity width may be about 1 m/s [full width at half maximum (FWHM)], which is of the order of the Doppler limit. To calculate the dashed curves in Fig. 2 we have assumed a Gaussian longitudinal velocity distribution. Furthermore, the target atoms may have a residual velocity width of 0.5 m/s (FWHM) which is typical for magneto-optically trapped Na atoms. We have taken this into account by a Monte-Carlo simulation and added a Gaussian velocity distribution to the scattered atoms (dotted curves in Fig. 2). Since the longitudinal veloc-

TABLE II. Resonances in the total scattering cross section.

$v_{\text{projectile}}$ (m/s)	Dominant partial wave	σ_{tot} (Å^2)
0	$\ell=0$	25232
1.2	1	20522
3.7	2	10816
10.48	6	7145
15.5	7	3007
20.3	8	2707
26.0	9	3759
31.8	12	2909
35.4	15	2811
44.7	16	1620

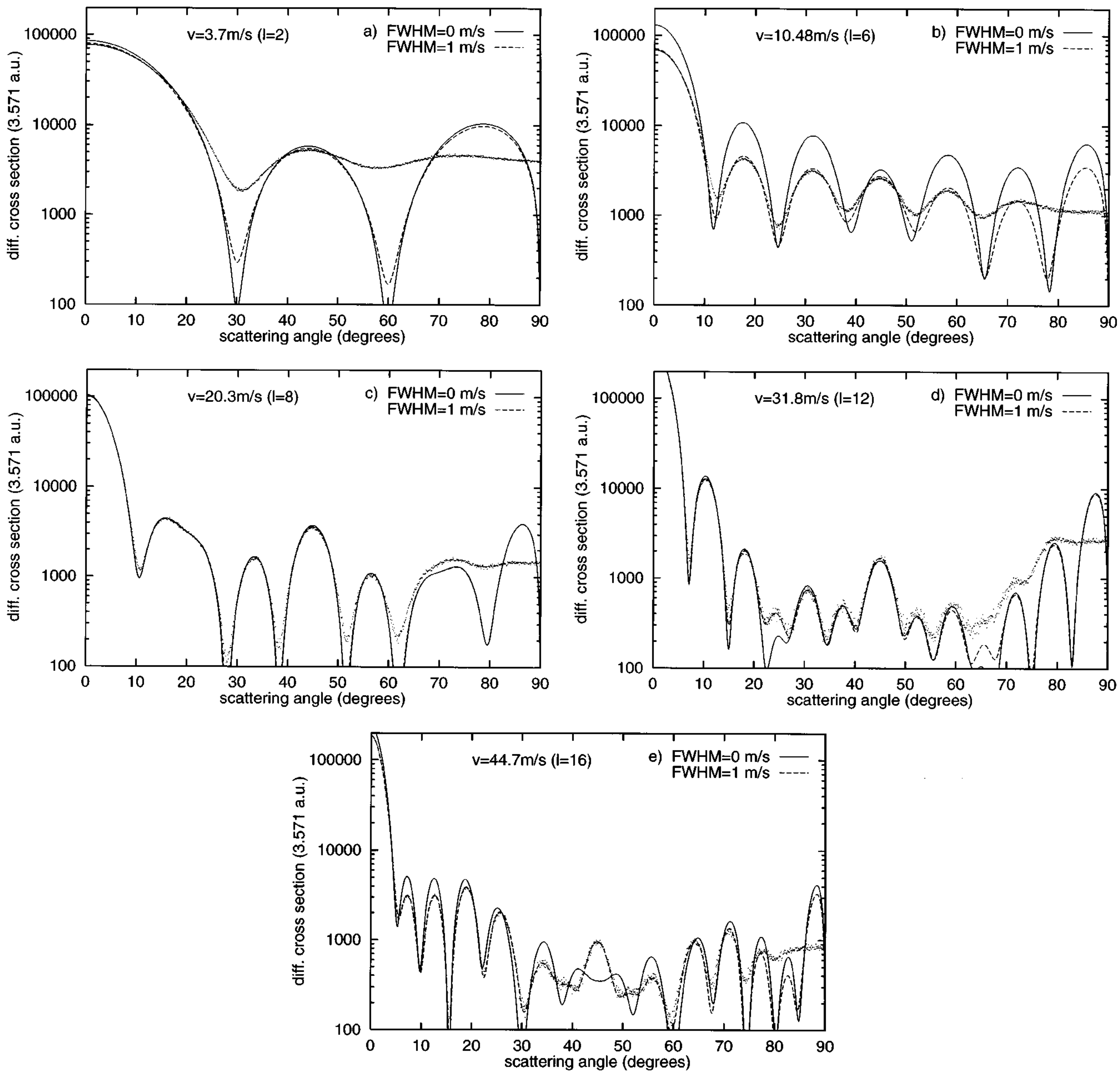

FIG. 2. Differential scattering cross sections (laboratory frame) of ground-state Na-Na collisions for five projectile velocities. Solid lines, sharp projectile velocity; dashed lines, projectile velocity width is 1 m/s (FWHM); dotted lines, projectile velocity width is 1 m/s (FWHM) and in addition a Monte Carlo simulated target velocity width of FWHM=0.5 m/s.

ity of the scattered atoms drops with the cosine of the scattering angle all structures in the DCS's are smeared for large angles.

II. EXPERIMENTAL PROSPECTS

Based on these calculations, and in particular on the differential scattering cross sections obtained, one can estimate the feasibility of an experiment. A beam of 10^7 cold polarized Na ground-state atoms $s^{-1}\,mm^{-2}$ in the velocity range of interest with a FWHM of 1 m/s can be generated nowadays with experimental techniques [25–28]. It is also possible to confine 10^7 cold, polarized Na ground-state atoms in a target volume of $1\,mm^3$, so that typical differential scattering rates of about 5000 atoms $s^{-1}\,sr^{-1}$ can be expected. The differential scattering into a solid angle of 10^{-3} sr thus yields with a detection efficiency of 1 a rate of a comfortable 5 counts per s. This requires a single atom detector [29] for ground-state atoms in the velocity region of interest. One can therefore conclude that the recent experimental advances now allow one to observe pronounced TCS resonances as a function of the collision velocity of the atoms and also the corresponding differential scattering distributions in order to improve the Na-Na triplet potential curve.

The concept of the scattering experiment discussed here is even more interesting for heavier alkali metals like ^{39}K, ^{85}Rb, ^{87}Rb, and ^{133}Cs since the ground-state potentials of these atoms are known very unsufficiently.

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