Sources of heading error of optically pumped magnetometers operated in the Earth’s magnetic field

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When optical pumped magnetometers are aimed for the use in Earth’s magnetic field, the orientation of the sensor to the field direction is of special importance to achieve accurate measurement result. Inaccuracy in relation to the heading of the sensor can be an even severe problem in the case of special operational configurations, such as for example the use of strong off-resonant pumping. We systematically study the main contributions to the heading error in systems that promise high field resolutions at Earth’s magnetic field strengths, namely the non-linear Zeeman splitting and the orientation dependent light shift. The good correspondence of our theoretical analysis to experimentally achieved data demonstrates that both of these effects are related to the modification of the interaction between laser light and dipole moment of the atoms when the heading is changed. Also our results promise a compensation of both effects when using both circular polarization directions.

I. INTRODUCTION

Optical pumped magnetometers (OPM) exploit the natural conversion of magnetic fields to frequencies by the Zeeman effect in alkali atoms [1]. Because in general frequencies can be determined with very high precision, magnetometers based on this effect offer the potential of very high sensitivities.

The development of OPMs over the last decades resulted in sensitivities that made them compatible with well established magnetometers based on superconducting systems such as SQUIDs [2–5]. Especially the so-called spin exchange relaxation-free (SERF) type [6,7] is nowadays increasingly applied for the detection of biomagnetic signals [8,9]. Additionally resulting from their working principle, OPMs offer the advantage to be used as total magnetic field sensor [10] which may be beneficial for a number of applications. Still, a vectorial characteristic is introduced because the laser light photons carry a certain momentum in parallel to the beam direction. Its alignment concerning the magnetic field direction can falsify the measurement result and influence sensitivity [11,12]. This so called heading error [1,13] leads to certain requirements for the operation of OPMs when used for geomagnetic surveys. For example their orientation concerning the Earth’s magnetic field is fixed during the measurement [14,15]. Thus, the study of orientational effects is an important step in the development of new detection concepts with atomic magnetometers and attracts increasing scientific interest [16–19].

Many application driven research on OPMs is orientated to biomagnetic fields. Therein the SERF operational regime allows for femtotesla sensitivities. However, because it requires an environmental field close to zero (well below 10 nT) [7], it sets strong requirements to magnetic shielding [20] or compensation of residual fields [21]. This limitation excludes the SERF-regime for a use in magnetically unshielded environments.

To overcome this obstacle, recently, the light narrowing (LN) [22] and light-shift dispersed $M_z$ (LSD-Mz) [23] operational modes have been developed. Both exploit a strong off-resonant pumping of buffer gas cells [24] for an optimal redistribution of population. This results in large output signal amplitudes. Additionally, the rather broad (about 1 kHz) magnetic resonances allow a comparable large bandwidth. In this paper, we analyze the heading error connected to the rather unusual parameters required for these operational modes. The rest of the paper is organized as follows: In Sec. II we theoretically discuss two effects expected to contribute mainly to the heading error for the mentioned operational modes. In Sec. III the experimental setup is demonstrated and measurement results are presented in Sec. IV in comparison to the calculations. We summarize the paper with a conclusion on the usability of the newly introduced operational modes.

II. ANALYSIS OF THE PROBLEM

The term heading error summarizes several effects associated with the change of orientation between the laser beam and the external magnetic field $B_0$ in OPMs [1]. For the LN [22] and LSD-Mz [23] operational modes two main sources can be identified. First, because the magnetometer is suggested to operate in ambient fields of the order of the Earth’s magnetic field, a significant contribution of the non-linear Zeeman splitting [19,25] can be expected. Secondly, the operation in these special modes is based on a strong off-resonant pumping at the optical transitions. This is connected to large light-shifts. Although attempts have been carried out to cancel the effect of non-linear Zeeman splitting by appropriate light-shift [16,26], such approach cannot easily be applied to the LN and LSD-Mz mode because large pump-laser powers are required for the latter to achieve good field resolutions.

II.a. Influence of the heading to atom-light coupling

The orientation dependence of both, the non-linear Zeeman splitting and light shift, can be understood by simple considerations: The direction of the magnetic field $B_0$ defines the quantization axis in the system. Further on, it is fixed along...
the z-axis. For alkali atoms that are usually used for optical magnetometers, its interaction with the atomic momentum \( \vec{F} \) as sum of the total electron momentum \( \vec{J} \) and the nuclear spin \( \vec{I} \) leads to the Zeeman splitting. That is the removal of the energetic degeneracy of the hyperfine levels. If the induced splitting is small compared to the hyperfine level splitting, meaning small magnetic fields, \( F \) is a good quantum number and the sub-levels can be labeled with different quantum numbers \( m_F \). Here, the latter is the quantized component of the atomic momentum on the quantization axis.

