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Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt

Magnetic-dipole-to-electric-quadrupole cross-susceptibilities for relativistic hydrogenlike atoms in some low-lying discrete energy eigenstates

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ARTICLE INFO

Article history:
Received 29 March 2016
Received in revised form
18 April 2016
Accepted 18 April 2016
Available online xxxx

Keywords:
Hydrogenlike atom
Electromagnetic moments
Quadrupole moment
Magnetic field

ABSTRACT

In this paper we present tabulated data for magnetic-dipole-to-electric-quadrupole cross-susceptibilities ($\chi_{M1\to E2}$) for Dirac one-electron atoms with a pointlike, spinless and motionless nucleus of charge Ze. Numerical values of this susceptibility for the hydrogen atom ($Z = 1$) and for hydrogenic ions with $2 \leqslant Z \leqslant 137$ are computed from the general analytical formula, recently derived by us (Stefanska, 2016), valid for an arbitrary discrete energy eigenstate. In this work we provide 30 tables with the values of $\chi_{M1\to E2}$ for the ground state, and also for the first, the second and the third set of excited states (i.e.: $2s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$, $3s_{1/2}$, $3p_{1/2}$, $3p_{3/2}$, $3d_{3/2}$, $3d_{5/2}$, $4s_{1/2}$, $4p_{1/2}$, $4p_{3/2}$, $4d_{3/2}$, $4d_{5/2}$, $4f_{5/2}$ and $4f_{7/2}$) of the relativistic hydrogenlike atoms. The value of the inverse of the fine-structure constant used in the calculations is $\alpha^{-1} = 137.035999139$, and was taken from CODATA 2014.

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http://dx.doi.org/10.1016/j.adt.2016.04.004
0092-640X/

Contents

1. Introduction

Theoretical investigation of atomic and molecular electromagnetic susceptibilities has been very commonly reported from early decades of the last century [1]. Most often, numerical computation of such quantities for many-electron atoms and molecules, as well as analytical calculations for simple systems, can be compared with experimental data, and sometimes they appear to be very helpful in the design of other experiments or improving those already used. Thus, in this work we provide theoretical study of the magnetic-dipole-to-electric-quadrupole cross-susceptibility for hydrogenlike atoms with a pointlike, spinless and infinitely heavy nucleus of charge Ze.

The phenomenon of inducing electric quadrupole moment $\mathcal{Q}$ in such systems by a perturbing uniform (dipole) magnetic field of a strength B was pointed out already in the mid-1950s by Coulson and Stephen [2]. Analytical derivation of the expression for this moment was reported also later by Potekhin and Turbiner [3,4]. However, in all these articles, calculations have been performed within the framework of the *nonrelativistic* quantum mechanics. First fully *relativistic* determination of that quantity has been carried out by us in 2012 [5]. Using the perturbation theory combined with the technique based on the Sturmian expansion of the generalized Dirac–Coulomb Green function [6], we have successfully derived the analytical expression for $\mathcal{Q}^{(1)}(B)$ (the first-order correction to the electric quadrupole moment as a function of the field strength B) induced in the *ground* state of Dirac one-electron atom (for other applications of this powerful technique to dipole electromagnetic properties of such system, see Refs. [7–13]).

Very recently, Szmytkowski and Łukasik considered analytically [14] and numerically [15] some families of *multipole* electric and magnetic susceptibilities for the ground state of relativistic hydrogenlike atoms. In particular, they pointed out that 2^λ-pole electric moments induced in the system by static 2^L-pole magnetic field are closely related to 2^L-pole magnetic moments induced in the atom by static 2^λ-pole electric field. To be precise, they indicated that the values of the magnetic-to-electric ($\chi_{\mathrm{ML}\to\mathrm{E}\lambda}$) and electric-to-magnetic ($\alpha_{\mathrm{E}\lambda\to\mathrm{ML}}$) cross-susceptibilities are *equal* for ions with the charge numbers from the whole range $1 \leqslant Z \leqslant 137$. This suggests that theoretical knowledge of such kind of quantities – in particular, the $\chi_{\mathrm{M1}\to\mathrm{E2}}$ susceptibility – may be doubly useful for experimentalists: those who would like to measure one of these atomic parameters but are unable to do that, may try to conduct another experiment which allows to determine the second of them.

Some time ago, we have discussed the aforementioned physical quantity in terms of another generalization. In [16] we derived analytically the expression for the magnetic-dipole-to-electric-quadrupole cross-susceptibility ($\chi_{\mathrm{M1}\to\mathrm{E2}}$) for the atom being in an *arbitrary* discrete energy eigenstate, characterized by the set of quantum numbers $\{n_r, \kappa, \mu\}$, in which n_r denotes the radial quantum number, the Dirac quantum number κ is an integer different form zero, whereas $\mu = -|\kappa| + \frac{1}{2}, -|\kappa| + \frac{3}{2}, \ldots, |\kappa| - \frac{1}{2}$ is the magnetic quantum number. The calculations for such general case were based on the Sturmian expansion of the generalized Dirac–Coulomb Green function [6] (for other applications of this method to another magnetic dipole properties of excited atomic states, see Refs. [17,18]). In view of the definition below:

