Frequency shifts of the magnetic resonance of Rb and K atoms in the K - Rb tandem magnetometer

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Abstract. Collisions of alkali atoms in the ground state are accompanied by the exchange of electron polarization between the colliding atoms, which lead to the polarization transfer between particles. As a result of this process, the electronic orientation is transferred from the spin oriented atoms to unpolarized atoms, along with the polarization transfer, the magnetic resonance frequency shifts of polarized atoms occur too. In this work the magnetic resonance frequency shifts of arising from spin exchange collisions in a mixture of alkali potassium and rubidium atoms at the optical orientation of atoms are calculated. The situation when optical pumping by resonant polarized radiation is carried out only for atoms of the one kind is considered. The spin exchange process between alkali atoms was described in the formalism of the complex cross section for spin exchange process. The real and imaginary parts of the complex cross section were calculated using the interaction potentials of alkali atom dimers. The calculation of the frequency shifts is carried out on the basis of data on the interaction potentials for the following pairs of alkali atoms K-K, K-Rb and Rb-Rb. Maxwell averaging of the cross sections over the velocities was done and the temperature dependences of the magnetic resonance frequency shifts for K and Rb atoms were plotted.

1. Introduction
It is known that quantum magnetometers with optical pumping currently play an important role in various magnetic measurements [1, 2]. In these magnetometers, alkali metal atoms in the ground state [3, 4], mixtures of alkali metal atoms and excited helium atoms in the $^2S_1$ metastable state [5], and excited helium atoms in the $^2S_1$ metastable state [6, 7] are used as the working media of such devices. To solve definite metrological problems, it is necessary to use a fast response device that can ensure high accuracy measurements. These properties are often difficult to implement in a single device; therefore, quantum magnetometers of a “tandem” type are used to solve such problems. The first “tandem” magnetometer was proposed in [8]. In this device the $^{87}$Rb isotope was used as a working media. At present, works with the “tandem” magnetometer using rubidium vapors is continued [9, 10]. Later, a “tandem” magnetometer based on a mixture of alkali atoms was suggested. The working chambers of this instrument contain a mixture of alkali metal atoms, in particular, $^{133}$Cs and $^{39}$K atoms [11]. In this case, the cesium atoms are used to construct a $M_x$ - type magnetometer and the potassium atoms are used to construct a $M_z$ - type magnetometer. At the same time, along with a pair of K-Cs, another pair of alkaline atoms, K-Rb, can also be used as a working medium of the magnetometers [12 - 14]. Due to the presence of the mixture of alkali metal atoms in the absorption chamber, both
collisions between the K atoms in the ground state, as well as collisions between the Rb atoms in the ground state, and collisions between the K and Rb atoms occur in the absorption chamber at the optical orientation of atoms.

In our work, the magnetic resonance frequency shifts in a mixture of $^{39}$K- $^{85}$Rb at the optical orientation of atoms are considered and the magnitude of the magnetic resonance frequency shifts for the case of a mixture of rubidium and potassium atoms in the absorption chamber is calculated.

2. Complex cross sections of spin exchange

The process of spin exchange during the collision of alkali atoms can be described in the formalism of the complex cross section for spin exchange process [15]

$$q = \bar{q} + i\bar{q}$$ .

The real and imaginary parts of the complex cross section can be calculated using the interaction potentials of alkali atoms.

The complex cross section for spin exchange can be represented in the following form through the scattering matrices $T$:

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

(2)

Here, $k_{AB}$ is the wave number, *) denotes the complex conjugation. The scattering matrix $T$ can be represented through the scattering phases ($\delta_{S}^{AB}(l)$) in the channel with full spin $S$ as follows:

$$T_{S}^{AB}(l) = \exp(2i\delta_{S}^{AB}(l)),$$

(3)

where $l$ is the orbital quantum number.