In dipole approximation the direction dependency of OPMs attributes to the interaction of the electric field of the laser beam \( \vec{E}(\vec{r}, t) \) with the dipole operator \( \vec{D} \) of the atom. The first may be described by a plane wave. We assume that its propagation direction is modified in the x-z-plane. Considering a circular polarization, as required for optical pumping, the electric field at the atom’s position \( \vec{r}_0 \) is given by

\[
\vec{E} = \frac{E_0}{\sqrt{2}} e^{i(\vec{k}\vec{r}_0 - \omega t)} (\cos \alpha \vec{e}_x \pm i \vec{e}_y + \sin \alpha \vec{e}_z). \tag{1}
\]

Here, \( \vec{k} \) and \( \omega t \) are the respective wave vector and circular frequency of the laser light, \( \vec{e}_x, \vec{e}_y, \vec{e}_z \) the respective unit vectors in \( x, y, \) and \( z \) direction, and \( \alpha \) the angle between the light propagation direction and the \( z \)-axis. The plus and minus sign applies respectively for left and right handed circular polarization. In the following, we refer to them as \( \sigma_+ \) and \( \sigma_- \) polarization, respectively.

Because the dipole operator is a vector, the matrix elements for optical transitions can be found following the Wigner-Eckart theorem \([27]\). Especially, when introducing \( D_x = D_x \pm i D_y \) the possible matrix elements for the \( F \leftrightarrow F' \) transition of the Cs-\( D_1 \) line are

\[
\begin{align*}
&\langle Fm_F | D_x | F'm_{F'} \rangle = c_{Fm_F,F'm_{F'}}^{(1)} \sqrt{2} \sum_{m_F} \langle J | D_x | J' \rangle , \\
&\langle Fm_F | D_- | F'm_{F'} \rangle = c_{Fm_F,F'm_{F'}}^{(-1)} \sqrt{2} \sum_{m_F} \langle J | D_+ | J' \rangle , \\
&\langle Fm_F | D_+ | F'm_{F'} \rangle = c_{Fm_F,F'm_{F'}}^{(0)} \sqrt{2} \sum_{m_F} \langle J | D_- | J' \rangle .
\end{align*}
\tag{2}
\]

The constants \( c \) depend on the quantum numbers \( F, F', m_F, \) and \( m_{F'} \) and can be found by reducing the dipole operator \([28]\) in terms of Wigner 3-j and 6-j symbols

\[
\begin{pmatrix}
F' & 1 & F \\
F_m & q & -m_F
\end{pmatrix}
\begin{pmatrix}
1/2 & 1/2 & 1 \\
F' & F & 7/2
\end{pmatrix}
\]

\[
\begin{pmatrix}
Fm_F, F' & m_{F'} & m_{F'}
\end{pmatrix}
\]

The above equations represent the optical selection rules \( \Delta m_F = 0 \) and \( q = 0 \) for linear as well as \( \Delta m_F = \pm 1 \) and \( q = \pm 1 \) for circular polarized light.

As a consequence, the interaction strengths are depending on the angle. They can be summarized as

\[
D \cdot \vec{E} = \frac{E_0}{2\sqrt{2}} e^{i(\vec{k}\vec{r}_0 - \omega t)} \left( \cos \alpha \vec{e}_x \pm i \vec{e}_y + \sin \alpha \vec{e}_z \right).
\]

where the driving amplitude

\[
\Omega = \frac{E_0}{2\sqrt{2h}} \langle J = 1/2 | D_x | J' = 1/2 \rangle
\]

\[
= \frac{1}{\hbar} \sqrt{\frac{P_L}{4\epsilon_0 c n A}} \langle J = 1/2 | D_0 | J' = 1/2 \rangle , \tag{5}
\]

depends on the transition dipole matrix element of the \( D_1 \) transition, the applied laser power \( P_L \), and its spot size \( A \). Also the speed of light \( c \), the permittivity \( \epsilon_0 \), and the refractive index \( n \) were introduced above and the double bars denote a reduced matrix element \([28]\).

