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# Magnetic resonance frequency shifts of alkali atoms in a K-Li mixture

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The calculation of the frequency shifts of the magnetic resonance of K and Li atoms in a K-Li mixture has been carried out. A significant difference in the behavior of the temperature dependences of the frequency shifts for the optical orientation of K or Li atoms is established.

**Keywords:** spin exchange, cross sections, frequency shifts.

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## Introduction

Quantum magnetometers with optical pumping currently play an important role in various magnetic measurements [1,2]. Working media of this kind of magnetometers can be atoms of alkali metals in the ground state [3], mixtures of alkali atoms of different sorts [4,5], mixtures of alkali atoms and excited atoms of Helium in the metastable $2^3S_1$-state [6], excited atoms of Helium in the metastable $2^3S_1$-state [7].

The interest in this kind of devices is due to, in particular, the use of quantum magnetometers for the purpose of applications as elements included in quantum gyroscopes and magnetoencephalographs. The use of alkali metals as working media in these devices results in certain problems. This is due to the fact that in absorption chambers alkali atoms collide to each other, atoms collide with chamber walls, alkali atoms collide with atoms of the buffer gas, if the latter is used for filling the absorption chambers. Since alkali atoms have uncompensated electronic spins ($S = 1/2$), then collisions of atoms with each other result in the process of electronic polarization exchange, if one of them was optically polarized before (so called spin exchange). Further, during the time between collisions the electronic polarization redistributed between electronic and nuclear degrees of freedom of the alkali atom due to the hyperfine interaction.

Along with the polarization transfer, a frequency shift of magnetic resonance of the colliding atoms takes place during the spin exchange. It is worth to note that in the case, when the spin exchange is accompanied by an inelastic process, i.e. chemoionization, as it takes place, for example, in [8], the latter process has a significant effect on both spin-exchange cross section and frequency shift of magnetic resonance [9].

In recent times attention is being increasingly focused on the devices that use mixtures of alkali atoms as their working media. In [10] a scheme of magnetometer was suggested with its working chamber filled with a mixture of alkali atoms of Cs and K. Polarized atoms of Cs were used to create a $M_x$-magnetometer, while polarized atoms of K were used to create a $M_z$-magnetometer. Both alkali atoms were in the condition of optic orientation. In [11] quantum magnetometers were considered that were based on a mixture of K and Rb alkali atoms with an addition of $^{21}$Ne inert gas that has $I = 3/2$ nuclear spin. This type of devices can be used to measure angular rotational rates. In these devices atoms of K are optically oriented. Further, due to the spin exchange during collisions of K and Rb atoms, Rubidium atoms are polarized, which, in turn, transfer the polarization to nuclear spins of $^{21}$Ne atoms.

As already mentioned, the presence of alkali atoms in the absorption chamber leads to the situation that in the condition of optical orientation in the chamber collisions take place between both atoms of the same sort and atoms of different sorts.

In this study we shall consider the effect of spin-exchange collisions between alkali atoms in a mixture of K and Li on the shift of magnetic resonant frequency of K and Li atoms in conditions of optical orientation of both K atoms and Li atoms.

## 1. Spin-exchange shifts of magnetic resonant frequency for a mixture of alkali atoms

Atoms of alkali metals in the ground state have an electronic spin of $S = 1/2$. Nuclear spin of $^{39}$K atoms considered in this study is $I_{\mathrm{K}} = 3/2$, while nuclear spin of $^7$Li atoms is $I_{\mathrm{Li}} = 3/2$. In [12] a theory was developed of magnetic resonant frequency shifts of alkali atoms in the conditions when one sort of alkali atoms in a mixture is optically oriented by the resonant polarized optical radiation. That is, the situation is similar to that implemented in [4,5]. In the model under consideration, in a system of two alkali atoms A and B optical orienting of atoms B is implemented and shifts of magnetic resonant frequency of atoms A are determined for two hyperfine states. In the process of spin-exchange collisions between atoms A and B the orientation is transferred from the optically polarized atom B to atoms A. In this case the evolution of density matrix of atoms A can be described by the following equation:

$$\frac{d}{dt}{}^{(A)}\rho = \left[\left(\frac{\partial}{\partial t}\right)_{AB} + \left(\frac{\partial}{\partial t}\right)_{AA} + \left(\frac{\partial}{\partial t}\right)_{AC} + \left(\frac{\partial}{\partial t}\right)_{D} + \left(\frac{\partial}{\partial t}\right)_{H}\right]^{(A)}\rho. \tag{1}$$

In accordance with the notation adopted in [12], we have the following: the first term describes collisions of different atoms (A and B), the second term describes collisions of atoms of the same type (A and A), the third term describes collisions of atoms A with buffer gas atoms C, the fourth term describes the diffusion to absorption chamber walls, the final term describes the interaction of atoms with constant magnetic field.

