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Collisions of spin-polarized alkali Na and Cs atoms in the ground state

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The paper considers collisions involving spin polarized alkali Na and Cs atoms in the ground state. The complex cross sections for spin exchange and the elastic scattering cross sections of the considered atoms are calculated in the energy range from 10^{-4} to 10^{-2} a.u

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Introduction

In recent years, the interest in studying the interactions between alkali metal atoms in the ground state has been renewed. This is true for the study of both homonuclear [1] and heteronuclear dimers of alkali metals [2]. The growth of the number of such studies is due to various factors, in particular, the interest in the properties of cold and ultracold collisions in gases of alkali metals in various types of traps [2,3], as well as the possibility of polarization transfer during collisions of spin-polarized alkali atoms with atoms of nuclear paramagnetic materials [4] with their subsequent use as working media in quantum magnetometers [5,6] and gyroscopes [7]. The interactions with spin-polarized alkali atoms involvement can be studied in experiments on the optical orientation of atoms. Optical orientation of atoms is the transfer of angular momentum from a polarized resonant radiation to an ensemble of atoms that are either in the ground state or in excited state and have an uncompensated electron spin. In this case, the polarization transfer is possible both between the electronic degrees of freedom of colliding atoms [8] and between the electronic and nuclear degrees of freedom [4,9].

Collisions of alkali metal atoms in the ground state with an electron spin of $S = 1/2$ are accompanied by the exchange of electronic coordinates between the colliding particles, which results in the transfer of polarization between them (i. e., to the well-known phenomenon of spin exchange). In addition, along with the transfer of polarization from one partner to another [8], the magnetic resonance lines of colliding atoms broaden and shift during the spin-exchange collisions [10,11]. The latter two processes depend, in particular, on the complex cross section of the spin exchange. 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, and the imaginary part, that is the shift cross section, determines the shift of the magnetic resonance frequency. When alkali atoms in the ground state collide, an elastic scattering also takes place, along with the spin exchange process.

The purpose of this study is to calculate the cross sections of collisions of Na and Cs alkali atoms. These include various cross sections: the elastic scattering cross section, the complex spin exchange cross section, consisting of real and imaginary parts. As it follows from the standard scattering theory, all of the above-mentioned cross sections can be calculated using the scattering phases on the corresponding terms of the NaCs dimer [12]. It should be noted that in collisions of alkali atoms at not too low temperatures, when the hyperfine interaction time $2\pi/\Delta\omega$ (for example, $\Delta\nu = 9192 \cdot 10^6$ Hz for ^{133}Cs and $\Delta\nu = 1771 \cdot 10^6$ Hz for ^{23}Na [13]) is significantly longer than the collision time, which is of the order of 10^{-12} s, the spin exchange process can only be considered as the evolution of electron spins during the collision. In other words, the total electron spin is assumed to be conserved during the collision. Between collisions, electron and nuclear spins interact. In this case, a molecule formed from two alkali atoms in the process of collision can be described in the ground state using two potentials corresponding to the total spins of the system: $S_1 = 0$ and $S_2 = 1$. Collision cross sections are calculated based on the information on singlet ($S = 0$, $X^1\Sigma^+$) and triplet ($S = 1$, $a^3\Sigma^+$) potentials describing the interaction of alkali atoms in the ground state [14].

1. Interaction potentials of the NaCs system

The interaction potentials of the NaCs system have been studied for quite a long time [14–17] and, as noted above, recently interest in the study of this system has grown significantly [3,17]. In this study, to calculate the cross sections of spin exchange and elastic scattering of interest to us, we will use the results of [14], where the singlet and triplet terms of the NaCs dimer were found on the basis of the experimental data obtained using Fourier spectroscopy. The potentials of interest were divided into three regions in accordance with the internuclear distance: the region of small internuclear distances ($R < R_{\mathrm{SR}}$), the region of large internuclear distances ($R > R_{\mathrm{LR}}$), the region of medium internuclear distances ($R_{\mathrm{SR}} \leq R \leq R_{\mathrm{LR}}$). The numerical values of the parameters R_{SR} and R_{LR} are given below. The region of small internuclear distances ($R < R_{\mathrm{SR}}$) is characterized by strong repulsion, the region of large internuclear distances ($R > R_{\mathrm{LR}}$) is due to van der Waals interaction, in the region of medium internuclear distances ($R_{\mathrm{SR}} \leq R \leq R_{\mathrm{LR}}$) singlet and triplet interaction potentials are characterized by the presence of a quantum well.

