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Nuclear magnetic shielding and quadratic Zeeman effect in helium-like ions

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Abstract. The quadratic Zeeman effect and hyperfine magnetic shielding are calculated in the ground $(1s)^2$ state of helium-like ions using perturbation theory. Numerical values are obtained for the nuclear charge range $Z = 6 - 32$. The Zeeman splitting is computed by solving the Dirac equation in the Coulomb field of an extended nucleus with B-splines from the DKB method. Leading-order contributions and one-photon-exchange corrections are treated within a rigorous QED approach. The calculated nuclear magnetic shielding constants can be used to determine nuclear magnetic moments, and the quadratic Zeeman effect is relevant for high-precision Penning-trap measurements of transition energies in He-like ions.

Keywords: Zeeman effect, *g* factor, highly charged ions, bound-state QED, nuclear magnetic shielding, hyperfine structure

Introduction

Bound-electron *g* factor, which mostly determines Zeeman splitting in highly charged ions, has been measured with increasing precision during the last two decades (Sturm et al. 2017). The relative experimental uncertainty has reached 2.4×10^{-11} in H-like carbon (Sturm et al. 2014), 0.7×10^{-10} in Li-like silicon (Glazov et al. 2019), and 0.24×10^{-9} in B-like tin (Morgner et al. 2025). The *g*-factor measurements already performed and anticipated in the near future, combined with the corresponding theoretical efforts, provide access to the fundamental constants and nuclear properties (Harman et al. 2018; Shabaev et al. 2015). In particular, nuclear magnetic moments can be determined with unprecedented precision from the *g* factors of few-electron ions (Quint et al. 2008; Werth et al. 2001). This task has become particularly relevant after a discrepancy was found between the recent measurement of the hyperfine splitting in H- and Li-like bismuth (Ullmann et al. 2017) and the most accurate theoretical prediction

(Volotka et al. 2012). This so-called 'hyperfine puzzle' has been resolved with the new value of ^{209}Bi nuclear magnetic moment (Skripnikov et al. 2018), which disagrees with the previously accepted one. The more general outcome of this work is that the uncertainty of the magnetic moment values determined by the nuclear magnetic resonance method can be significantly underestimated. Recently, a new value for ^{207}Pb has been determined (Fella et al. 2020) in strong disagreement with the tabulated value. The nuclear magnetic shielding for a bound electron in the 1s and some excited states was studied using a fully relativistic approach in Refs. (Moore 1999; Pyper 1999; Pyper, Zhang 1999). Later, detailed theoretical investigations have been presented for the ground state of H-like (Moskovkin, Shabaev 2006; Moskovkin et al. 2004; Yerokhin et al. 2011; 2012), He-like (Yerokhin et al. 2024), Li-like (Moskovkin et al. 2008a; 2008b), and B-like ions (Volchkova et al. 2017). In this work, we study the nuclear magnetic shielding for the ground state of He-like ions. The total magnetic moment is fully determined by the nucleus and the shielding constant in this case. Despite certain experimental difficulties, this allows one, in principle, to access directly the nuclear magnetic moment in high-precision Penning-trap measurements.

The nonlinear contributions to the Zeeman splitting can play an important role in high- precision measurements. In particular, the second- and third-order effects can be detected in the Penning-trap experiments with B-like ions (von Lindenfels et al. 2013). Recent measurement of the ground-state g factor in $^{40}Ar^{13+}$ (Arapoglou et al. 2019) was sensitive to the third-order contribution (Glazov et al. 2013; Varentsova et al. 2017; 2018). Subtraction of the second-order contribution (Agababaev et al. 2017; Glazov et al. 2013; Varentsova et al. 2018) was required to obtain the most precise up-to-date experimental value of the fine-structure transition energy in B-like argon (Egl et al. 2019; Micke et al. 2020).

The nonlinear Zeeman effects are enhanced by the closely spaced levels of the same parity — $^2P_{1/2}$ and $^2P_{3/2}$ in B-like ions — which are mixed by the external magnetic field. The same can happen with $n = 2$ levels in low- and middle-Z He-like ions. The quadratic Zeeman shift can thus be relevant for future high-precision measurements. Transition energies in He-like ions serve as a perfect probe of the many-electron QED effects and therefore attract much experimental and theoretical interest: see, e. g., Refs. (Beiersdorfer, Brown 2015; Epp et al. 2015; Kozhedub et al. 2019; Loetzsch et al. 2024; Machado et al. 2018; Malyshev et al. 2019; 2023; Yerokhin, Surzhykov 2019; Yerokhin et al. 2022) and references therein. In this work, we investigate the second-order Zeeman effect for the ground state of low- and middle-Z He-like ions. The excited states of He-like ions will be the subject of our future work.