Equation \((4)\) describes a \( \sin\alpha \) dependence of the interaction strength for an effective \( \pi \) transition, meaning \( m'_{F'} = m_F \). Such linear pumping is therefore maximal at angles of 90 degree. On the other hand, for parallel orientation the ground states levels \( m_F \) are coupled to the excited states \( m_F \pm 1 \) with different angle dependent weights for respective circular polarized light and optical pumping is achieved.

\[ W_{m_F,m_F} = \pi \frac{1}{2\hbar^2} \langle 4m_F | \vec{D} \cdot \vec{E} | 3m_F \rangle^2 \int_0^\infty \rho(\omega) s(\omega) d\omega. \tag{6}\]

Therein, the last term accounts for spectral distribution of the laser light given by \( \rho(\omega) \) and broadened transitions lines \([29]\). Each of this distribution functions is normalized. The discussed term can be deduced from strict quantum mechanical calculation \([30]\) or by Fermi golden rule type arguments.
There $s(\omega)$ defines the spectral distribution of light spontaneous emitted by the considered transition. On the other hand, the laser light will have a narrow spectral width, allowing to set $\rho(\omega) = \delta(\omega - \omega_L)$. Further, we assume a Lorentzian line shape for the optical transition with an in general doppler broadened linewidth $\gamma_{m_F,m_F}$. Thus the integral in Eq. [6] simplifies to the factor $2/\pi \gamma_{m_F,m_F}$. Then Eq. [6] is simplified to

$$W_{m_F,m_F} = c_{m_F,m_F}(\alpha) \frac{\Omega^2}{\gamma_{m_F,m_F}},$$

(7)

where the angle dependence and the exact value of the transition matrix element are summarized in the factor $c_{m_F,m_F}$. Following Eq. [4], at perpendicular orientation, namely when $\cos \alpha = 0$, no pumping to the dark states remains and the population is distributed along the levels of the ground state. On the other hand, a clear pumping to the levels with high absolute quantum numbers $|m_F|$ is found close to heading angles $\alpha$ of 0 and 180 degree.

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**FIG. 1.** Transition elements of the $F = 4$ to $F' = 3$ transition of Cs. The different colors are used for visual separation of the $\Delta m_F = 0, \pm 1$ transitions.

The pumping is illustrated in the level diagram of Fig. [1] where the Zeeman-split states of the $F = 4$ ground and $F' = 3$ excited state are shown. The ground and excited states are coupled by transition elements that yield from the dipole moment. As a result from (2), the picture illustrates the allowed transitions with $\Delta m_F = 0, \pm 1$. Their strength is indicated by the saturation of the colors. This difference in the coupling strength of ground and excited states for different magnetic sub-levels results in a similar dependence for the rates of spontaneous emission. Note, that there is no additional dependence of this emission on the orientation of the laser beam to the magnetic field.

On the other hand, as found by Eq. [4], all these illustrated transitions are relevant for optical pumping of a magnetometer that is rotated in a magnetic field $\vec{B}_0$. Hereafter, we neglect the stimulated emission because the rate for spontaneous emission is assumed to be much larger. Starting with an angle $\alpha = 0$ between the magnetic field and the laser beam direction and assuming $\sigma_+$ polarization, only the blue transitions in Fig. [1] remain and the population is transferred towards the $m_F = 4$ level. With increasing angle the linear polarized component corresponding to the black lines in the figure is increased with a factor of $\sin \alpha$. In addition, the pumping to large numbered $m_F$ levels is decreased with $\cos \alpha + 1$ and also the inverse pumping increases with $1 - \cos \alpha$. Therefore at an angle of $\alpha = 90$ degree, transitions with $\Delta m_F \neq 0$ dominate while the transitions to higher and lower magnetic quantum numbers have an equal orientational factor of one. Thus the latter only depends on the values of the constants $c_{F,m_F,F',m_F}$.

We illustrate the effect of this orientation-dependent pumping to the population of the levels by the use of rate equations including spontaneous emission and absorption of the laser light. For the calculation, we normalize the rate of laser absorption $\Omega^2/\gamma_{m_F,m_F}$ to the rate of spontaneous emission $\gamma_s$. Note, for a more realistic picture we included coupling of neighboring ground states with a constant rate $\Gamma$. This simplified estimation leads to a level occupation as shown in Fig. [2].

The natural linewidth corresponding to the rate of spontaneous emission of the $D_1$ transition takes a value of 4.5 MHz [28]. For the calculation of the plots in Fig. [2] we used a natural line width of $\gamma_s/2\pi = 4.2$ MHz, a doppler broadened linewidth of $\gamma_{m_F,m_F} = 350$ MHz, and a reduced dipole moment of $\langle J = 1/2 \mid D \mid J' = 1/2 \rangle = 2.7 \times 10^{-29}$ cm that relates the laser powers to the driving amplitudes $\Omega^2/\gamma_{m_F,m_F} \gamma_s$.

The latter as well as the ground state redistribution rate are at least four orders of magnitude smaller so that no population is acquired in the excited states.

