Optics and Spectroscopy, 2025, Vol. 133, No. 4

01

Cross sections of spin exchange, magnetic resonance frequency shift and elastic scattering in collisions of alkali atoms Na-Rb

© V.A. Kartoshkin

Ioffe Institute, St. Petersburg, Russia
e-mail: victor.kart@mail.ioffe.ru

Received December 26, 2024
Revised December 26, 2024
Accepted March 21, 2025

The article studies interactions involving spin-polarized alkali metal atoms in the ground state. The calculation of spin exchange and elastic scattering cross sections for the Na-Rb pair is performed. The calculation of the cross sections is carried out for the range of atomic collision energies from 10^{-4} to 10^{-2} a. u energy. The presented calculation allows for the first time to obtain the temperature dependences of the cross sections under consideration, which in turn can be used to consider the kinetics of polarization transfer during optical neutron scattering of atoms.

Keywords: collisions of polarized atoms, indirect polarization, cross sections.

DOI: 10.61011/EOS.2025.04.61405.7506-24

Introduction

Quantum electronics devices operating based on the principle of optical orientation of atoms attract research interest due to the possibility of their use in general-purpose high-precision sensitive instruments. Above all, this applies to quantum magnetometers with optical orientation of alkali atoms [1,2], which serve as key elements in the design of magnetoencephalographs [3], magnetocardiographs [4], quantum gyroscopes [5], and quantum frequency and time standards [6]. The key factors affecting the performance of such devices are the signal-to-noise ratio and the accuracy of measuring the magnetic resonance line frequency. The width and frequency of the magnetic resonance line are determined, among other things, by the cross sections of interest to us.

These cross sections result from spin-exchange collisions in the working chamber. The spin exchange process may be characterized by a complex spin exchange cross section [7]. It follows from [7] that, knowing the interaction potentials of the NaRb dimer, one may calculate the phases of scattering by the corresponding terms and use them to determine the sought-for cross sections. A collision of Na and Rb atoms leads to the formation of the NaRb quasimolecule (dimer) with total electron spins $S = 0$, 1 that correspond to singlet and triplet terms, respectively.

Depending on the objective, studies into optical orientation of alkali atoms may utilize same-type alkali atoms [8] or a mixture of alkali atoms [9]. In the present study, we discuss a mixture of Na and Rb atoms.

Since a mixture of Na and Rb atoms is present in the working chamber, collisions of both identical and different atoms occur within its volume. Quasimolecules produced in such collisions may be represented by two terms corresponding to total spins $S = 0$ and $S = 1$ of the system. These terms are characterized by deep potential wells. In view of this, noticeable concentrations of diatomic molecules are present within the working chamber. Specifically, the pressure of Rb_2 vapor at room temperature is $7.046 \cdot 10^{-12}$ mmHg; Na_2 – $5.751 \cdot 10^{-14}$ mmHg at 325 K [10].

Spin-exchange collisions have already been studied for different atoms. Collisions between Na atoms were considered in [11], while collisions between Rb atoms were analyzed in [12]. In the present study, we examine collisions between Na and Rb atoms and calculate the cross sections resulting from these collisions.

Interaction potentials of the Na-Rb dimer

When Na and Rb atoms collide in the S state, a dimer is formed in the singlet $^1\Sigma$ or triplet $^3\Sigma$ states. The authors of [13] have used the results of Fourier spectroscopy experiments for the NaRb dimer to obtain data on the singlet and triplet potentials with their short-range parts ($U_{SR}(R)$) set in tabular form within the range of internuclear distances from 2.1 to 11 Å for the singlet term and from 2.94444 to 11 Å for the triplet term and the long-range parts ($U_{LR}(R)$) presented in analytical form. It follows from [13] that the sought-for potentials $U_{LR}(R)$ in the region of large internuclear distances ($R > 11$ Å) are written as

$$U_{LR}(R) = U_\infty - C_6/R^6 - C_8/R^8 - C_{10}/R_{10} \pm E_{exch}, \quad (1)$$

where the exchange interaction contribution (E_{exch}) was presented as

$$E_{exch} = A_{ex} R^\gamma \exp(-\beta R), \quad (2)$$

E_{exch} and has (+) and (−) signs in the triplet and singlet potentials, respectively. The coefficients in (1) and (2)

