Interaction between spin polarized alkali atoms

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Abstract. Collisions of alkali-metal atoms in the ground state with the electron spin S = 1/2 are accompanied by exchange of electron coordinates between colliding particles, which leads to polarization transfer between them (i.e., to the well-known phenomenon of spin exchange). In addition, along with the polarization transfer from one partner to another, the magnetic resonance lines of colliding atoms are broadened and shifted in spin-exchange collisions. In particular the last two processes depend on the complex spin-exchange cross section. The real part of the cross section determines the so-called “spin-exchange cross section,” which is responsible for the broadening of magnetic resonance lines, while the imaginary part determines the shift cross section, which governs the frequency shift of magnetic resonance.

In order to describe the spin-exchange process one have to know complex spin-exchange cross sections. Complex spin-exchange cross sections are calculated on the basis of the data on the singlet (X1Σ+) and triplet (a3Σ+) potentials describing the interaction alkali-metal atoms in the ground state.

Collisions of alkali-metal atoms Cs, Rb, K, Na in the ground state are considered in the energy interval of 10^{-4}–10^{-2} au.

1. Complex cross sections of spin-exchange

It is known that, when two atomic particles with nonzero electron spins collide, electron exchange process can occur and, if one of the particles was initially polarized, the particles can exchange electron polarization. This process can conditionally be represented as follows:

\[ A(\uparrow) + B(\downarrow) \leftrightarrow A(\downarrow) + B(\uparrow). \] (1)

The arrows show here possible electron polarization of the particles.

The spin exchange process can be described using the complex cross section of the spin exchange:

\[ q^{AB} = q^{AB} + i \cdot q^{AB}. \] (2)

The real part of a cross section determines the orientation transfer upon collision of particles, relaxation, and the formation of the high rank polarization moments (alignment and hyperfine polarization) [1]. The imaginary part of the cross section determines shifts of a magnetic-resonance-frequency in the system of both Zeeman and hyperfine levels of atoms. Consequently, knowledge of a
spin-exchange complex cross section allows one to completely describe the processes occurring upon spin-exchange collisions. The complex cross section of the spin exchange can be represented in a standard way by the scattering matrix \( S(l) \) as follows:

\[
q^{AB} = \frac{\pi}{k_{AB}^2} \sum_{l=0}^{\infty} (2l + 1) \cdot \left[ 1 - T_0^{AB}(l) \cdot T_1^{AB}(l)^* \right].
\]

Here, \( k_{AB}^2 = \frac{\hbar^2}{\mu_{AB}} \) is the wave vector, \( \mu_{AB} \) is the reduced mass of the colliding particles A and B, \( v_{AB} \) is the mean relative velocity of the colliding atoms, and the asterisk denotes complex conjugation.

The scattering matrix can be written by the scattering phases \( \delta^{AB}_S(l) \) in the channel with the total spin \( S \) as follows:

\[
T_S^{AB}(l) = \exp(2i\delta^{AB}_S(l)),
\]

It follows from expression (3) that the real and imaginary parts of the complex cross section have the form

\[
\overline{q}^{AB} = \frac{\pi}{k_{AB}^2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \left[ \delta^{AB}_1(l) - \delta^{AB}_0(l) \right],
\]

\[
\overline{q}^{AB} = \frac{\pi}{k_{AB}^2} \sum_{l=0}^{\infty} (2l + 1) \sin 2 \left[ \delta^{AB}_1(l) - \delta^{AB}_0(l) \right].
\]

Thus, to calculate the considered cross sections, it is necessary to calculate the scattering phases at the singlet and triplet terms.