As already shown in [13], contributions from three last terms in (1) are small. Therefore in this study we shall consider the effect of the first two terms in (1) on shifts of magnetic resonant frequency, i. e. the effect of collisions of atoms of the same type and collisions of different atoms between themselves. The use of absorption chambers with anti-relaxation coating all the more leads to the situation that terms 3 and 4 in (1) can be neglected. In this context, we shall consider cases when either K atoms or Li atoms are optically oriented, and frequency shifts are determined either for Li atoms or for K atoms, respectively.

In this case, according to [12] the consideration of spin-exchange collisions only results in the following expressions for shifts of magnetic resonant frequency of two hyperfine states of an alkali atom:

$$\Delta\omega(\pm) = \delta^{(1)}\omega(\pm) + \delta^{(2)}\omega. \tag{2}$$

Here the first term is due to the emergence of an addition to the transverse component of orientation for atom A in collisions with longitudinally oriented atoms B, and the second term is due to the transfer of transverse orientation from one sublevel $F$ of atom A to another as a result of collisions. The shifts represented in (2) in accordance with [12] have the following form:

$$\delta^{(1)}\omega(+) = -\frac{P_z(B)}{2(2I_A+1)}\left[\bar{\bar{\gamma}}_{AB} - \bar{\bar{\gamma}}_{AA}B_-\left(\frac{2I_A-1}{2I_A+1}\right)^{1/2}\right], \tag{3}$$

$$\delta^{(1)}\omega(-) = -\frac{P_z(B)}{2(2I_A+1)}\left[\bar{\bar{\gamma}}_{AB} + \bar{\bar{\gamma}}_{AA}B_+\left(\frac{2I_A+3}{2I_A+1}\right)^{1/2}\right], \tag{4}$$

$$\delta^{(2)}\omega = -\frac{C}{\bar{\omega}_0}\left\{(2\bar{\gamma}_{AA} + 3\bar{\gamma}_{AB})^2 - [\bar{\bar{\gamma}}_{AA}P_z(B)]^2\right\}. \tag{5}$$

In this study the subscript A is referred to Li or K atoms (depending on which atom is optically oriented), while the subscript B is referred to $^{39}$K or $^{7}$Li atoms, respectively. Then $\delta^{(1)}\omega(+)$ — magnetic resonant frequency shift for the $F = S + I$ hyperfine state (where $S$ — electronic spin, which is equal to 1/2 for alkali atoms, and $I$ — nuclear spin of alkali atom (in our case it is $I = 3/2$)), $\delta^{(1)}\omega(-)$ — magnetic resonant frequency shift for the $F = S - I$ hyperfine state, $P_z(B)$ — polarization of particle B (as it is noted earlier, spin-exchange shifts are calculated when atoms B are subjected to optical orientation), $I_{\mathrm{A}}$ — nuclear spin of particle A (Li atom) is equal to 3/2 and 3/2, when atoms B are $^{39}$K atoms, $\bar{\bar{\gamma}}_{AB}$ and $\bar{\bar{\gamma}}_{AA}$ — imaginary components of complex spin-exchange rate $\gamma$, that can be expressed through imaginary parts of the complex spin-exchange cross section ($\gamma_{AB} = \langle v_{AB}\rangle N_B\sigma_{AB}$, $N_{\mathrm{B}}$ — concentrations of particle sort B, $\langle v_{AB}\rangle$ — mean relative thermal velocity of colliding particles, $\sigma_{AB}$ — spin-exchange cross section of colliding particles), $\bar{\omega}_0 = H_0|g_S|\mu_B/\hbar$ (frequency of electronic precession), $H_0$ — constant magnetic field, $g_s$ — $g$-factor of electron, $\mu_{\mathrm{B}}$ — Bohr magneton. Subscripts AA and AB are referred to collisions between the same or different atoms, $\mathrm{B}_\pm$ can be represented as follows in accordance with [12]:

$$B_+ = \frac{2I_A+2}{6}\left(\frac{2I_A+3}{2I_A+1}\right)^{1/2},$$

$$B_- = \frac{2I_A}{6}\left(\frac{2I_A-1}{2I_A+1}\right)^{1/2}, \tag{6}$$

$$C = \frac{2I_A(2I_A+2)(2I_A+3)(2I_A-1)}{288(2I_A+1)^4}. \tag{7}$$

Thus, to calculate the magnetic resonant frequency shifts in question, which are caused by the spin exchange, in accordance with (3)−(5) it is necessary to know complex spin-exchange cross sections (first of all their imaginary parts, and in case of the shift defined by (5), also real parts of complex cross sections) for the following pairs of atoms: Li-Li, Li-K, and K-K.