In the low pumping case, a rather weak redistribution of the population is found. Furthermore for angles close to zero degree, the population is shifted towards the levels with high magnetic quantum numbers $m_F$ as expected when pumping with $\sigma_+$ circular polarization. Still the strongest population differences are not found for transitions incorporating sub-level with largest $m_F$ but rather around $m_F = 3$. When the magnetic field $\vec{B}_0$ is perpendicular to the beam direction, only linear pumping remains and alignment, that is the concentration of population to states with large absolute quantum numbers $|m_F|$, can be found. In our simulation for perpendicular configuration, indeed the largest population differences are found close to the levels with large absolute magnetic quantum numbers $|m_F|$. If the pumping is substantially increased, as shown in the lower plot of Fig. [2], a clear pumping to the dark state is achieved. It is best for angles close to zero degree. If the orientation is changed to 90 degree, only alignment remains. Note, due to the pumping of the $F = 4 \rightarrow F' = 3$ transition in principle two dark states are found for optimal $\sigma_+$ pumping. This fact leads to the large population of the $m_F = 3$ levels at $\alpha = 0$ and makes pumping to the dark state with $m_F = 4$ even more efficient if a small linear polarized component remains in the laser beam. The discussed modifications in the population of states influence to the observable magnetic rf-resonance.
The position amplitude is given by the perpendicular component to the modulation of the Larmor frequency. This part can be treated by the Bloch equation \cite{36}. They might also be decomposed into a parallel and a perpendicular component to the \(\vec{B}_0\) field as

\[
\vec{B}_{\perp} = \frac{\Gamma}{\Gamma_r \Gamma_\varphi + \Omega_{rf}^2}. \tag{9}
\]

Here \(\delta = \omega_0 - \omega_{rf}\) is the detuning between the rf-field and Larmor frequency and \(\Gamma_\varphi' = (\Gamma_\varphi^2 + \delta^2) / \Gamma_\varphi\). Depending on the detection technique, either the unmodulated population \(\langle \sigma_z \rangle\) or the off-diagonal components that are modulated with the \(B_1\) field can be reconstructed. These methods correspond respectively to the so-called \(M_2\) and \(M_x\) operation modes of atomic magnetometers. Because the different components are connected to magnetization along different axes (given by the index of the Pauli operators) their detection is again direction dependent.

In principle one can separate the description of the pumping and the probing of the atomic magnetization. The detection is assumed by a circularly polarized probe laser. If the latter is for instance orientated perpendicular to the magnetic field \(\vec{B}_0\), its intensity after transmission through the medium is modulated with \(\omega_{rf}\) because of the coupling to the modulated field along the x-axis (proportional to \(\langle \sigma_x \rangle\)). By using homodyne detection, the in- and out-of-phase components give a dispersive \(\propto \delta\) and absorptive Lorentzian like signal. They are respectively named \(Y\) and \(X\). A fitting of the experimental curves for varying \(B_1\)-frequency can then be used to extract the Larmor frequency from resonant conditions where \(\delta = 0\) and \(\langle \sigma_z \rangle\) becomes maximum.

The additional direction dependence that results from probing the spin dynamics can be found similar to \cite{4} with a change of the quantization axis to the x-direction but is neglected here. The population as plotted in Fig. 2 corresponds to the steady state population due to optical pumping. The corresponding rates, namely the pumping and the emission are of the order of tens of kHz and MHz, respectively and thus much larger as the dissipative rates \(\Gamma_r\) and \(\Gamma_\varphi\) as well as the driving amplitude \(\Omega_{rf}\) of the magnetic resonance that both are assumed well below 10 Hz for a vacuum cell \cite{38}. Note latter driving amplitude should not exceed several Hz because otherwise the magnetic resonance curve is significantly broadened.

With these ratios of the corresponding rates, one can safely assume that the steady state population as calculated in Fig. 2 is unchanged by the \(B_1\) field because the other processes leading to it are much faster. Still, the applied \(B_1\) field tends to equalize the population of neighboring magnetic sub-levels. Therefore, to keep the steady state population, also the laser absorption needs to be increased depending on the resonance condition between \(B_1\) and the Larmor frequency.

Additionally, a difference in the splitting of the magnetic sub-levels is found that is caused by the non-linear Zeeman effect.
effect and can be calculated by the Breit-Rabi equation [39]. Therefore we estimate the measurement results of an $M_e$ atomic magnetometer rotated in the Earth’s magnetic field by the following equation

$$X = \sum_{m_F = -4:3} -\beta(m_F, \theta) \frac{\Gamma_r \Omega_f}{\Gamma_r F' \wp(\omega_0(m_F))) + \Omega_r^2}$$  \hspace{1cm} (10)

Here, the factor $\beta$ is the population difference of the magnetic transition $m_F \leftrightarrow m_F + 1$ and the change of the Larmor frequency due to the non-linear Zeeman effect is included into $\Gamma_r$. In Fig. 3 we extracted the center frequency of the line-shape described in (10) by a Lorentzian fitting. Therewith the plot describes the heading error of the Larmor frequency due to the non-linear Zeeman splitting.