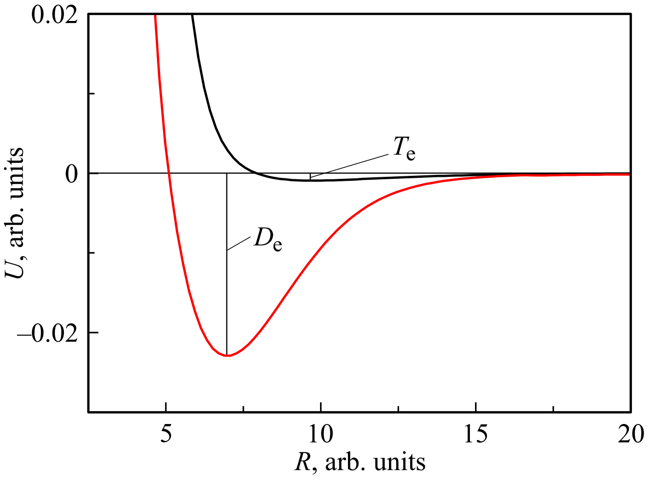

Figure 1. Potentials of interaction of Na and Rb atoms in the ground state (atomic system of units). Data were taken from [13].

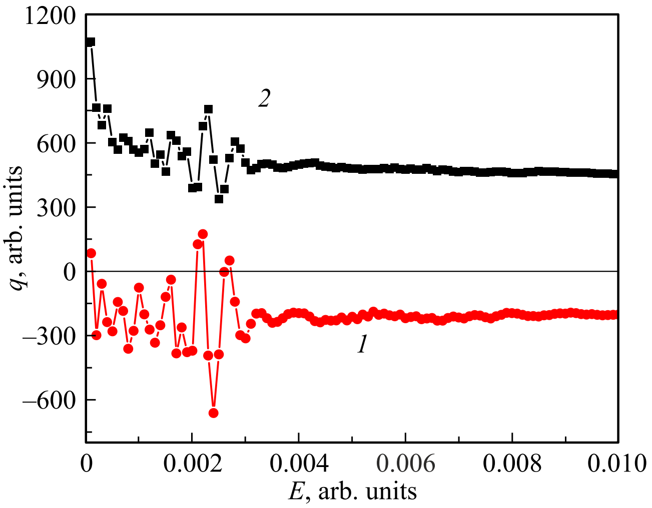

Figure 2. Real (2) and imaginary (1) parts of the spin exchange cross section for ^{23}Na—^{85}Rb in the atomic system of units.

assume [13] the following values: $U_\infty = 5030.50235\,\mathrm{cm}^{-1}$, $R_0 = 11.2967\,\text{Å}$, $C_6 = 1.3237\cdot 10^7\,\mathrm{cm}^{-1}\text{Å}^6$, $A_{ex} = 2.8609\cdot 10^4\,\mathrm{cm}^{-1}\text{Å}_\gamma$, $C_8 = 2.9889\cdot 10^8\,\mathrm{cm}^{-1}\text{Å}^8$, $\gamma = 5.0081$, $C_{10} = 1.5821\cdot 10^{10}\,\mathrm{cm}^{-1}\text{Å}^{10}$, $\beta = 2.2085\,\text{Å}^{-1}$, $T_e^X = 0\,\mathrm{cm}^{-1}$, $R_e^X = 3.6434\,\text{Å}$, $D_e^X = 5030.502(50)\,\mathrm{cm}^{-1}$, $D_0^X = 4977.187(50)\,\mathrm{cm}^{-1}$ for the singlet potential; in the triplet potential: $R_o = 11.3370\,\text{Å}$, $T_e^a = 4827.14727\,\mathrm{cm}^{-1}$, $R_e^a = 5.6003\,\text{Å}$, $D_e^a = 203.355(50)\,\mathrm{cm}^{-1}$, $D_0^a = 193.365(50)\,\mathrm{cm}^{-1}$. Here, D_e^X is the potential well depth for term $^1\Sigma$, and D_e^a is the depth for term $^3\Sigma$. Accordingly, R_e^X and R_e^a are the positions of energy minima for terms $^1\Sigma$ and $^3\Sigma$, and D_0^X and D_o^a are the dissociation energies relative to the lower vibrational-rotational levels.

The data from [13] were used to plot the interaction potentials in the atomic system of units. The method of spline approximation of the tabular data on potentials from [13] was used in calculations within the distance interval of $11\,\text{Å} \geq R$. The dependences obtained this way are presented in Fig. 1.