In [14], the singlet and triplet potentials were represented in analytical form as follows.

For small internuclear distances ($R < R_{\mathrm{SR}}$), the potential had the form of repulsion:

$$U_{\mathrm{SR}}(R) = A + \frac{B}{R^3}, \tag{1}$$

where $A = -0.121078258 \cdot 10^5\,\mathrm{cm}^{-1}$, $B = 0.278126476 \cdot 10^6\,\mathrm{cm}^{-1}\text{Å}^3$ for the singlet term and $A = -0.147429182 \cdot 10^4\,\mathrm{cm}^{-1}$, $B = 0.160029429 \cdot 10^6\,\mathrm{cm}^{-1}\text{Å}^3$ for the triplet term.

For large internuclear distances ($R > R_{\mathrm{LR}}$), the potential was described by the van der Waals interaction taking into account the term describing the exchange interaction:

$$U_{\mathrm{LR}} = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} \pm E_{\mathrm{ex}}. \tag{2}$$

The exchange interaction E_{ex} is included with the sign $(+)$ in the triplet term and with the sign $(-)$ in the singlet term; its explicit form is presented in [14]:

$$E_{\mathrm{ex}} = A_{\mathrm{ex}} R^{\gamma} \exp(-\beta R). \tag{3}$$

For distances of $R_{\mathrm{SR}} < R < R_{\mathrm{LR}}$, the potential was presented in the following form:

$$U_{\mathrm{IR}}(R) = \sum_{k=0}^{n} a_k x^k, \tag{4}$$

where $x = \frac{R-R_m}{R+bR_m}$, a_i are fitting coefficients, R_m is distance close to the equilibrium, equal to 3.85062906 Å for the singlet term and 5.75585938 Å for the triplet term. The explicit form of the parameters in expressions (1)–(4) is tabulated in [14]. Using expressions (1)–(4) and the parameters included in them, given in [14], we have built up the interaction potentials of the NaCs dimer in the atomic system of units (Fig. 1). Knowing the singlet and triplet terms of the NaCs dimer in the ground state, we can proceed to the calculation of the cross sections of interest to us.

In [14], the dissociation energy of the NaCs molecule and the equilibrium distance were also determined: for the singlet term $D_e = 4954.237(10)\,\mathrm{cm}^{-1}$, $R_e = 3.8506$ Å, for the triplet term $T_e = 217.168(10)\,\mathrm{cm}^{-1}$, $R_e = 5.7448$ Å. Moreover,$R_{\mathrm{SR}} = 2.8435$ Å, $R_{\mathrm{LR}} = 10.2$ Åfor the singlet term, $R_{\mathrm{SR}} = 4.78$ Å, $R_{\mathrm{LR}} = 10.2$ Åfor the triplet term.

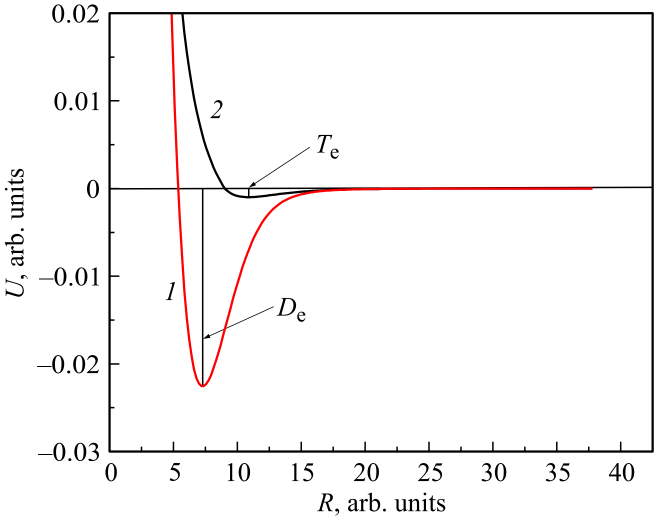

Figure 1. Singlet (*1*) and triplet (*2*) potentials of the NaCs dimer according to [14] in the atomic system of units.