![Graph showing Larmor frequency as a function of orientation angle α.](image)

**FIG. 3.** (Color online) The Larmor frequency as expected from a measurement as a function of the orientation angle $\alpha$. The calculations are carried out for different laser powers as presented in the legend in $\mu W$ assuming a circular beam shape with constant intensity and an diameter of 4 mm. The left and right picture assume respectively a redistribution of population between neighboring and from one to all other ground states. Note, only negative angles are shown for simplicity because the curves have an even symmetry and the lines for highest laser powers in the left image overlap.

For the calculations resulting in Fig. 3 we assumed $\sigma_+$ polarization of the laser, a magnetic field $B_0 = 50 \mu T$ and transverse as well as longitudinal relaxation times of $T_1 = 40$ ms and $T_2 = 20$ ms, respectively. These are slightly increased compared to the values as for example given in Ref. [38], but fit better to the experiment as shown below. We investigated two cases, namely a redistribution of the ground state population only between neighboring and from one to all the other ground states as shown in the left and right graphs of Fig 3, respectively.

Depending on the laser intensity, proportional to $\Omega^2$, in both cases quite different dependencies are found. In common, for strong pumping (light blue curves in Fig. 3) we observe the smallest magnetic resonance frequencies in a region between -90 and 90 degree, were an effective pumping to the $m_F = 4$ dark state is achieved. Contrary between -180 to -90 as well as 90 to 180 degree the system is effectively pumped with $\sigma_-$, because the direction of the laser beam to the $B_0$ field is inverse. Therefore, at these angles the largest Larmor frequencies are expected namely the one between the $m_F = -4 \leftrightarrow m_F = -3$ levels. The peculiarities at 0 and 180 degree are connected to the use of the $F = 4 \rightarrow F' = 3$ transition for optical pumping. The occurrence of two dark states that is found if the linear pumping component in Eq. (3) is missing, allows two magnetic transition frequencies instead of only one. This results in the peak of population at 0 degree at the $m_F = 3$ ground state in the lower plot of Fig. 3 and a shifted reconstructed mean value for the Larmor frequency (to lower values at 180 and higher values at zero degree). It could be avoided by solely pumping to the $F' = 4$ excited state.

For lower laser intensities we observe for both redistribution models similar expected Larmor frequencies at angles $\alpha$ of 0 and 180 degree. Additionally, they are increased and decreased when approaching 90 degree. This is due to only small modifications in population compared to the undisturbed system by the optical pumping. The effect of redistribution of population is increased if the linear polarized component is increased and, thus, if the angles are approaching -90 and 90 degree. Then, the comparable small effect of the circular polarization components influences strongly to the expected resonance frequencies. By that, the strong angle dependence close to 90 degree can be understood. We conclude that an accurate description of the population’s redistribution process in the ground state including spin-exchange as well as the influence of the $B_1$ field (as for example in Ref. [40]) is required for a more precise prediction of the angle dependence in the case of small laser intensities. Because of the non-linearity of these processes this can not easily be achieved in frame of rate equations.

**II.c. Light shift**

An operation with reasonable sensitivity at Earth’s magnetic field strengths is possible in the LN and LSD-Mz operational mode. Still both of them require a strong pumping. To empty the $F = 3$ ground state the large intensity laser is tuned close to this $D_1$ transition. Thus, the measurable dark state is achieved in the $F = 4$ ground state. Due to the strong detuned laser light the Zeeman split $F = 4$ ground state levels will be effected by a strong light shift. The latter is given by [41]

$$\Delta \omega_{m_F} = -\frac{1}{4\hbar^2} \sum_{F', m_{F'}} \text{Re} \left( \frac{\langle 4m_F | \vec{E} \cdot \vec{D} | F', m_{F'} \rangle}{\omega_{F' m_{F'}} - \omega_{4m_F} - i\gamma_{F' m_{F'}} m_{F'}/2} \right)^2$$

$$- \frac{\langle 4m_F | \vec{E} \cdot \vec{D} | F', m_{F'} \rangle}{\omega_{F' m_{F'}} - \omega_{4m_F} + i\gamma_{F' m_{F'}} m_{F'}/2} \right)^2 \right).$$  \hspace{1cm} (11)