Cross sections of spin exchange and elastic scattering for the Na and Rb pair

The cross sections of interest to us were calculated in the scattering matrix representation $T_S^{AB}(l)$, where S corresponds to the total spin of the system (1 or 0) and l is the orbital quantum number [6.7]. The complex spin exchange cross section is

$$q_{se}^{AB} = \frac{\pi}{k_{AB}^2}\sum\nolimits_{l=0}^{\infty}(2l+1)[1 - T_0^{AB}(l)T_1^{AB}(l)^*], \qquad (3)$$

and elastic scattering cross sections are

$$q^{s,t} = \frac{\pi}{k_{AB}^2}\sum\nolimits_{l=0}^{\infty}(2l+1)|1 - T_{s,t}^{AB}(l)|^2. \qquad (4)$$

Here, $k_{AB} = \mu_{AB}\upsilon_{AB}/\hbar$ is the wave vector, μ_{AB} is the reduced mass of colliding particles A and B, υ_{AB} is the average relative velocity of colliding particles, the asterisk denotes complex conjugation, and l is the orbital angular momentum.

The representation of scattering matrix $T_S^{AB}(l)$ through phases of scattering $(\delta_S^{AB}(l))$ by the corresponding terms takes the form

$$T_S^{AB}(l) = \exp(2i\delta_S^{AB}(l)). \qquad (5)$$

The real $(\overline{q}^{AB})$ and imaginary $(\overline{\overline{q}}^{AB})$ cross sections of spin exchange and the cross sections of elastic scattering by the singlet (q^0) and triplet (q^1) terms may then be written as [14]

$$\overline{q}^{AB} = \frac{\pi}{k_{AB}^2}\sum_{l=0}^{\infty}(2l+1)\sin^2[\delta_1^{AB}(l) - \delta_0^{AB}(l)] \qquad (6)$$

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

$$q^{0,1} = \frac{\pi}{k_{AB}^2}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_{0,1}^{AB}(l)) \qquad (7)$$

Following [15], we find that the total cross section of elastic scattering in collisions of different atoms has the form

$$q_{tot} = \frac{1}{4}(q^0 + 3q^1). \qquad (8)$$

The data from [13] were used to calculate the corresponding cross sections, which are presented in the atomic system of units in Fig. 2.

The calculated dependences of cross sections on the collision energy are shown in Figs. 2–4: $\overline{q}^{AB}$ and $\overline{\overline{q}}^{AB}$ in Fig. 2, q^0 and q^1 in Fig. 3, and q_{tot} in Fig. 4. It follows from

Velocity-averaged values of the cross sections presented in Figs. 2–4

T,K	Q^0, 10^{-16} cm^2	Q^1, 10^{-16} cm^2	Q_{tot}, 10^{-16} cm^2	$\overline{Q}^{AB}$, 10^{-16} cm^2	$\overline{\overline{Q}}^{AB}$, 10^{-16} cm^2
300	325.3	314.1	316.9	156.6	−54.2
320	321.5	311.1	313.7	155.8	−54.5
340	317.9	308.3	310.7	154.0	−54.8
360	314.5	305.6	307.8	152.9	−55.1
380	311.4	303.0	305.1	151.7	−55.3
400	308.3	300.5	302.5	150.6	−55.5

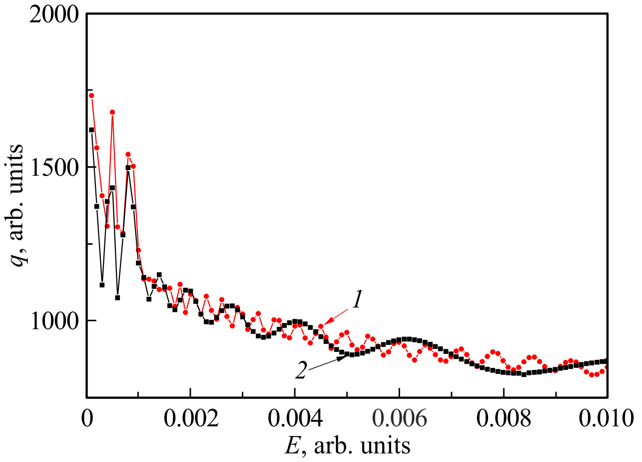

Figure 3. Dependences of elastic scattering cross sections q^0 and q^1 on the collision energy for the ^{23}Na$-^{85}$Rb pair in the atomic system of units.