2. Calculation of scattering phases for the singlet and triplet terms

As can be seen from the previous section, the real and the imaginary parts of the complex spin exchange cross section (2) can be expressed by the scattering phases at the singlet and triplet terms of the alkali dimer in correspondence with formulas (5) and (6). The scattering phases were determined by the Jeffreys approximation modified by Langer as follows [2]:

\[
\delta_l = \int_{R_0^{-}}^{R} F_l(R) dR - \int_{R_0^{-}}^{R} F_0(R) dR,
\]

where

\[
F_l(R) = \left[ 2\mu_{AB} E - V(R) - \frac{(l + 1/2)^2}{2\mu R^2} \right],
\]

\[
F_0(R) = \left[ 2\mu_{AB} E - \frac{(l + 1/2)^2}{R^2} \right].
\]

Here, \( E \) is the collision kinetic energy, \( R_0 \) and \( R \) are roots of the equations \( F_l(R) = 0 \) and \( F_0(R) = 0 \) (for \( F_l^2 \), one should take the largest root); and \( V(S) \) is the interaction potential for the singlet (\( S = 0 \)) or triplet (\( S = 1 \)) terms. The use of the quasiclassical approximation in the calculation of scattering phases is quite substantiated because, in the case of alkali atom dimers with a large reduced mass \( \mu_{AB} \).
the centrifugal barrier $\left(\frac{l + \frac{1}{2}}{2\mu_{AB}R^2}\right)$ varies slowly (as compared to the kinetic energy) with an increase of the orbital quantum number $l$. This leads to a contribution to the values of the cross sections (5) and (6) from a large number of partial waves. To use the cross sections obtained in subsequent calculations or compare them to the experimental data, it is necessary to perform Maxwellian averaging of cross sections over velocities.

3. Spin-exchange interaction between alkali atoms

3.1. K-K system

The potentials of interaction in a $K_2$ molecule were investigated in numerous papers. The parameters for the singlet [3, 4] and triplet terms [5, 6] of the dimer were obtained from the analysis of the experimental data. In [3], information about the singlet ($X^1\Sigma^+$) potential of interaction up to $v = 75$ ($v$ is a vibration quantum number) was obtained from analysis of the laser induced spectra of fluorescence at the $A^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$ transitions of the $^{39}K$ isotope. Figure 1 presents the calculated dependences of the real and imaginary parts of the complex cross section on the collision energy. As is seen from Fig. 1, the cross section of the frequency shift oscillates and tends toward the range of negative values as the collision energy increases.

![Figure 1](image1.png)

Figure 1. Dependence of the real (1) and imaginary parts (2) of the complex cross section of spin exchange on collision energy in the system of two $^{39}K$ atoms [7].

3.2. K-Rb system

The singlet ($X^1\Sigma^+$) state of the KRb molecule has been studied fairly well both experimentally and theoretically [8–10]; investigations of the triplet state of the KRb molecule were performed significantly more rarely and, as for the interaction potential describing the $a^3\Sigma^-$-state of the molecule, the data on it are considerably fewer. In [11], the singlet and triplet states of the KRb molecule were simultaneously studied by Fourier spectroscopy, and the singlet and triplet interaction potentials were constructed using the experimental data. Figure 2 presents the calculated dependences of the real and imaginary parts of the complex cross section on the collision energy.

![Figure 2](image2.png)
3.3. \textit{Na-Na} system.

By now, there are many works in which parameters of the singlet and triplet interaction potentials of the Na$_2$ dimer were determined. In particular, an empirical potential for the $a^3\Sigma^+$ state was constructed in [13]; in [14], parameters of the singlet ($X^1\Sigma^+$) state were determined. In this work, the cross sections that we are interested in were calculated using interaction potentials obtained in [15], as well as a combination of the singlet [15] and triplet [13] interaction potentials. This choice was based on the fact that the sought interaction potentials describe the interaction of Na atoms in a wide range of inter-nuclear distances, which makes it possible to calculated cross sections in question in a wide range of collision energies. The Figure 3 presents the real and imaginary parts of the complex spin-exchange cross section calculated as functions of the collision energy.