Here, the energy of the i-th state is given by $\hbar \omega_i$. For simplicity the detuning between the transition frequency of the $F = 4, m_F$ ground to $F', m_{F'}$ excited state $\omega_{4m_F, F' m_{F'}} =$
\( \omega_{F'm_F'} - \omega_{4m_F} \) and the laser frequency \( \omega_L/2\pi \) is set to be constant for all of the transitions to a \( F' \) excited state \( \delta_{4m_F,F'm_F'} = \omega_{F'm_F'} - \omega_{4m_F} - \omega_L = \delta_{F'} \). This approximation is justified because the latter is for the considered operational modes significantly larger than the Zeeman splitting of the ground and excited state. Additionally, one can neglect the second term in the brackets of Eq. (11) since it is significantly smaller than the first. With assuming a constant width of each of the transitions \( \gamma \), Eq. (11) takes the compact form

\[
\Delta \omega_{m_F} = \frac{-1}{4\hbar^2} \sum_{F'm_{F'}} \text{Re} \left( \left| \frac{\langle pF'm_F'| \vec{E} \cdot \vec{D} |4m_F \rangle}{\delta_{F'} - i\gamma/2} \right|^2 \right).
\]

Above equation can easily be interpreted when reminding the light shift of a two level system. The latter is easily reconstructed by expanding the generalized Rabi frequency \( \lambda \) for small interaction energies \( \hbar \Omega_0 \) compared to the energetic detuning \( \hbar \delta \)

\[
\Omega_R = \sqrt{\Omega_0^2 + \delta^2} \approx \delta + \frac{\Omega_0^2}{2\delta} + O(x^4).
\]

Note that the energetic shift for one of the levels is \( \Omega_R/2 \) and that the second term describes the power dependent shift of the energy levels. Also these oscillations get damped by a dephasing \( \gamma \) leading to a smaller measured splitting as found in Eq [12]. Therefore, the Eq (12) describes the sum of all the measurable energetic shifts induced by the coupling of a single ground state level to all allowed excited states. This shift is increased by larger intensities \( \propto \vec{E}^2 \) or smaller detuning. Note, instead of using the expansion in Eq [13] the use of the generalized Rabi frequency in principle allows a description for arbitrary detuning, namely in frame of dressed states. The selection rules are included in the matrix elements of \( \vec{E} \cdot \vec{D} \). Their modification by the change of orientation of the laser light concerning the \( \vec{B}_1 \) direction is responsible for the heading dependent light shift and already given in Eq. [3]. In Fig. 4 the shifts of the energy \( F = 4 \) ground states are plotted for different angles between magnetic field and laser beam direction.

Here, for each \( F = 4 \) ground state level the sum given by Eq. (12) is calculated taking into account all transitions to the \( F' = 3,4 \) excited states that have non-zero Matrix elements \( \langle 4 \rangle \) in the dipole approximation. The respective detunings of the laser to the transitions frequencies are \( \delta_{3}/2\pi = -8.6 \text{ GHz} \) and \( \delta_{4}/2\pi = -9.8 \text{ GHz} \). Also a transition linewidth \( \gamma/2\pi = 4 \text{ GHz} \) and driving amplitude of \( \Omega/2\pi = 4 \text{ MHz} \) were used. The latter corresponds to a laser power of 1.3 mW estimated for a perfect circular beam shape on a spot size of 4 mm diameter.

In Fig. 4 we observe all the light shifts discussed in literature [3]. First, all energy levels are shifted by a constant value that is about 3 kHz for an orientation of 90 degree and else is slightly smaller. This effect corresponds to the scalar light shift. Secondly, the vector part is most pronounced at 0 degree, that is at positions where optimal circular pumping is achieved. It describes a shift of the energy levels proportional to the magnetic quantum number \( m_F \). The direction of this shift is changed between the two different circular polarizations. This vector light shift can be interpreted as additional magnetic field \( \vec{B}_{LS} \) that is added to \( \vec{B}_0 \) shifting the Larmor frequencies. Finally, the tensor part is most pronounced at an angle of 90 degree and corresponds to a small shift for large absolute magnetic quantum numbers \( |m_F| \).

![FIG. 4. (Color online) Light shift of the energy levels for the \( F \) = 4 ground state levels. They are respectively plotted for \( \sigma_- \) and \( \sigma_+ \) polarized light in red and blue. The solid, dotted, and dashed line styles correspond to orientation angles of 0, 45, and 90 degree between magnetic field and laser beam direction. The parameters for this plot are given in the main text.](image)

![FIG. 5. (Color online) Expected reconstructed Larmor frequencies as a function of the direction angle \( \alpha \). They are influence by a strong light shift due to the strong off-resonant pumping that is modified due to the change of interaction matrix elements, see Eq. [4]. The same parameters as for Fig 4 have been used.](image)
respectively for $\sigma_+$ and $\sigma_-$ circular polarized light in dependence on the angle range. Two possible ranges are required to be considered, namely [-90 to 90] degree and the rest. The choice of these ranges occurs from the fact that the population is shifted due to the strong driving to the corresponding dark states. Therefore, one special transition is selected to be measured as we explained in the previous section. In other words, when the system is rotated over -90 and 90 degree the role of $\sigma_+$ and $\sigma_-$ polarization are exchanged.

