Available online at www.sciencedirect.com

SCIENCE DIRECT

Chemical Physics Letters 419 (2006) 537–539

CHEMICAL PHYSICS LETTERS

www.elsevier.com/locate/cplett

Relationship between the static dipole polarizability and the static dipole magnetizability of the relativistic hydrogen-like atom

Radosław Szmytkowski *

Atomic Physics Division, Department of Atomic Physics and Luminescence, Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Narutowicza 11/12, PL 80-952 Gdańsk, Poland

Received 21 October 2005; in final form 3 December 2005
Available online 4 January 2006

Abstract

We show that the ground-state static dipole polarizability $\alpha_{\mathrm{d}}(Z)$ and the ground-state static dipole magnetizability $\chi_{\mathrm{d}}(Z)$ of the relativistic hydrogen-like atom, with a spinless and point-like nucleus of charge $+Ze$, are related through the formula

$$\alpha_{\mathrm{d}}(Z) = -3(\gamma_1 - 2)^2(\alpha Z)^{-2}\chi_{\mathrm{d}}(Z) - a_0^3 Z^{-4}(\gamma_1 + 1)(2\gamma_1 + 1)(14\gamma_1^3 - 63\gamma_1^2 + 55\gamma_1 - 24)/36,$$

where α and a_0 are, respectively, the Sommerfeld fine-structure constant and the Bohr radius, while $\gamma_1 = \sqrt{1 - (\alpha Z)^2}$.

The ground-state static dipole polarizability α_{d} and the ground-state static dipole magnetizability χ_{d} are among the most important electromagnetic properties of atoms and molecules [1]. Calculations of these quantities for the simplest atomic system – the hydrogen-like atom – were done, with a neglect of relativistic effects, already in the earliest days of quantum mechanics (cf. Ref. [2] and references therein). Counterpart calculations for a Dirac one-electron atom, with a spinless and point-like nucleus of charge $+Ze$, have been carried out since the mid 1970s, and are still being pursued (for a comprehensive up-to-date bibliography of the subject, see Refs. [3–5]). They resulted in a variety of expressions, usually differing one from each other, but possessing a common feature of being much more complicated functions of the nuclear charge Z than their nonrelativistic counterparts.

One of the simplest expressions found so far for the static dipole polarizability of the relativistic hydrogen-like atom is [5]

$$\alpha_{\mathrm{d}}(Z) = a_0^3 Z^{-4}\left[-\frac{(\gamma_1+1)(2\gamma_1+1)(32\gamma_1^5 - 80\gamma_1^4 - 408\gamma_1^3 - 376\gamma_1^2 + 163\gamma_1 + 324)}{36(4\gamma_1+1)^2} + \frac{(\gamma_1-2)^2\Gamma^2(\gamma_1+\gamma_2+2)}{6(\gamma_2-\gamma_1)(\gamma_2-\gamma_1-2)^2\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)}\,{}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-2,\gamma_2-\gamma_1-2,\gamma_2-\gamma_1\\ \gamma_2-\gamma_1+1,2\gamma_2+1\end{matrix};1\right)\right], \tag{1}$$

while the simplest among the known formulas for the static dipole magnetizability of such an atom is [4,6,7]

* Fax: +004858347 2821.
E-mail address: radek@mif.pg.gda.pl.

0009-2614/$ - see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.cplett.2005.12.031

$$\chi_{\mathrm{d}}(Z)=\alpha^2 a_0^3 Z^{-2}\Bigg[-\frac{(\gamma_1+1)(4\gamma_1^2-1)}{18} -\frac{\Gamma^2(\gamma_1+\gamma_2+2)}{72(\gamma_2-\gamma_1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \times {}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-1,\gamma_2-\gamma_1-1,\gamma_2-\gamma_1\\ \gamma_2-\gamma_1+1,2\gamma_2+1\end{matrix};1\right)\Bigg]. \tag{2}$$

In Eqs. (1) and (2), and hereafter,

$$a_0=(4\pi\epsilon_0)\frac{\hbar^2}{me^2} \tag{3}$$

is the Bohr radius,

$$\alpha=(4\pi\epsilon_0)^{-1}\frac{e^2}{c\hbar} \tag{4}$$

is the Sommerfeld fine-structure constant,

$$\gamma_\kappa=\sqrt{\kappa^2-(\alpha Z)^2}, \tag{5}$$

while ${}_3F_2$ is the special case of the generalized hypergeometric series

$${}_pF_q\left(\begin{matrix}a_1,\ldots,a_p\\ b_1,\ldots,b_q\end{matrix};z\right) =\frac{\Gamma(b_1)\cdots\Gamma(b_q)}{\Gamma(a_1)\cdots\Gamma(a_p)}\sum_{n=0}^{\infty}\frac{\Gamma(a_1+n)\cdots\Gamma(a_p+n)}{\Gamma(b_1+n)\cdots\Gamma(b_q+n)}\frac{z^n}{n!}. \tag{6}$$