Both the nuclear magnetic shielding and the quadratic contribution in a magnetic field represent the terms of the second order of perturbation theory. In addition to the one- electron part, we consider the first-order interelectronic-interaction correction. The results are obtained within the perturbation theory using the finite basis sets.

Relativistic units ($\hbar = 1$, $c = 1$, $m_e = 1$) and Heaviside charge unit [$\alpha = e^2/4\pi$, $e < 0$] are employed throughout the paper; $\mu_B = |e|/2m_e$ denotes the Bohr magneton, m_p is the proton mass, and m_e is written for clarity in the electron-to-proton mass ratio m_e/m_p.

Relativistic theory for He-like ions

We consider a helium-like ion in the ground $(1s)^2$ state. The relativistic perturbation theory offers the following expression for the ground-state energy, to first order in $1 / Z$:

$$E_{1s^2} = 2E_{1s}^{(0)} + \Delta E_{1ph}^{(1)} + \ldots, \tag{1}$$

where $E_{1s}^{(0)}$ is the single-electron energy in the 1s state. The one-photon-exchange correction is given by

$$\Delta E_{1ph}^{(1)} = \langle ab|I(0)|ab\rangle - \langle ba|I(\Delta_{ab})|ab\rangle. \tag{2}$$

Here, a and b represent electron states — 1s with angular momentum projection ± 1/2, and $\Delta_{ab} = E_a - E_b$ is zero in the present case. The operator I is the interelectronic-interaction operator, which in the Feynman gauge takes the form

$$I(\omega, r_{12}) = \alpha(1 - \alpha_1 \cdot \alpha_2)\frac{exp(i|\omega|r_{12})}{r_{12}}. \tag{3}$$

Below, we focus on various aspects of the Zeeman effect in helium-like ions, such as the second-order shift in a magnetic field and nuclear magnetic shielding. These problems have been addressed before, including the second-order Zeeman effect in hydrogen-like ions (Feinberg et al. 1990; Grozdanov, Taylor 1986; Manakov, Zapryagaev 1976; Manakov et al. 1974; Szmytkowski 2002a; 2002b), the second- and third-order Zeeman effects in boron-like ions (Agababaev et al. 2017; Glazov et al. 2013; von Lindenfels et al. 2013; Varentsova et al. 2017; 2018), and the Zeeman splitting in hydrogen-, helium-, lithium-, and boron-like ions with nonzero nuclear spin (Moskovkin, Shabaev 2006; Moskovkin et al. 2004; 2008a; 2008b; Volchkova et al. 2017; Yerokhin et al. 2011; 2012; 2024). The present work brings into focus two-electron systems and computes the first-order electron-electron interaction, namely one-photon-exchange contribution.

For this purpose, we employ the complete spectrum of the one-electron Dirac equation

$$\widehat{H}_0\psi\left(r\right)=\varepsilon\psi\left(r\right) \tag{4}$$

with the zeroth-order Hamiltonian:

$$\widehat{H}_0=\boldsymbol{\alpha}\,\boldsymbol{p}+\beta+V_{nuc}\left(r\right), \tag{5}$$

where α and β are the Dirac matrices, and $V_{nuc}(r)$ is the spherically symmetric electrostatic nuclear potential. The interaction between electrons is treated within the framework of perturbation theory (PT). To describe the ground state of a helium-like ion, we specifically take the sum of two one-electron zeroth-order energies and account for the electron-electron interaction in first-order PT.

Quadratic contribution to the Zeeman effect

Consider a bound electron in the presence of an external magnetic field. The system is described by the stationary Dirac equation (4), and the magnetic field is treated as a perturbation V_m:

$$V_m=\lambda U,\quad \lambda=\mu_B B,\quad U=\left[\boldsymbol{r}\times\boldsymbol{\alpha}\right]_z. \tag{6}$$

Within the perturbation theory, the energy $E(\lambda)$ can be expanded in a power series in λ,

$$\begin{aligned}E\left(\lambda\right)&=E^{(0)}+\Delta E^{(1)}+\Delta E^{(2)}+\ldots\\&=E^{(0)}+\lambda g^{(1)}+\lambda^2 g^{(2)}+\ldots.\end{aligned} \tag{7}$$