3.4. \textit{Cs-Cs, Rb-Rb, and Rb-Cs} systems. Shifts of magnetic-resonance-frequencies in Cs-Rb.
A number of specific features should be taken into account in calculating the magnetic-resonance-frequency shifts and in comparing the calculated results with experimental findings. In particular, the spin-exchange process in collisions of alkali-metal atoms and its influence on the magnetic-resonance-frequency shifts were theoretically considered in [17]. Note that the expressions for the magnetic-resonance frequency shifts caused by spin-exchange collisions were derived taking into account not only the spin-exchange process, but also the influence of diffusion to the walls of an absorption chamber, collisions with atomic particles of a buffer gas, and the presence of a constant magnetic field. In addition, the expressions obtained take into account the complicated system of alkali-metal atomic levels.

Taking into account only spin-exchange collisions leads to the following expressions for the shifts [17]:

\[
\delta^{(1)}\omega(+) = -\frac{P_{e}(B)}{2(2I_{A} + 1)} \left[ \gamma_{AB} - \gamma_{AA} B_{-} \left( \frac{2I_{A} - 1}{2I_{A} + 1} \right)^{1/2} \right],
\]

\[
\delta^{(1)}\omega(-) = -\frac{P_{e}(B)}{2(2I_{A} + 1)} \left[ \gamma_{AB} - \gamma_{AA} B_{+} \left( \frac{2I_{A} + 3}{2I_{A} + 1} \right)^{1/2} \right].
\]

According to the designations accepted in [17], here, \(\delta^{(1)}\omega(+)\) is the magnetic-resonance-frequency shift for the hyperfine state \(F = S + I\) (where \(S\) is the electron spin equal to 1/2 in the case of alkali atoms and \(I\) is the nuclear spin of an alkali atom), \(\delta^{(1)}\omega(-)\) is the magnetic-resonance-frequency shift for the hyperfine state \(F = S - I\), \(P_{e}(B)\) is the polarization of particle \(B\), \(I_{A}\) is the nuclear spin of particle \(A\), and \(\gamma_{AB}\) and \(\gamma_{AA}\) are the imaginary parts of the complex spin exchange rate \(\gamma\), which can be expressed through the complex cross section of spin exchange (1).

In order to calculate frequency shifts of Cs and Rb atoms one have to know the imaginary part of the cross section. Consequently, knowledge of the spin-exchange complex cross section allows one to completely describe the processes occurring upon spin-exchange collisions. Earlier the complex cross sections of the spin-exchange processes for Cs-Cs [18], Cs-Rb [19], and Rb-Rb [20] systems were calculated. The magnetic-resonance-frequency shifts were obtained for \(^{87}\text{Rb}\) and \(^{133}\text{Cs}\) atoms in a mixture of Cs–Rb in the atmosphere of the buffer gas (N\(_2\)).

![Figure 4](image-url)

Figure 4. Temperature dependences of the doubled absolute values of magnetic-resonance-frequency shifts for the hyperfine states of \(^{87}\text{Rb}\) atoms [21]. The calculated values (solid curves): (1) \(F = 2\) [23], (2) \(F = 1\) [23], (3) \(F = 2\) [24], and (4) \(F = 1\) [24]. Experimental values (symbols): (○) \(F = 1\) [21], (■) \(F = 2\) [21].
The results of such calculation for electron polarization $P_z(B) = 0.3$ of atom B (in our case, this is a Cs atom) are presented in the Figure 4 for Rb and Figure 5 for Cs. The values obtained are compared with the data measured in experiments on optical orientation of Cs atoms [21] and Rb atoms [22].

Fig. 5. Temperature dependences of the doubled absolute values of magnetic-resonance-frequency shifts for the hyperfine states of $^{133}$Cs atoms [25]. The calculated values (solid curves): (1) $F = 3$ (this work), (2) $F = 4$ (this work), experimental values (symbols): (○) $F = 1$ [21], (■) $F = 2$ [21].

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