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# Magnetizabilities of relativistic hydrogenlike atoms in some arbitrary discrete energy eigenstates

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## ARTICLE INFO

*Article history:*

Received 10 September 2015

Received in revised form

19 September 2015

Accepted 19 September 2015

Available online xxxx

*Keywords:*

Hydrogenlike atom

Magnetizability

Electromagnetic moments

Dipole moment

Magnetic field

Green function

## ABSTRACT

We present the results of numerical calculations of magnetizability ( $\chi$ ) of the relativistic one-electron atoms with a pointlike, spinless and motionless nuclei of charge  $Ze$ . Exploiting the analytical formula for  $\chi$  recently derived by us Stefańska (2015), valid for an arbitrary discrete energy eigenstate, we have found the values of the magnetizability for the ground state and for the first and the second set of excited states (i.e.:  $2s_{1/2}$ ,  $2p_{1/2}$ ,  $2p_{3/2}$ ,  $3s_{1/2}$ ,  $3p_{1/2}$ ,  $3p_{3/2}$ ,  $3d_{3/2}$ , and  $3d_{5/2}$ ) of the Dirac one-electron atom. The results for ions with the atomic number  $1 \leq Z \leq 137$  are given in 14 tables. The comparison of the numerical values of magnetizabilities for the ground state and for each state belonging to the first set of excited states of selected hydrogenlike ions, obtained with the use of two different values of the fine-structure constant, i.e.:  $\alpha^{-1} = 137.035999139$  (CODATA 2014) and  $\alpha^{-1} = 137.035999074$  (CODATA 2010), is also presented.

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1. Introduction

Interaction of atoms and molecules with electromagnetic field is undoubtedly one of the most commonly reported physical processes, both theoretically and experimentally. For the simplest systems, like one-electron atoms, there are some analytical methods of calculating many atomic parameters, such as the polarizability or the magnetizability. One of such useful tools is the Sturmian expansion of the first-order generalized Dirac–Coulomb Green function [1], proposed by Szymtkowski in 1997. In the series of papers [2–9] published by his group over the period of past several years, it has been used in perturbation-theory calculations of some electromagnetic properties of the relativistic hydrogenlike atoms in the ground state, with a pointlike, spinless and motionless nuclei of charge  $Z$ .

Recently, we have shown that the usefulness of this method goes beyond the study of the atomic ground state. In Ref. [10] we derived analytically an expression for the magnetizability of the Dirac one-electron atom (with regard to its nucleus we impose the same assumptions as above) in an arbitrary discrete energy eigenstate, characterized by the set of quantum numbers  $\{n, \kappa, \mu\}$ , in which  $n$  denotes the radial quantum number, the Dirac quantum number  $\kappa$  is an integer different from zero, whereas  $\mu = -|\kappa| + \frac{1}{2}, -|\kappa| + \frac{3}{2}, \dots, |\kappa| - \frac{1}{2}$  is the magnetic quantum number. The final result has the following form

$$\begin{aligned}
 \chi &\equiv \chi_{n\kappa\mu} \\
 &= \frac{\alpha^2 a_0^3}{Z^2} \frac{1}{128(4\kappa^2 - 1)^2 N_{n\kappa}} \left\{ \Theta_{n\kappa\mu}^{(I)} + \sum_{\kappa'} \frac{\eta_{\kappa\mu}^{(+)} \delta_{\kappa', -\kappa+1} + \eta_{\kappa\mu}^{(-)} \delta_{\kappa', -\kappa-1}}{N_{n\kappa} + \kappa'} \right. \\
 &\times \left[ \Theta_{n\kappa}^{(II)} + \frac{n!(n^2 + 2n\gamma_\kappa + \kappa^2) \Gamma(n + 2\gamma_\kappa + 1)}{(N_{n\kappa} - \kappa)(\gamma_{\kappa'} - \gamma_\kappa - n + 1) \Gamma(2\gamma_{\kappa'} + 1)} \right. \\
 &\times \sum_{k=0}^n \sum_{p=0}^n \tilde{Z}_{\kappa\kappa'}^n(k) \tilde{Z}_{\kappa\kappa'}^n(p) \\
 &\left. \left. \times {}_3F_2 \left( \begin{matrix} \gamma_{\kappa'} - \gamma_\kappa - k - 1, \gamma_{\kappa'} - \gamma_\kappa - p - 1, \gamma_{\kappa'} - \gamma_\kappa - n + 1 \\ \gamma_{\kappa'} - \gamma_\kappa - n + 2, 2\gamma_{\kappa'} + 1 \end{matrix} ; 1 \right) \right] \right\}, \quad (1)
 \end{aligned}$$