The first-order contribution, which is conveniently expressed via the g factor,

$$E^{(1)}=\lambda g^{(1)}\left(M_J\right)=\mu_B B g M_J, \tag{8}$$

and the second-order term can also be written in terms of a dimensionless quantity — the g^2 coefficient,

$$E^{(2)}=\lambda^2 g^{(2)}\left(M_J\right)=(\mu_B B)^2 g^{(2)}(M_J). \tag{9}$$

These calculations are carried out here for the 1s state using the previously developed numerical approach (Varentsova et al. 2018). We then turn to the ground state of He-like ions, evaluating the contribution from electron-electron interaction. In this case, the linear Zeeman effect vanishes, and the second-order coefficient is expressed as

$$g^{(2)}\left[\left(1s\right)^2\right]=g_0^{(2)}\left[\left(1s\right)^2\right]+\Delta g_{1ph}^{(2)}\left[\left(1s\right)^2\right], \tag{10}$$

where $g_0^{(2)}[(1s)^2] = 2g^{(2)}[1s]$ corresponds to the non-interacting electron case and follows from the second-order perturbation theory expression:

$$g^{(2)}\left(1s\right)=\Sigma_n'\frac{\langle a|U|n\rangle\langle n|U|a\rangle}{\varepsilon_a-\varepsilon_n}, \tag{11}$$

where $|a\rangle$ denotes the one-electron [1s] state, and the summation extends over the complete Dirac spectrum of states $|n\rangle$, excluding the reference state $|a\rangle = |1s\rangle$. The resulting coefficient $g^{(2)}$ is an even function of the angular momentum projection: $g^{(2)}(M_J) = g^{(2)}(-M_J)$.

The one-photon exchange correction to the $g^{(2)}$ coefficient is obtained from the set of diagrams displayed in Fig. 1. To evaluate this correction, we employ formal expressions derived within a rigorous QED framework. Up to symmetry coefficients, these expressions coincide with those in Ref. (Moskovkin et al. 2008a) after replacing the hyperfine interaction potential with the magnetic-field interaction potential appropriate for the quadratic Zeeman effect.

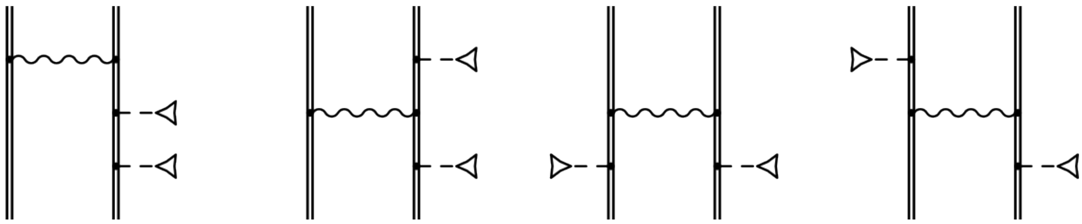

Fig. 1. Illustration of the one-photon exchange correction to the $g^{(2)}$ coefficient. In the diagram, the double line represents the electron propagator in the field of the nucleus $V_{nuc}(r)$, the wavy line corresponds to the photon propagator, and the dashed line terminating in a triangle denotes the interaction with the magnetic field as given in Eq. (6)

Zeeman splitting of the hyperfine structure levels

A rigorous treatment of the hyperfine interaction necessitates incorporating nuclear variables into the Hamiltonian. Nevertheless, after constructing the proper states of the system with a definite total angular momentum **F** = **J** + **I**, the hyperfine interaction can be represented by an effective term within the Dirac Hamiltonian for the bound electron:

$$V_{hfs} = \mu W, \qquad \mu = \frac{\alpha}{2}\frac{m_e}{m_p} g_I I, \qquad W = \frac{[\boldsymbol{r}\times\boldsymbol{\alpha}]_z}{r^3}, \tag{12}$$

where I denotes the nuclear spin and g_I is the nuclear g factor. Note that μ represents a dimensionless parameter proportional (though not equal) to the nuclear magnetic moment.

Zeeman splitting of the hyperfine levels is then described by V_m in Eq. (6). The total perturbation potential in the Dirac equation is $V_m + V_{hfs}$. Within perturbation theory, the zeroth-order Hamiltonian remains that of Eq. (4), whereas the perturbation comprises two distinct contributions, V_m and V_{hfs}. These are governed by two independent parameters, λ and μ, which 'tune' the magnetic and hyperfine interactions, respectively.