2. Calculation of scattering phases during collisions of Na and Cs atoms

As it follows from the theory of scattering, the calculation of cross sections is conditioned by the knowledge of scattering phases ($\delta_l^{s,t}$) (here the superscript s is referred to the singlet term, t is referred to the triplet term) on the corresponding terms. The amplitude of the scattered wave on the triplet (f_t) and singlet (f_s) terms is determined by the following expression through the scattering phases [18,19]:

$$f_{t,s} = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)[\exp(2i\delta_l^{t,s}) - 1] P_l(\cos\theta), \tag{5}$$

The scattering phase $\delta_l^{s,t}$ can be obtained from a regular solution to the equation of partial waves:

$$\frac{d^2 g_l^{t,s}}{dR^2} + \left[k^2 - V_{t,s} - \frac{l(l+1)}{R^2}\right] g_l^{t,s} = 0. \tag{6}$$

For large values of R, the $g_l^{t,s}$ function has the following asymptotic form:

$$g_l^{t,s} \sim k^{-1} \sin\left(kR - \frac{1}{2} l\pi + \delta_l^{t,s}\right). \tag{7}$$

Here l is orbital momentum, k is wave vector, $V_{t,s}$ is triplet (or singlet) interaction potential, P_l is Legendre polynomial.

The scattering phases were calculated in a quasi-classical approximation based on the Jeffreys method modified by Langer [18], in the collision energy range of $E = 10^{-2}$–10^{-4} a.u. In accordance with this method, the scattering phase on the potential V_s can be represented in the following form:

$$\delta_l = \int_{R_0}^{\infty} F_1(R)dR - \int_{R_0'}^{\infty} F_0(R)dR, \tag{8}$$

where

$$F_1^S(R) = \left[2\mu(E - V_S(R) - \frac{(l+1/2)^2}{2\mu R^2}\right], \ S = s, t, \tag{9}$$

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

Here E is collision energy, R_0 and R_0' are roots of the equations $F_1^S(R) = 0$, $F_0(R) = 0$ (and for $F_1^S(R)$ the largest root is taken), $V_S(R)$ is interaction potential corresponding to the total spin S (0 or 1).

3. Calculation of cross sections for collisions of Na and Cs atoms

Complex spin exchange cross sections and elastic scattering cross sections can be calculated based on the standard theory of scattering. The calculation of complex cross sections for spin exchange in collisions of sodium and cesium atoms was carried out similarly to how it was done, for example, in collisions of rubidium isotopes [20]. When two atomic particles with electron spins collide, an exchange of electrons is possible, and if one of the particles was previously polarized, then an exchange of electron polarization is possible as well. Such a process can be notionally represented as follows:

$$A(\uparrow) + B(\downarrow) \leftrightarrow A(\downarrow) + B(\uparrow), \tag{10}$$

in this representation arrows indicate the possible electronic polarization of the atom.

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

$$q^{AB} = \overline{q}^{AB} + i\overline{\overline{q}}^{AB}. \tag{11}$$

At the same time, knowing the interaction potentials of Na and Cs atoms, it is also possible to determine the cross sections for elastic scattering at each potential.

The complex spin exchange cross section can be represented in a standard way through the scattering matrix $T_S^{AB}(l)$ [12]:

$$q^{AB} = \frac{\pi}{k_{AB}^2}\sum_{l=0}^{\infty}(2l+1)[1 - T_0^{AB}(l)T_1^{AB}(l)^*]. \tag{12}$$

Here k_{AB}^2 is wave number, * means complex conjugation, S is total spin of the system. The scattering matrix can be represented in terms of scattering phases $\delta_S^{AB}(l)$ in a channel with total spin S as follows:

$$T_S^{AB}(l) = \exp(2i\delta_S^{AB}(l)), \tag{13}$$

where l is orbital quantum number. In this case, the elastic scattering cross section can be represented [12] in the following form:

$$q^{s,t} = \frac{\pi}{k_{AB}^2}\sum_{l=0}^{\infty}(2l+1)|1 - T_{s,t}^{AB}(l)|^2. \tag{14}$$

In thus representation subscripts s and t correspond to scattering on singlet ($S = 0$) term or triplet ($S = 1$) term.