It is worth noting that coefficient C in formula (7) is considerably less than one, and expression (5) includes squares of imaginary and real parts of complex spin-exchange rates. Therefore the $\delta^{(2)}\omega$ frequency shift can be neglected in comparison with $\delta^{(1)}\omega(+)$ ans $\delta^{(1)}\omega(-)$ frequency shifts.

## 2. Optical orientation of K atoms. Magnetic resonant frequency shift of Li atoms

Let us consider the situation when optical orienting of Potassium atoms takes place in the mixture of alkali atoms of K and Li. In accordance with (3) and (4), we need to know temperature dependencies of imaginary parts of complex spin exchange rate ($\bar{\bar{\gamma}}_{AB} = \langle v_{AB}\rangle N_B\bar{\bar{\sigma}}_{AB}$ and $\bar{\bar{\gamma}}_{AA} = \langle v_{AA}\rangle N_A\bar{\bar{\sigma}}_{AA}$) for the case when atom B is an atom of Potassium, and atom A is an atom of Lithium. In [14–16], temperature dependencies of real and imaginary parts of the complex spin-exchange cross section were calculated for K-K, K-Li, and Li-Li pairs. Results of Maxwellian

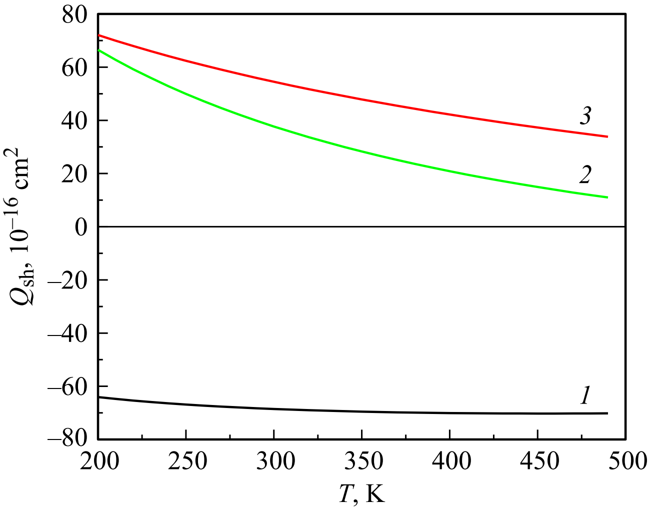

**Figure 1.** Imaginary part of complex spin-exchange cross section as a function of temperature: *1* — K-Li system according to [13], *2* — Li-Li system according to [14], *3* — K-K system according to [15].

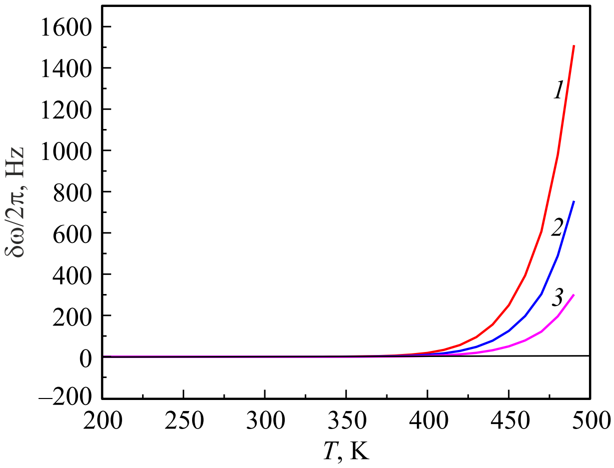

**Figure 2.** Shift of magnetic resonant frequency $\delta^1\omega(+)$ and $\delta^1\omega(-)$ of Li atoms as a function of temperature in the mixture of alkali atoms of K and Li at $P$ optical orientation of K atoms: $P = 100$ (*1*), 50 (*2*), 20% (*3*).

averaging of imaginary part of the complex cross section are shown in Fig. 1. As it follows from the figure, imaginary parts of spin-exchange cross sections for pairs of the same atoms, K-K and Li-Li, are positive and reduce as the temperature increases. At the same time, the imaginary part of spin-exchange cross section for the pair of K-Li grows in magnitude and remains negative throughout the entire range of temperatures.

Fig. 2 shows the calculation of magnetic resonant frequency shifts of Li atoms in a situation when optical orientation of K atoms takes place. The calculation was performed in accordance with formulae (3)–(6) using the information on the imaginary parts of complex spin-exchange cross sections shown in Fig. 1. Since expressions (3), (4) include temperature dependencies of imaginary parts of complex spin-exchange rate, then to calculate the shifts it is necessary to know the concentrations of alkali atoms in the absorption chamber. To calculate the concentrations, tables from [17] were used. Since this study considers the case of alkali atoms mixture, then to change over from temperature of the absorption chamber to concentration of alkali atoms in the chamber it is necessary to use Raoult's law for saturated-vapor pressure above the melt of metal mixture.