$$\mathcal{Q}^{(1)} = \mathrm{sgn}(\mu)(4\pi\epsilon_0)c\,\chi_{\mathrm{M1}\to\mathrm{E2}}B, \tag{1}$$

where c is the speed of light, while $\mathcal{Q}^{(1)} \equiv \mathcal{Q}^{(1)}_{20}$ is the only one of the spherical components $\mathcal{Q}^{(1)}_{2M}$ $(M = 0, \pm1, \pm2)$ of the quadrupole electric moment tensor which can be induced in the atom by the perturbing magnetic field $\boldsymbol{B} = B\boldsymbol{n}_z$ (for details, see Ref. [16]), the formula for the atomic parameter under study can be written as follows: (see Box I).

Here α is the Sommerfeld's fine structure constant, a_0 denotes, as usually, the Bohr radius, $\Gamma(\zeta)$ is the Euler's gamma function and ${}_3F_2$ is the generalized hypergeometric function, while

$$\eta^{(\pm)}_{\kappa\mu} = \frac{2\kappa \pm 1}{2\kappa \mp 3}\left[(2\kappa \mp 1)^2 - 4\mu^2\right], \tag{3}$$

$$\begin{aligned}\Theta^{(\mathrm{I})}_{n_r\kappa\mu} &= 32\,(\alpha Z)^2\,\kappa^2(4\kappa^2 - 12\mu^2 - 1)\\ &\times \left\{(5n_r^2 + 10n_r\gamma_\kappa + 4\gamma_\kappa^2 + 1)N^2_{n_r\kappa} - \kappa(n_r + \gamma_\kappa)\right.\\ &\times \left.\left[2\kappa(n_r + \gamma_\kappa) + 3N_{n_r\kappa}\right]\right\},\end{aligned} \tag{4}$$

$$\begin{aligned}\Theta^{(\mathrm{II})}_{n_r\kappa} &= 6(N_{n_r\kappa} - \kappa)N^2_{n_r\kappa}\left\{4\kappa(n_r + \gamma_\kappa)^2\right.\\ &\times \left[7(n_r + \gamma_\kappa)^2 - 3\gamma_\kappa^2 + 5\right]\\ &+ N_{n_r\kappa}\left[63(n_r + \gamma_\kappa)^4 + 70(n_r + \gamma_\kappa)^3\right.\\ &- 21(2\gamma_\kappa^2 - 5)(n_r + \gamma_\kappa)^2 - 10(3\gamma_\kappa^2 - 5)(n_r + \gamma_\kappa)\\ &+ \left.\left.3(\gamma_\kappa^2 - 1)(\gamma_\kappa^2 - 4)\right]\right\},\end{aligned} \tag{5}$$

$$\begin{aligned}\mathcal{X}(k) &= \frac{(-)^k}{k!(n_r - k)!}\,\frac{\Gamma(\gamma_\kappa + \gamma_{\kappa'} + k + 3)}{\Gamma(k + 2\gamma_\kappa + 1)}\\ &\times \left[C^{(1)}_k(N_{n_r\kappa} + \kappa') - C^{(2)}_k(n_r - k - 3)\right],\end{aligned} \tag{6}$$

$$\begin{aligned}\mathcal{Y}(p) &= \frac{(-)^p}{p!(n_r - p)!}\,\frac{\Gamma(\gamma_\kappa + \gamma_{\kappa'} + p + 2)}{\Gamma(p + 2\gamma_\kappa + 1)}\\ &\times \left[(n_r - p)(\kappa + \kappa') + 2(N_{n_r\kappa} - \kappa)\right],\end{aligned} \tag{7}$$

with

$$\begin{aligned}C^{(1)}_k &= (n_r - k) + \frac{n_r + \gamma_\kappa}{N_{n_r\kappa}}\left(\kappa - N_{n_r\kappa}\right),\\ C^{(2)}_k &= \frac{n_r + \gamma_\kappa}{N_{n_r\kappa}}(n_r - k) + \left(\kappa - N_{n_r\kappa}\right),\end{aligned} \tag{8}$$

$$N_{n_r\kappa} = \sqrt{n_r^2 + 2n_r\gamma_\kappa + \kappa^2} \tag{9}$$

and

$$\gamma_\kappa = \sqrt{\kappa^2 - (\alpha Z)^2}. \tag{10}$$

In Ref. [16] we have shown that the expression from Eq. (2) remains valid for an *arbitrary* discrete energy eigenstate of the atom. Nevertheless, we realize that its quite complexity form might be perceived by someone as inconvenient for calculations. Such our thoughts, as well as the lack of any tabulated data in the aforementioned article, were the main reasons for which we decided to perform numerical calculations of that quantity. In the next section we will discuss briefly our results.

Please cite this article in press as: P. Stefańska, Magnetic-dipole-to-electric-quadrupole cross-susceptibilities for relativistic hydrogenlike atoms in some low-lying discrete energy eigenstates, Atomic Data and Nuclear Data Tables (2016), http://dx.doi.org/10.1016/j.adt.2016.04.004