Taking into account (2) and (3), the real and imaginary parts of the complex cross section can be represented as:

$$q_{R}^{AB} = \frac{\pi}{k_{AB}} \sum_{l=0}^{\infty} (2l+1) \sin^2 \left[\delta_{1}^{AB}(l) - \delta_{0}^{AB}(l) \right],$$

(4)

$$q_{I}^{AB} = \frac{\pi}{k_{AB}} \sum_{l=0}^{\infty} (2l+1) \sin 2 \left[\delta_{1}^{AB}(l) - \delta_{0}^{AB}(l) \right].$$

(5)

Hence, knowing the singlet and triplet interaction potentials of the $^{39}$K$_2$, $^{85}$Rb$_2$, and KRb dimers, one can calculate the scattering phases at the singlet and triplet terms and determine the cross sections we are interested in.

In the collision of alkali atoms in the ground state with an electron spin $S = 1/2$ a molecule is formed. This molecule is described by two potentials corresponding to the total spins of the system $S=0$ (singlet term) and $S = 1$ (triplet term). In [16–18], interaction potentials describing the $^{39}$K$_2$ dimers were presented. In [19, 20] the potentials for the $^{85}$Rb$_2$ were presented, and in [21] the potentials were received for the $^{39}$K$^{85}$Rb dimer. Based on the presented interaction potentials, in [22–24], the real and imaginary parts of the complex spin exchange cross sections were calculated for the systems under study. The calculations were carried out in accordance with expressions (4) and (5). To pass from the dependences of the complex cross sections on the collision energy to the temperature dependences in the absorption chamber, Maxwell averaging of the cross sections over the velocities was done.

Figures 1 and 2 show the temperature dependences of the real and imaginary parts of the complex cross section $^{39}$K$_2$ [22], $^{85}$Rb$_2$ [23], and $^{39}$K$^{85}$Rb [24] averaged over the velocities.
Figure 1. Temperature dependences of the real part of the complex spin-exchange cross section in collisions of K atoms with Rb (1) [24] and K (2) [22] atoms, and Rb atoms with Rb (3) [23] atoms.

Figure 2. Temperature dependences of the imaginary part of the complex spin-exchange cross sections of K atoms with Rb (1) [24] and K (2) [22] atoms, and Rb atoms with atoms Rb (3) [23] atoms.

3. Magnetic resonance frequency shifts due to spin exchange between K and Rb atoms

In experiments with alkaline atoms, which are the working media of quantum magnetometers with optical pumping, one of the main processes leading to the transfer of polarization between colliding atoms, relaxation, and shift of the magnetic resonance frequency is the spin exchange process. That is, the process of exchange of electronic degrees of freedom between colliding atoms. In the general case, the description through the density matrix of the processes occurring in the absorption chamber and affecting the evolution of the density matrix includes, in accordance with [25], the following processes: collisions of alkali atoms with each other, collisions of alkaline atoms with atoms of a buffer gas, diffusion of atoms to the absorption chamber walls, the interaction of atoms with a constant magnetic field. In this work we consider the situation when optical pumping by resonant polarized radiation is carried out only for atoms of the one kind. In this case, the polarization of atoms of the second kind is due to the spin exchange process. If a mixture of alkaline atoms is contained in the working chamber, then collisions of alkaline atoms of different kinds between themselves are also added to the processes indicated above. Typically, in order to reduce relaxation in the working chamber, various kinds of anti-relaxation coatings are used (primarily paraffin). In this case a buffer gas is not used and diffusion and collisions with the atoms of the buffer gas can be neglected.

In accordance with [25], taking into account only spin exchange collisions leads to the following expressions for the magnitudes of the magnetic resonance frequency shifts of two hyperfine states of the alkali atom:

$$\Delta \omega(\pm) = \Delta \omega^{(1)}(\pm) + \Delta \omega^{(2)},$$  \hspace{1cm} (6)

where, the first term is due to the appearance of an addition to the transverse component of orientation of atoms 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 presented in (6) in accordance with [25] have the following form:
\[
\delta^{(1)} \omega(+) = -\frac{P_z(B)}{2(2I_A + 1)} \left[ \gamma_{AB} - \gamma_{AA} B \left( \frac{2I_A - 1}{2I_A + 1} \right)^{1/2} \right],
\]