In the figure we observe a large measurable light shift at angles of 0 and 180 degree. There its vector component becomes maximal due to optimal circular pumping. It is then reduced reaching values of [90] degree. Still, because a tensor component of the lightshift remains, an overshooting of the corresponding curves is visible at these angles. Note, for the figure the operational mode is not of importance.

**III. EXPERIMENTAL METHOD**

**III.a. Measurement setup**

For an experimental investigation we created a special setup as shown in a schematic drawing accompanied with a photographic image in Fig. 6. Laser light for pumping the cesium atoms with a wavelength of 895 nm is supplied to the setup by a polarization maintaining fiber. By a combination of a lens, a linear polarizer, and a quarter-lambda plate the pump laser is collimated and circular polarization is created. The beam diameter is adjusted to 4 mm. This beam is passed either through a vacuum glass cell or a micro fabricated magnetometer cell both filled with Cs. The latter additionally exploits a rather high buffer gas pressure of 200 mbar as necessary for both, LN and LSD-Mz operational mode.

The transmitted laser beam is measured by a photodiode behind the cell. An additional bandpass filter avoids unwanted light on the diode.

The micro-fabricated magnetometer cell is heated by an additional heating laser beam at a wavelength of 978 nm applied perpendicular to the pump laser at the side of the cell. Three coils are mounted around the cell allowing the application of magnetic $B_1$-fields in three perpendicular directions.

The described setup is mounted on top of a rotational table inside of a 3D Helmholtz coil system and three layers of mu-metal shielding. By that the influence of external magnetic fields is reduced and arbitrary magnetic fields $B_0$ can be applied. In the experiment the direction of this field is kept in $z$-direction and only its strength is set to either 5 or 50 $\mu$T. Note, we decided to rotate the magnetometer and not adjust the magnetic field direction as for example in Refs. [44, 45] to avoid unwanted strain fields and allow a more realistic experiment compared to exploration applications. Our setup is adjusted in a way to ensure the magnetometer cell to stay in the middle of the $B_0$ coil setup during rotation. Therewith the whole setup reflects an atomic magnetometer rotated in an external magnetic field. The alignment of the magnetometer setup to the magnetic field can be controlled from outside the shielding by a cable pull. This setup is somehow comparable to one presented earlier, where the OPM is rotated in the Earth’s magnetic field [44, 46], but it excludes external interferences and is variable in the magnetic field strength.

The current measured by the photodiode is amplified by a trans-impedance amplifier before it is demodulated to its X and Y component by a lock-in amplifier or directly digitized respectively for $M_x$ or $M_z$ operation, compare to Eq. 9. A radio frequency generator serves as local oscillator for the demodulation and is used also to apply the $B_1$ field utilizing one of the coils.

**III.b. Characterization of experimental setup**

A first measurement series is aimed for the characterization of the measurement setup and basic limitations. Therefore, the vacuum cell and a $B_0$ field of 5 $\mu$T are used in the classic $M_x$ regime. With this rather small magnetic field the influence of the non-linear Zeeman splitting is reduced. In addition, the pump laser is adjusted to the $F = 4 \rightarrow F' = 3$ transition; and low powers of about 10 $\mu$W reduce the influence of light shifts. Furthermore, these and subsequent measure-
ments are carried out in 10 degree steps over a full rotation of the setup inside the magnetic field. To evaluate the influence of low frequency drifts the heading angle is first rotated counter clockwise starting at 180 degree and measuring in 20 degree steps. The intermediate points are then recorded by consequent clockwise rotation. In Fig. 7 the measured Larmor frequencies are plotted as a function of the orientation $\alpha$ of the laser beam direction to the $B_0$ field.

Experimentally we observe a sinusoidal dependence of the Larmor frequency on the orientation. Its amplitude has a value of 1.6 Hz. Despite of a careful design of the experimental setup, we assume a parasitic field located on the rotating table as cause of this dependency added and subtracted to the $B_0$ field at different angles. In addition, while the back and forward measurements (marked by circles and crosses, respectively) give almost the same results close to -180 degree, a large deviation of about 2 Hz is found between the start and end point at 180 degree. We account this to a low frequency drift of the $B_0$ field that is likely caused by thermal variations at the current sources for the coils or the Helmholtz system itself. In principle the observed remaining orientation dependence is limiting the evaluation of the orientation dependence.

IV. EXPERIMENTAL FINDINGS

IVa. Influence of the non-linear Zeeman splitting

In a further experiment the $B_0$ field is increased to 50 $\mu$T while the vacuum cell and the rest of the experimental parameters is kept. This setup should allow to determine the heading error caused by the non-linear Zeeman splitting. In our investigations we used both possible circular polarizations, left and right handed. In between the experimental setup had to be modified, namely the orientation of the quarter wave plate had to be adjusted. To do so the mu-metal shielding was opened resulting in an magnetic offset field. Therefore, a constant deviation between the Larmor frequencies of both circular polarizations is expected accounting for the magnetic field change due to the rearrangement of the setup. Experimentally it takes a value of 100 Hz. The observed Larmor frequency as a function of the orientation angle is shown in Fig. 8.