Taking a glance at Eqs. (1) and (2), one realizes that although the expressions displayed therein contain different ${}_3F_2$ functions, nevertheless these ${}_3F_2$ functions are structurally similar one to each other, as do Eqs. (1) and (2) as wholes. These similarities motivate one to pose the following question: is it possible to transform one of these equations so that it contains the same ${}_3F_2$ function (and no other nontrivial ${}_pF_q$ function) as the other? Apart from fulfilling aesthetic needs for a maximal symmetry between the expressions for $\alpha_{\mathrm{d}}(Z)$ and $\chi_{\mathrm{d}}(Z)$, achieving such a goal would have also some practical consequences, implying the existence of a particular relationship between the two susceptibilities of the form

$$\alpha_{\mathrm{d}}(Z)=f(Z)\chi_{\mathrm{d}}(Z)+g(Z), \tag{7}$$

with the functions $f(Z)$ and $g(Z)$ being expressible in terms of some elementary functions of Z and, possibly, the Euler gamma function. It is the purpose of this note to show that the answer to the above posed question is affirmative, that the consequent expression for $\alpha_{\mathrm{d}}(Z)$ in terms of ${}_3F_2(\gamma_2-\gamma_1-1;\ \gamma_2-\gamma_1-1,\ \gamma_2-\gamma_1;\ \gamma_2-\gamma_1+1,\ 2\gamma_2+1;1)$ is much simpler than the one in Eq. (1), and that the coefficients $f(Z)$ and $g(Z)$ in the resulting relationship of the form (7) are even simpler than expected, containing only elementary functions of Z.

Consider at first the generalized hypergeometric function ${}_3F_2(a_1+1,a_2,a_3;a_3+1,b;z)$. From the definition (6), from the obvious relationship

$$\Gamma(a_1+1+n)\Gamma(a_3+n) =\Gamma(a_1+n)\Gamma(a_3+1+n)+(a_1-a_3)\Gamma(a_1+n)\Gamma(a_3+n), \tag{8}$$

and from the property

$${}_3F_2\left(\begin{matrix}a_1,a_2,a_3\\ a_3,b\end{matrix};z\right)={}_2F_1\left(\begin{matrix}a_1,a_2\\ b\end{matrix};z\right), \tag{9}$$

one finds that the following recurrence relation holds:

$${}_3F_2\left(\begin{matrix}a_1+1,a_2,a_3\\ a_3+1,b\end{matrix};z\right)=\frac{a_3}{a_1}{}_2F_1\left(\begin{matrix}a_1,a_2\\ b\end{matrix};z\right) +\frac{a_1-a_3}{a_1}{}_3F_2\left(\begin{matrix}a_1,a_2,a_3\\ a_3+1,b\end{matrix};z\right) \times(a_1\neq 0). \tag{10}$$

Replacing in Eq. (10) a_2 by a_2+1 and transforming the right-hand side of the resulting equation again with the aid of Eq. (10), but this time with a_1 interchanged with a_2, leads to

$${}_3F_2\left(\begin{matrix}a_1+1,a_2+1,a_3\\ a_3+1,b\end{matrix};z\right) =\frac{a_3(a_1-a_3)}{a_1a_2}{}_2F_1\left(\begin{matrix}a_1,a_2\\ b\end{matrix};z\right)+\frac{a_3}{a_1}{}_2F_1\left(\begin{matrix}a_1,a_2+1\\ b\end{matrix};z\right) +\frac{(a_1-a_3)(a_2-a_3)}{a_1a_2}{}_3F_2\left(\begin{matrix}a_1,a_2,a_3\\ a_3+1,b\end{matrix};z\right) \times(a_1\neq 0,a_2\neq 0). \tag{11}$$

Hence, it follows that

$${}_3F_2\left(\begin{matrix}a_1,a_2,a_3\\ a_3+1,b\end{matrix};z\right) =-\frac{a_3}{a_2-a_3}{}_2F_1\left(\begin{matrix}a_1,a_2\\ b\end{matrix};z\right)-\frac{a_2a_3}{(a_1-a_3)(a_2-a_3)} \times{}_2F_1\left(\begin{matrix}a_1,a_2+1\\ b\end{matrix};z\right)+\frac{a_1a_2}{(a_1-a_3)(a_2-a_3)} \times{}_3F_2\left(\begin{matrix}a_1+1,a_2+1,a_3\\ a_3+1,b\end{matrix};z\right)(a_1\neq a_3,a_2\neq a_3). \tag{12}$$