It follows from expressions (12)−(13) that the real and imaginary parts of the complex spin exchange cross section have the following form:

$$\overline{q}^{AB} = \frac{\pi}{k_{AB}^2}\sum_{l=0}^{\infty}(2l+1)\sin^2[\delta_1^{AB}(l) - \delta_0^{AB}(l)], \tag{15}$$

$$\overline{\overline{q}}^{AB} = \frac{\pi}{k_{AB}^2}\sum_{l=0}^{\infty}(2l+1)\sin 2[\delta_1^{AB}(l) - \delta_0^{AB}(l)]. \tag{16}$$

In this case, the elastic scattering cross section on the singlet and triplet terms can be represented as follows:

$$q^{0,1} = \frac{\pi}{k_{AB}^2}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_{0,1}^{AB}(l)). \tag{17}$$

In accordance with [21], the total elastic scattering cross section in the case of collisions of dissimilar atoms can be represented in the following form:

$$q_{el} = (1/4)(q^0 + 3q^1). \tag{18}$$

Thus, to calculate the cross sections of interest to us using expressions (15)−(18), it is necessary to calculate the scattering phases on the singlet and triplet terms presented in Section 1.

4. Calculation of elastic scattering cross sections and complex spin exchange cross sections in collisions of Na and Cs atoms

In the quasi-classical approximation, based on expressions (8) and (9) and interaction potentials from [14], the scattering phases were calculated in the collision energy range from 10^{-4} to 10^{-2} a.u. The possibility of using the quasi-classical approximation is due to the fact that a large number of scattering phases contribute to the cross sections even at a minimum collision energy. Fig. 2 shows the dependences of real and imaginary parts of the complex spin exchange cross section on the collision energy, obtained on the basis of relationships (15) and (16). Fig. 3 shows the dependences of the elastic scattering cross sections on the singlet and triplet terms as function of the collision energy, obtained on the basis of relationships (17).

To proceed to the temperature dependences of the desired cross sections, it is necessary to carry out Maxwellian averaging over velocities in accordance with the following expression:

$$\sigma^{AB}(T) = \frac{\langle q^{AB}(E)v_{AB}\rangle}{\langle v_{AB}\rangle}$$

$$= \frac{1}{(kT)^2}\int_0^{\infty} q^{AB}(E)E\exp\Big(-\frac{E}{kT}\Big)dE. \tag{19}$$

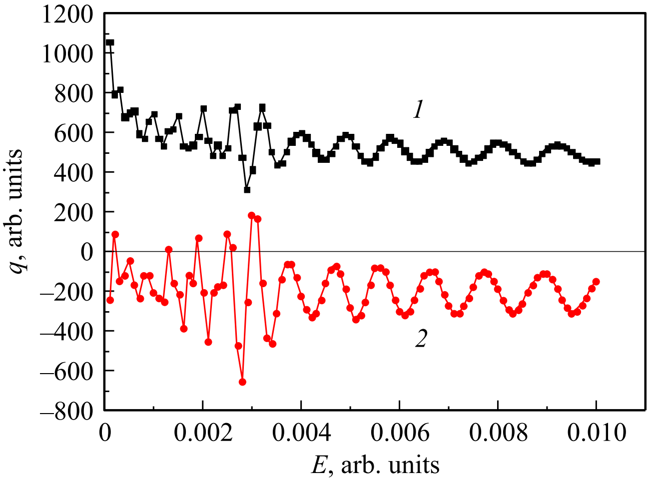

Figure 2. Dependence of the real (*1*) and imaginary (*2*) parts of the complex cross section of spin exchange on the collision energy during collisions of Na and Cs atoms in the ground state.

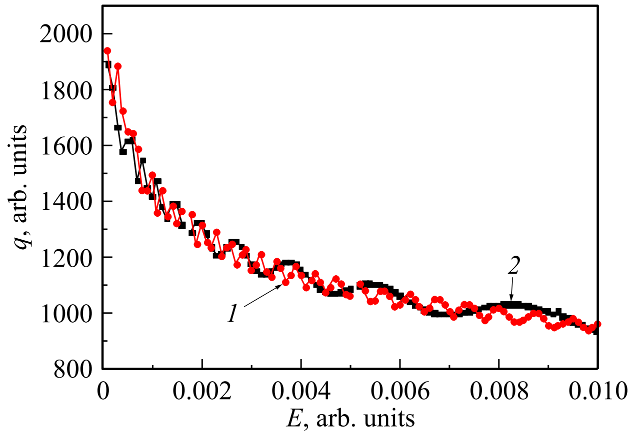

Figure 3. Dependence of elastic scattering cross sections on collision energy: *1* — scattering cross section on a singlet term (■), *2* — scattering cross section on a triplet term (•).