In the present work, we consider the weak-magnetic-field regime, where the Zeeman splitting is significantly smaller than the hyperfine splitting. In this limit, the linear Zeeman shift is characterized by the g factor of the electron-nucleus system, which takes the form (Moskovkin et al. 2004; Yerokhin et al. 2012):

$$g_F = g_J \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)} - (1-\sigma)\frac{m_e}{m_p} g_I \frac{F(F+1) + I(I+1) - J(J+1)}{2F(F+1)}, \tag{13}$$

where g_J is the electronic g factor, while m_e and m_p denote the electron and proton masses, respectively. The nuclear magnetic shielding constant σ arises from the mixed second-order contribution involving the perturbations V_m and V_{hfs}. We compute σ for the 1s state using perturbation theory, following the previous work of our group (Volchkova et al. 2017). In the one-electron approximation, it is conveniently characterized by the relativistic factor $A(\alpha Z)$ (Shabaev 1994; Volotka et al. 2008), which can be expressed as:

$$A = \frac{3}{8(\alpha Z)^3 M_J}\langle a|W|a\rangle . \tag{14}$$

The expression for σ in the ground state of He-like ions is written as:

$$\sigma\left[(1s)^2\right]=\sigma_0\left[(1s)^2\right]+\Delta\sigma_{1ph}\left[(1s)^2\right], \tag{15}$$

where $\sigma_0[(1s)^2] = 2\sigma[1s]$ is obtained from the second-order perturbation theory term:

$$\sigma_0[1s]=\Sigma'_n\frac{\langle a|U|n\rangle\langle n|W|a\rangle}{\varepsilon_a-\varepsilon_n}\quad , \tag{16}$$

where the summation extends over the complete spectrum of states $|n\rangle$, omitting the reference state $|a\rangle = |1s\rangle$, as in Eq. (11). Note that the first term in Eq. (13) vanishes because $J = 0$ in this case.

The diagrams illustrating the one-photon-exchange corrections to the nuclear magnetic shielding are shown in Fig. 2. Their explicit form can be found in Ref. (Moskovkin et al. 2008a).

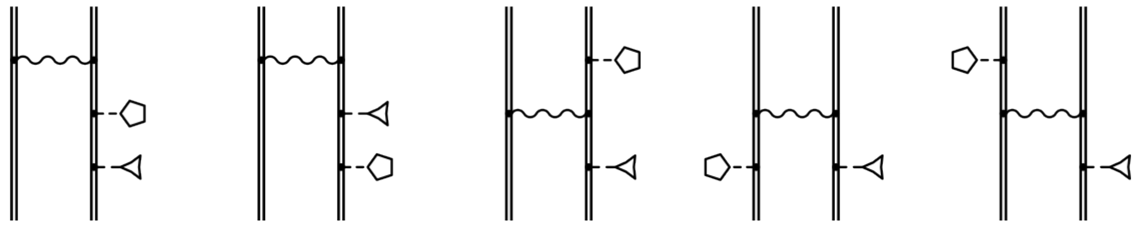

Fig. 2. Illustration of the one-photon-exchange correction to the nuclear magnetic shielding. Here, the hyperfine interaction potential (Eq. (12)) is represented by a dashed line terminating in a pentagon. The remaining notation is the same as in Fig. 1

Discussion

In this section, we present the results of our calculations for nuclear charge Z varying from 6 to 32. All the calculations were performed using B-splines obtained by the dual-kinetic-balance method (Shabaev et al. 2004). All calculations were performed for an extended nucleus, employing the homogeneously charged sphere model for the nuclear charge distribution.

Table 1 presents the values of the coefficient $g^{(2)}$, its one-photon-exchange correction, and their sum for the ground $(1s)^2$ state of helium-like ions. For convenience, g factor values for hydrogen-like ions are also listed. As expected from Eq. (11), $g^{(2)}$ scales as $(\alpha Z)^{-2}$ with increasing Z. It is important to note that the contribution of the negative-energy spectrum to this coefficient is dominant. The one-photon-exchange correction behaves as$1/Z$ as expected. Moreover, its relative magnitude is smaller than in the case of p states, where the coefficient is mainly determined by a single contribution whose energy denominator depends strongly on the interelectronic interaction.