Finally, we particularize to the case $z=1$. Exploiting the Gauss' identity [8]

$${}_2F_1\left(\begin{matrix}a_1,a_2\\ b\end{matrix};1\right)=\frac{\Gamma(b)\Gamma(b-a_1-a_2)}{\Gamma(b-a_1)\Gamma(b-a_2)} \times(\mathrm{Re}(b-a_1-a_2)>0) \tag{13}$$

reduces Eq. (12) to

$${}_3F_2\left(\begin{matrix}a_1,a_2,a_3\\ a_3+1,b\end{matrix};1\right) =-\frac{a_3[a_1a_2+(a_1+a_2-a_3)(b-a_1-a_2-1)]}{(a_1-a_3)(a_2-a_3)} \times\frac{\Gamma(b)\Gamma(b-a_1-a_2-1)}{\Gamma(b-a_1)\Gamma(b-a_2)}+\frac{a_1a_2}{(a_1-a_3)(a_2-a_3)} \times{}_3F_2\left(\begin{matrix}a_1+1,a_2+1,a_3\\ a_3+1,b\end{matrix};1\right) \times(a_1\neq a_3,a_2\neq a_3,\mathrm{Re}(b-a_1-a_2-1)>0). \tag{14}$$

After these preparatory steps, we turn our attention to Eq. (1). Making use, therein, of the recurrence (14), after somewhat tedious manipulations, one derives the following alternative formula for the static dipole polarizability of the Dirac one-electron atom:

$$\alpha_d(Z) = a_0^3 Z^{-4}\left[-\frac{\gamma_1(\gamma_1+1)(2\gamma_1+1)(2\gamma_1^2-9\gamma_1-17)}{36} + \frac{(\gamma_1-2)^2\Gamma^2(\gamma_1+\gamma_2+2)}{24(\gamma_2-\gamma_1)\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)} \times {}_3F_2\left(\begin{matrix}\gamma_2-\gamma_1-1, \gamma_2-\gamma_1-1, \gamma_2-\gamma_1 \\ \gamma_2-\gamma_1+1, 2\gamma_2+1\end{matrix}; 1\right)\right]. \quad (15)$$

Apart from being structurally much simpler than Eq. (1), the expression (15) possesses the advantage that the ${}_3F_2$ function appearing in it is just the same one which enters the formula (2) for the static dipole magnetizability $\chi_d(Z)$. Exploiting this particular feature, we may combine Eqs. (2) and (15), arriving at

$$\alpha_d(Z) = -3(\gamma_1-2)^2(\alpha Z)^{-2}\chi_d(Z) - a_0^3 Z^{-4} \times \frac{(\gamma_1+1)(2\gamma_1+1)(14\gamma_1^3-63\gamma_1^2+55\gamma_1-24)}{36}, \quad (16)$$

which is the sought relationship of the form (7), linking $\alpha_d(Z)$ and $\chi_d(Z)$, with the coefficients being manifestly elementary functions of Z. The relation (16) enables one to calculate straightforwardly one of the susceptibilities when the value of the other is known.

It remains to investigate the nonrelativistic limit of Eq. (16). Denoting respectively by $\overline{\alpha}_d(Z)$ and $\overline{\chi}_d(Z)$ the leading terms in the expansions of $\alpha_d(Z)$ and $\chi_d(Z)$ in terms of powers of α, and exploiting the fact that

$$\gamma_\kappa \overset{c\to\infty}{\longrightarrow} |\kappa|, \quad (17)$$

from Eq. (16) we find

$$\overline{\alpha}_d(Z) = -3(\alpha Z)^{-2}\overline{\chi}_d(Z) + 3a_0^3 Z^{-4}. \quad (18)$$

Eq. (18) is evidently valid since it is well known [2] (cf. also the nonrelativistic limits of Eqs. (1) and (2)) that

$$\overline{\alpha}_d(Z) = \frac{9}{2}a_0^3 Z^{-4} \quad (19)$$

and

$$\overline{\chi}_d(Z) = -\frac{1}{2}\alpha^2 a_0^3 Z^{-2}. \quad (20)$$

References

[1] P. Lazzeretti, in: S. Wilson (Ed.), Handbook of Molecular Physics and Quantum Chemistry, vol. 3, Wiley, Chichester, 2003 (Chapter 3).

[2] J.H. Van Vleck, The Theory of Electric and Magnetic Susceptibilities, Oxford University Press, Oxford, 1932.

[3] R. Szmytkowski, J. Phys. B 30 (1997) 825, 2747.

[4] R. Szmytkowski, J. Phys. B 35 (2002) 1379.

[5] R. Szmytkowski, K. Mielewczyk, J. Phys. B 37 (2004) 3961.

[6] Ya.I. Granovskii, V.I. Nechet, Yad. Fiz. 19 (1974) 1290.

[7] N.L. Manakov, S.A. Zapryagaev, Phys. Lett. A 58 (1976) 23.

[8] I.S. Gradshteyn, I.M. Ryzhik, Table of Integrals, Series, and Products, fifth edn., Academic Press, San Diego, 1994 (Eq. (9.122)).