We reconstructed the Larmor frequency in the $M_x$ mode from the in- and out-of-phase signals by a linear fitting of the ratio $X/Y$. According to Eq. (9) the total population difference $\langle r_2 \rangle$ is canceled and only

$$X/Y = -\frac{\omega - \omega_0}{\Gamma_\varphi}$$

remains. Then the only remaining fitting parameters are the Larmor frequency $\omega_0/2\pi$ and the resonance width $\Gamma_\varphi/2\pi$.

The experimentally observed curve corresponds roughly to the theoretical one for the smallest laser intensities (compare to Fig. 7). That roughly agrees to the value set in the experiment that was about 10 $\mu$W. Herein, we additionally assumed a circular laser spot with equal power distribution of 4 mm diameter.

In Fig. 9 we show example measurement curves for the X signal. They nicely demonstrate the measured shift of the resonance line as mainly caused by a broadening of the Lorentzian curve. Therefore, a distributed population allows an overlay of several Lorentzian curve with shifted center frequencies as a result of the non-linear Zeeman splitting occurring in the case of moderate pumping intensities and therefore several populated ground-state levels in the steady state. Note, the asymmetry of curves results from the same overlay of Lorentzian lines with different center frequencies [1].
FIG. 9. (Color online) Example measurement results for the X signal measured at a magnetic field of 50 µT on the vacuum cell. The blue and red color are used for $\sigma_+$ and $\sigma_-$ circular polarization of the laser light, respectively. The angle $\alpha$ between the light propagation direction and the magnetic field at which the curves are measured is given in the legend.

IV.b. Light shift in the LN and LSD-Mz operational mode

For the following measurements the experimental setup as shown in Fig. 6 is extended for the simultaneous recording of both circular polarizations. Thus, a polarizing beam splitter and a deflecting prism are used to create two beams. An additional linear polarizer in the straight beam is used for intensity adjustment. Both of them are circular polarized by separate quarter-lambda plates and passed through microfabricated vapor cells that share the same reservoir. In the experiments with micro-fabricated cells we observe optical linewidths in the order of several GHz due to the high buffer gas pressure [22]. Therefore, while the ground state hyperfine splitting is resolved the excited states of the $D_1$ transition overlap. The wavelength of the pump laser is stabilized to the $F = 3 \rightarrow F' = 4$ transition on a doppler free absorption spectrum of an additional vacuum cell. This modification of the wavelength is required to effectively empty the $F = 3$ ground state as required by the LN and LSD-Mz operational modes. Due to the slightly overlapping absorption lines, the same laser optically pumps the $F = 4$ levels to the dark states $\Delta m_F = \pm 1$ depending on its circular polarization. By such strong off-resonant pumping a large light shift of the energy levels observable in the magnetic transition between the Zeeman split states is additionally created.

We present measurements of the orientation dependency of the measured Larmor frequencies for the LN and LSD-Mz mode in Figs. 10 and 11 respectively. In both cases a large light shift of the order of 1 kHz for each of the two circular polarizations is observed. Note, optical pumping in both cases works well at 0 and 180 degrees but also the largest light shifts are observed at these angles. Secondly, at these angles the LN-signal is minimal, because the modulated components are observed best in the x-y plane as found in Eq. (9). This is most probable causing the discrepancy of the curve of the measured Larmor frequencies in this $M_x$ method compared to the expected results of Fig. 5 as well as the experimental dependence observed in the LSD-Mz mode. Nevertheless, the experimental results correspond qualitatively as well as quantitatively very well to our calculations. Furthermore, the laser power of about 2 mW in the experiment is in the same range as the one used for the calculation.

Additionally, we experimentally observe a larger light shift for the $\sigma_-$ polarization compared to that of $\sigma_+$ that most probable is related to a not exact adjustment of laser intensities and/or polarizations of the two beams. Therefore, especially in Fig. 11 an angle dependence of the mean Larmor frequency of the two polarization directions remains.
CONCLUSION

We investigated main contributions to the heading error for operation of optical pumped magnetometers with strong off-resonant pumping in Earth’s magnetic field strengths. A dedicated experimental setup is used for a most realistic measurement environment, namely a well defined magnetic field in which the alignment of a magnetometer can be adjusted. In two separated experiments we evaluate the influence of the non-linear Zeeman splitting and of light shifts. As our theoretical model suggest, the first results from a redistribution of the ground states population and thus the experimental de-
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