(7)

\[
\delta^{(1)} \omega(-) = -\frac{P_z(B)}{2(2I_A + 1)} \left[ \gamma_{AB} + \gamma_{AA} B \left( \frac{2I_A + 3}{2I_A + 1} \right)^{1/2} \right],
\]

(8)

\[
\delta^{(2)} \omega = -\frac{C}{\omega_0} \left\{ (2\gamma_{AA} + 3\gamma_{AB})^2 - \left[ \gamma_{AA} P_z(B) \right]^2 \right\}.
\]

(9)

In accordance with the notation adopted in [25] here: \( \delta^{(1)} \omega(+) \) is the magnetic resonance frequency shift for the hyperfine state \( F = S + I \) (where \( S \) is the electron spin and in the case of alkaline atoms it is \( 1/2 \), and \( I \) is the nuclear spin of the alkali atom. In the case of isotopes \(^{39}\text{K}\) and \(^{85}\text{Rb}\), the nuclear spins are \( 3/2 \)), \( \delta^{(1)} \omega(-) \) is the magnetic resonance frequency shift for the hyperfine state \( F = S - 1 \), \( P_z(B) \) is the polarization of particle \( B \) (Particle \( B \) is polarized by circularly polarized resonant radiation.), \( I_A \) 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 the spin exchange \( (\gamma_{AB} = \langle v_{AB} \rangle N_B q_{AB}, N_B \) is the concentration of particles \( B \), \( \langle v_{AB} \rangle \) is the average relative velocity of the colliding particles, \( q_{AB} \) is the spin exchange cross section, \( \omega_0 = \frac{H_0 g_s \mu_B}{\hbar} \) is the electron precession frequency, \( H_0 \) is the constant magnetic field, \( g_s \) is the electron g-factor, and \( \mu_B \) is the Bohr magneton. Letters \( AA \) and \( AB \) correspond to collisions between the same or different alkaline atoms, the values of \( B_\pm \) in accordance with [25] have the form:

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

(10)

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

\[
C = \frac{2I_A(2I_A + 2)(2I_A + 3)(2I_A - 1)}{288(2I_A + 1)^4}.
\]

(11)

It can be shown that the magnitude of the shift determined by relation (11) is significantly less than the magnitudes of the shifts (10). In the future, we will not consider them.

Thus, in order to calculate the shifts of the magnetic resonance frequency that are of interest to us due to the spin exchange, in accordance with (7) - (8), we need to know the values of the complex cross sections of the spin exchange (primarily their imaginary parts) for the following pairs of atoms: Rb-Rb, Rb-K and K-K.

To calculate the frequency shifts, it is necessary to know the concentration of alkaline K and Rb atoms in the absorption chambers. The calculation of the concentration of atoms was carried out according to [26]. Using a mixture of alkali atoms in the absorption chamber one has to know the
concentration of each atom in the absorption chamber. In order to know the concentration of alkali atoms in the chamber, it is necessary to use the Raoult law for the pressure of saturated vapor over the melt of a mixture of metals. In the calculation, it was assumed that potassium and rubidium atoms were in the melt in equal weight ratios.

Using the data of complex spin exchange cross sections presented in Part 2, we calculated the magnitudes of the magnetic resonance frequency shifts for Rb and K atoms in accordance with relations (7), (8), (10). Figures 3 and 4 show the results of the calculation of the shifts for the degree of polarization of the atoms (atoms B) equal to 20% and 50%.

Figures 3 and 4 show that with an increase in temperature there is a sharp increase in the magnitude of the shifts. This is due to the temperature dependence of the pressure of alkali atoms over the melt. The frequency shifts of the magnetic resonance of rubidium atoms have different signs for the two hyperfine states $F = 2$ and $F = 1$. For the hyperfine state $F = 2$, the frequency shift is negative, while for the hyperfine state $F = 1$ it is positive. At the same time, the frequency shifts of the magnetic resonance of potassium atoms also have different signs for the two hyperfine states $F = 2$ and $F = 1$. For the hyperfine state $F = 1$, the frequency shift is negative, while for the hyperfine state $F = 2$ it is positive.

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