Here k is Boltzmann's constant, E is collision energy, v_{AB} is relative thermal velocity of colliding particles. Fig. 4 shows the results of Maxwellian averaging of the energy dependences of the cross sections presented in Fig. 2 and 3, including the total elastic scattering cross section, which is expressed through the elastic scattering cross sections on the triplet and singlet terms in accordance with (18). Since the elastic scattering cross sections on the singlet and triplet terms are close to each other (Fig. 3), and in accordance with (18) the contribution from scattering on the triplet term prevails in the value of the total cross section, it turns out that the total cross section and the scattering cross section on the triplet term are weakly differ, as it follows from Fig. 4.

Indeed, as can be seen, for example, from [19], in the collision of two lithium atoms in the ground state with Maxwellian averaging of the cross sections in the temperature interval of 1−100 K scattering cross sections on the singlet and triplet terms coincide, and the spin exchange cross section (real part) is significantly smaller than them. The main difference between the cross sections for elastic scattering on the singlet and triplet terms takes place in the region of low temperatures (less than 1 K).

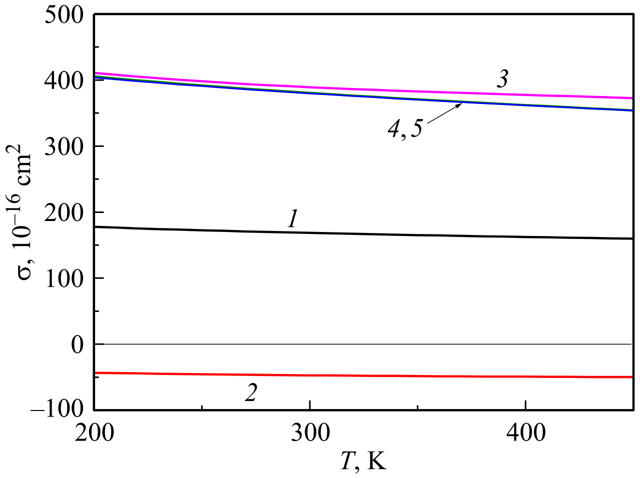

Figure 4. Temperature dependences of the cross sections: *1* — real part of the spin exchange cross section, *2* — imaginary part of the spin exchange cross section, *3* — scattering cross section on the singlet term, *4* — scattering cross section on the triplet term, *5* — total scattering cross section on the singlet and triplet terms.

Conclusion

As can be seen from Fig. 4, the real part of the spin exchange cross section $(\overline{q}^{AB})$ is quite large and falls within the range from $1.8 \cdot 10^{-14}$ to $1.6 \cdot 10^{-14}$ cm ^{2}. At the same time, the imaginary part of the cross section $(\overline{\overline{q}}^{AB})$, responsible for shifts in the magnetic resonance frequency, is, firstly, negative throughout the entire temperature range, and secondly, varies from $-4 \cdot 10^{-15}$ to $-5 \cdot 10^{-15}$ cm^2. The magnitude and sign of the cross section are significant when calculating the frequency shift of magnetic resonance in the collision of polarized alkali metal atoms in the ground state. In particular, the behavior of the frequency shift as a function of temperature for two hyperfine states of alkali atoms depends on them.

Spin exchange cross sections make it possible to describe the process of spin exchange during the collision of two alkali metal atoms in the ground state. As already noted, the process of spin exchange leads both to the transfer of polarization between colliding particles and to the broadening of the magnetic resonance line of colliding atoms. In addition, along with the transfer of polarization from one partner to another, the magnetic resonance lines of colliding atoms broaden and shift during spin-exchange collisions. These processes depend, in particular, on the complex cross sections of spin exchange. 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, and the imaginary part, „the shift cross section" determines the shift of the magnetic resonance frequency. The spin-exchange broadening of the magnetic resonance line affects the accuracy of quantum electronics devices such as quantum frequency standards and magnetometers, which are built using the optical orientation of atoms.

Conflict of interest

The author declares that he has no conflict of interest.

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