Table 1. The g factor for the $1s$ state and the second-order Zeeman effect for the ground $(1s)^2$ state of helium-like ions are expressed in terms of $g^{(2)}$ coefficient, comprising the leading-order term $g_0^{(2)}$, the one-photon-exchange correction $\Delta g_{1ph}^{(2)}$, and their sum $g^{(2)}$

Z	$g[1s]$	$g_0^{(2)}[(1s)^2]$	$\Delta g_{1ph}^{(2)}[(1s)^2]$	$g^{(2)}[(1s)^2]$
6	1.998721	1040.605	138.744	1179.349
10	1.996445	372.913	30.038	402.951
12	1.994878	258.154	17.410	275.564
14	1.993024	188.959	10.984	199.943
16	1.990881	144.049	7.374	151.423
18	1.988448	113.259	5.191	118.450
20	1.985723	91.236	3.794	95.030
26	1.975782	52.906	1.767	54.673
32	1.963138	34.032	0.945	34.977

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Table 2 presents data on the hyperfine magnetic shielding for the ground $(1s)^2$ state of helium-like ions, defined by the coefficient σ, as well as the one-photon-exchange correction to it and the sum of these contributions. The values of the coefficient $A(\alpha Z)$ for the hydrogen-like ion are given for comparison. As expected from (16), the coefficient σ scales linearly with Z. The one-photon-exchange correction behaves as $1/Z$ relative to σ, meaning that its absolute value does not vary significantly with Z.

Table 2. The factor $A(\alpha Z)$ for the $1s$ state and the nuclear magnetic shielding constant σ for the ground $(1s)^2$ state of helium-like ions. Presented here are the leading-order term $\sigma_0[(1s)^2]$, the one-photon-exchange correction $\Delta\sigma_{1ph}[(1s)^2]$, and their sum $\sigma[(1s)^2]$. The $1s$ results from Ref. (Moskovkin, Oreshkina, Shabaev et al. 2004) are shown for comparison ($\sigma_0[(1s)^2] = 2\sigma[1s]$). The values of σ are given in 10^{-3} units

Z	$A(\alpha Z)$	$\sigma_0[(1s)^2] \times 10^3$	$\Delta\sigma_{1ph}[(1s)^2] \times 10^3$	$\sigma[(1s)^2] \times 10^3$
6	1.002332	0.214108	–0.011041	0.203067
		0.214109[b]		
10	1.006906	0.360134	–0.010944	0.349190
	1.006911[a]	0.360135[b]		
12	1.010201	0.434893	–0.010875	0.424018
	1.010204[a]			
14	1.014136	0.511171	–0.010792	0.500379
	1.014133[a]			
16	1.018689	0.589235	–0.010693	0.578542

Note: [a]From Ref. (Volotka et al. 2008), [b]from Ref. (Moskovkin et al. 2004).

For comparison, we also present the values of the hyperfine-splitting factor A obtained in this work using perturbation theory, alongside those from Ref. (Volotka et al. 2008), as well as the values of $\sigma[1s]$ from Ref. (Moskovkin et al. 2004). One can see that these coefficients are in good agreement. The remaining discrepancies can be attributed to the fact that the coefficients in Refs. (Moskovkin et al. 2004; Volotka et al. 2008) were calculated for a pure Coulomb potential, whereas our values were computed for a finite nucleus.

It should be noted that our calculations account for the finite nuclear size (employing the finite-size nuclear potential V_{nucl}), but neglect the effect of the finite nuclear magnetic moment distribution (the Bohr–Weisskopf effect). Consequently, the quantity we report is actually $A(\alpha Z)(1 - \delta)$, where δ represents the nuclear size correction (Shabaev 1994; Volotka et al. 2008).

Conclusion

This work reports on the calculation of the quadratic Zeeman effect and hyperfine magnetic shielding in helium-like ions using perturbation theory. We have obtained numerical values for the ground $(1s)^2$ state in the nuclear charge range $Z = 6 - 32$. The DKB method to solve the Dirac equation in the Coulomb field with an extended nucleus has been applied to evaluate the Zeeman splitting in helium-like ions. We provide the leading-order contributions as well as the one-photon-exchange corrections, the latter being derived within a rigorous QED approach. The results for the nuclear magnetic shielding constant can be used to determine the nuclear magnetic moments. The quadratic Zeeman effect can be relevant for high-precision Penning-trap measurements of the transition energies in He-like ions. To provide complete theoretical background, corresponding calculations for excited states are needed, which is the subject of our future investigations.

Conflict of Interest

The authors declare that there is no conflict of interest, either existing or potential.

Author Contributions

All authors made an equivalent contribution to the preparation of the publication.

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