As can be seen from Fig. 2, $\delta^{(1)}\omega(+)$ and $\delta^{(1)}\omega(-)$ shifts of Li atoms coincide with each other in magnitude and sign in the entire range of temperatures under consideration. The coincidence of shifts is caused by the fact that the imaginary parts of complex spin-exchange rate included in (3) and (4) ($\overline{\overline{\gamma}}_{AA} = \langle v_{AA}\rangle N_A \overline{\overline{\sigma}}_{AA}$ and $\overline{\overline{\gamma}}_{AB} = \langle v_{AB}\rangle N_B \overline{\overline{\sigma}}_{AB}$) depend on the concentration of alkali atoms, the corresponding cross section, and the relative velocity of colliding atoms. Moreover, while velocities of the collision and cross sections (shown in Fig. 1) are nearly equal to each other, the concentrations of Li and K atoms are different by several orders of magnitude, with concentration of K atoms is higher than that of Li. Thus, in (3) and (4) prevailing are the first terms in brackets, that depend on the concentration of K atoms and define both the absolute values and sign of the magnetic resonant frequency shift.

## 3. Optical orientation of Li atoms. Magnetic resonant frequency shifts of K atoms

In the case of optical orientation of Li atoms in the K-Li mixture, shifts of magnetic resonant frequencies of Potassium atoms as function of temperature were calculated for two hyperfine states: $F = 2$ and $F = 1$. Fig. 3 shows shifts of magnetic resonant frequencies as function of

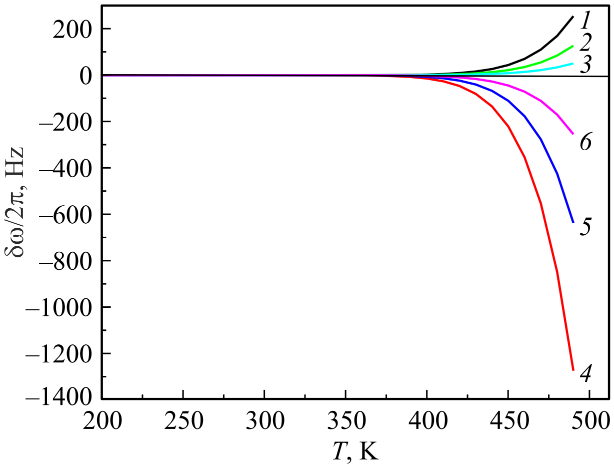

**Figure 3.** Dependence of magnetic resonant frequency shift of Potassium atoms in the mixture of K and Li alkali atoms at $P$ optical orientation of Li atoms: $\delta^1\omega(+)$ for $P = 100$ (*1*), 50 (*2*), 20%(*3*); $\delta^1\omega(-)$ for $P = 100$ (*4*), 50 (*5*), 20%(*6*).

temperature for two hyperfine states: $F = 1$ and $F = 2$ of $^{39}$K atom, calculated on the basis of relationships $(3)-(6)$ and the information on imaginary parts of spin-exchange cross sections for K-K and K-Li pairs from Fig. 1. As it follows from Fig. 3, temperature dependencies of magnetic resonant frequency shifts for K atom in the ground state are considerably different from similar dependencies of Lithium atom (Fig. 2). This is due to the fact that in the case of optical orientation of Li atoms and a shift observed for Potassium atoms, the second term in (4) plays a significant role because it is this term that depends on concentration of Potassium atoms in the absorption chamber. As already mentioned, the concentration of Potassium atoms in the absorption chamber is much higher than the concentration of Li atoms at the same temperatures. The difference between $\delta^{(1)}\omega(+)$ and $\delta^{(1)}\omega(-)$ dependencies is due to the difference between coefficients $B_-$ and $B_+$, explicit form of which is represented by expressions (6), and signs between the first and the second terms in expression (4).

## Conclusion

As already mentioned in the Introduction, shifts of magnetic resonant frequency play a significant role in devices, which operation principle is based on the optical orientation of alkali metal atoms. At the same time the behavior of frequency shifts depends on the complex spin-exchange cross section, which is defined by interaction potentials of the atoms used in absorption chambers as working media. Interaction potentials of alkali atoms define both absolute imaginary part of the complex spin-exchange cross section and its sign, which can be clearly seen in Fig. 1. In addition, the shifts are considerably contributed by concentrations of atomic particles in the working chamber. The impact of these factors is evidently seen in Fig. 2 and 3. The $\delta^{(2)}\omega(+)$ shift of magnetic resonant frequency, as defined by relationships (5) and (7), is considerably less than $\delta^{(1)}\omega(+)$ and $\delta^{(1)}\omega(-)$ frequency shifts, and therefore can be neglected in the temperature range under study at a magnetic field strength of $H_0 = 1\,\mathrm{Oe}$.

### Conflict of interest

The author declares that he has no conflict of interest.

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