where  $\alpha$  is the Sommerfeld’s fine structure constant,  $\Gamma(\zeta)$  denotes the Euler’s gamma function,  ${}_3F_2$  is the generalized hypergeometric function, while

$$\eta_{\kappa\mu}^{(\pm)} = (4\kappa^2 - 1)^2 - 4\mu^2(2\kappa \pm 1)^2, \quad (2)$$

$$\begin{aligned}
 \Theta_{n\kappa\mu}^{(I)} &= -256\kappa^2 \mu^2 \left[ 2\kappa^2(n + \gamma_\kappa)^3 + (n + \gamma_\kappa)(5n^2 + 10n\gamma_\kappa \right. \\
 &\quad \left. + 2\gamma_\kappa^2 - 2\kappa^2 + 1)N_{n\kappa}^2 \right. \\
 &\quad \left. - \kappa(3n^2 + 6n\gamma_\kappa + 4\gamma_\kappa^2 - \kappa^2)N_{n\kappa} \right], \quad (3)
 \end{aligned}$$

$$\begin{aligned}
 \Theta_{n\kappa}^{(II)} &= 2(2n + 2\gamma_\kappa + 1)(\kappa - N_{n\kappa})N_{n\kappa}^2 \\
 &\quad \times [5(n + \gamma_\kappa)(n + \gamma_\kappa + 1) - 3(\gamma_\kappa^2 - 1)], \quad (4)
 \end{aligned}$$

$$\begin{aligned}
 \tilde{Z}_{\kappa\kappa'}^n(k) &= \frac{(-)^k [2(N_{n\kappa} - \kappa) + (n - k)(\kappa + \kappa')]}{k!(n - k)!} \\
 &\quad \times \frac{\Gamma(\gamma_\kappa + \gamma_{\kappa'} + k + 2)}{\Gamma(k + 2\gamma_\kappa + 1)} \quad (5)
 \end{aligned}$$

and analogously for  $\tilde{Z}_{\kappa\kappa'}^n(p)$ , with

$$N_{n\kappa} = \sqrt{n^2 + 2n\gamma_\kappa + \kappa^2}, \quad (6)$$

and

$$\gamma_\kappa = \sqrt{\kappa^2 - (\alpha Z)^2}. \quad (7)$$

The above result has been exhaustively verified by us, both analytically and numerically. In Ref. [10] we have shown that it remains valid for an arbitrary discrete energy eigenstate. However, the aforementioned article contains only two representational tables with values of the relativistic magnetizabilities for some excited states of selected hydrogenlike ions. In this work, we present a more comprehensive numerical data in the form of 14 tables comprising the results for the atomic ground state  $1s_{1/2}$  and for each state belonging to the first and second set of excited states, i.e.:  $2s_{1/2}, 2p_{1/2}, 2p_{3/2}, 3s_{1/2}, 3p_{1/2}, 3p_{3/2}, 3d_{3/2}$  and  $3d_{5/2}$ , having regarded all possible values of the magnetic quantum number.

Present calculations have been performed with the current value 137.035 999 139 of the inverse of the fine-structure constant recommended by the Committee on Data for Science and Technology (CODATA) [11], in contrast to those described in Ref. [10], in which we have used  $\alpha^{-1} = 137.035 98 95$  (CODATA 1986), to be able to compare our results with the previous results of other authors [12]. To show how the change in the value of the fine structure constant affects the value of the magnetizability, additionally, we performed calculations for  $\chi$  with  $\alpha^{-1} = 137.035 999 074$ , recommended by CODATA 2010 (i.e. immediately before the currently valid value of this constant) and compared them with the corresponding values from Tables 1–5. The appropriate juxtaposition of numerical values of  $\chi$  for the ground state and the first excited states of selected hydrogenlike ions is shown in Table 15. (See Tables 6–14.)

Acknowledgment

I wish to thank Professor R. Szymtkowski for many stimulating discussions, especially for every advice he gave me during the preparation of this work.

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