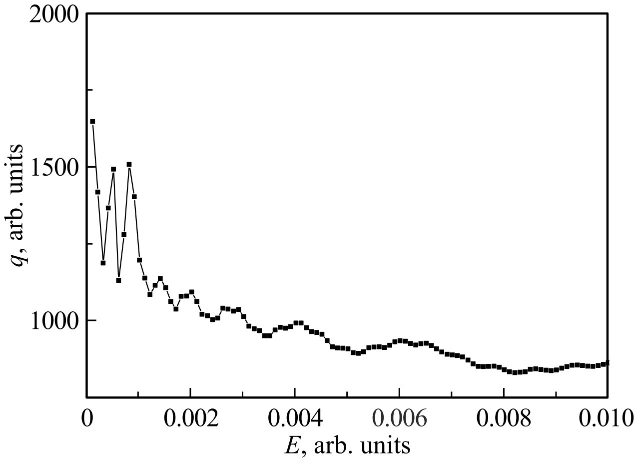

Figure 4. Dependence of the total elastic scattering cross section (q_{tot}) on the collision energy for the ^{23}Na$-^{85}$Rb pair in the atomic system of units.

relation (8) that the main contribution to the total elastic scattering cross section is produced by the cross section of scattering by the triplet term.

In order to use the obtained cross sections in experiments on optical orientation of atoms, one needs to pass from energy to temperature dependences of the cross sections. The results of averaging the cross sections by velocity are listed in the table.

It can be seen that elastic scattering cross sections Q^0 (singlet term) and Q^1 (triplet term) differ only slightly. Cross section Q_1 produces the dominant contribution to Q_{tot}. The value of the frequency shift cross section remains negative within the entire temperature range.

Conclusion

The obtained cross sections and the earlier data on Na-Na and Rb-Rb collisions may be used to analyze the kinetics of polarization transfer processes in a mixture of alkali Na-Rb atoms with optical orientation of atoms. Collisions of optically oriented alkali atoms in mixtures affect significantly the shifts in the magnetic resonance frequency of atoms that are induced by spin exchange. Contributions to these shifts are produced by collisions of both identical and different atoms. These contributions, in turn, depend both on the absolute values of cross sections and on their signs, as well as on the concentration of alkali atoms in the working chamber. Notably, there are feasible scenarios in which the spin-exchange shift changes sign and passes through zero.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] M.V. Romalis. In *Flexible high performance magnetic field sensors*. Ed by E. Labyt, T. Sander, R. Wakai (Cham: Springer, 2022). P. 3.
[2] T. Sander, A. Jodko-Władzi'nska, S. Hartwig, R. Brühl, T. Middelmann. Adv. Opt. Technol.,**9** (5), 247 (2020). DOI: 10.1515/aot-2020-0027
[3] A.K. Vershovskii, M.V. Petrenko. Techn. Phys. Lett., **49** (3), 77 (2023). DOI: 10.21883/TPL.2023.03.55693.19378

[4] K. Jensen, M.A. Skarsfeldt, H. Staerkind, J. Arnbak, M.V. Balabas, S-P. Olesen, D.H. Bentzen, E.S. Polzik. Sci. Rep., **8** (1), 16218 (2018). DOI: 10.1038/s41598-018-34535-z

[5] M. Lipka, A. Sierant, C. Troullinou, M.W. Mitchell. Phys. Rev. Appl., **21**, 034054 (2024). DOI: 10.1103/PhysRevApplied.21.034054

[6] V.N. Baryshev, D.S. Kupalov, A.V. Novoselov et al. Measur. Techn., **59** (12), 1286(2017). DOI: 10.1007/s11018-017-1130-6

[7] V.A. Kartoshkin. In *Alkali metals: new research* (2023) P. 1.

[8] C. Abel, S. Afach, N.Phys. Rev. A, **101** (5), 053419 (2020). DOI: 10.1103/PhysRevA.101.053419

[9] Yan Lu, Yueyang Zhai, Yong Zhang, Wenfeng Fan, Li Xing, Wei Quan. Chin. Phys. B, **29** (4), 043204(2020). DOI: 10.1088/1674-1056/ab75d3

[10] A.N. Nesmeyanov. *Vapor Pressure of the Elements* (Academic, N.Y, 1963).

[11] V.A. Kartoshkin. Opt. Spectr., **119** (4), 594 (2015). DOI: 10.1134/S0030400X1510015X.

[12] V.A. Kartoshkin. Opt. Spectrosc., **116** (4), 548 (2014). DOI: 10.1134/S0030400X14030096.

[13] A. Pashov, O. Docenko, M. Tamanis, R. Ferber, H. Knöckel, E. Tiemann. Phys. Rev. A, **72**, 062505 (2005). DOI: 10.1103/PhysRevA.72.062505

[14] S. Sunakawa. *Kvantovaya teoriya rasseyaniya* (Mir, M., 1979) (in Russian).

[15] H.O. Dickinson, M.R. Rudge. J. Phys. B, **3**, 1448 (1970).

Translated by D.Safin