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TOROID POLARIZABILITY OF HYDROGEN-LIKE ATOMS

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A closed formula is obtained for the frequency-dependent toroid dipole polarizability $\gamma(\omega)$ of a (nonrelativistic, spinless, ground-state) hydrogen-like atom. The static result reads $\gamma(\omega=0)=(23/60)\times \alpha^2 Z^{-4} a_0^5$ (α - fine structure constant, Z - nucleus charge number, a_0 - Bohr radius). This is the toroid analog of the well-known static electric dipole polarizability $\alpha(\omega=0)=(9/2)Z^{-4}a_0^3$.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Тороидная поляризуемость водородоподобных атомов

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Получена замкнутая формула для динамической тороидной дипольной поляризуемости $\gamma(\omega)$ /нерелятивистского, бесспинового/ водородоподобного атома в основном состоянии. Статический результат имеет вид $\gamma(\omega=0)=(23/60)\alpha^2 Z^{-4} a_0^5$ /α - константа тонкой структуры, Z - зарядовое число ядра, a_0 - боровский радиус/ и является аналогом известной статической электрической дипольной поляризуемости $\alpha(\omega=0)=(9/2)Z^{-4}a_0^3$.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

As is shown in refs.1, an external magnetic field $\vec{H}^{ext}$ (time-dependent, in general) of nonvanishing $\nabla\times\vec{H}^{ext}$ (i.e., an external conduction ($\vec{J}^{ext}$) or displacement ($(4\pi)^{-1}d\vec{D}^{ext}/dt$) current) induces in a system a toroid dipole moment of Fourier components $T_i^{ind}(\omega)=\Sigma_j \gamma_{ij}(\omega)\cdot[\nabla\times\vec{H}^{ext}(\omega)]_j$, (i,j = 1,2,3), where, in the quantum case, the dynamic (i.e., frequency (ω) dependent) toroid (dipole) polarizability $\gamma_{ij}(\omega)$ is given by the following formula:

$$\gamma_{ij}(\omega)=\sum_n\left[\frac{<0|T_i|n><n|T_j|0>}{E_n-E_0-\hbar\omega-i\epsilon}+\frac{<0|T_j|n><n|T_i|0>}{E_n-E_0+\hbar\omega+i\epsilon}\right]. \quad (1)$$

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E_0, E_n denote the energies of the ground and excited states of the unperturbed Hamiltonian, the sum extends over all excited states (in the discrete and continuous spectrum), while T_i (i = 1,2,3) stands for the operator of the toroid dipole moment. The toroid dipole moment of a current distribution $\vec{j}(\vec{x}, t)$ is defined as[2]

$$T_i(t) = \frac{1}{10c} \int \{x_i[\vec{x}\cdot\vec{j}(\vec{x}, t)] - 2\vec{x}^2 j_i(\vec{x}, t)\} d^3x. \qquad (2)$$

$\gamma_{ij}(\omega)$ characterizes the response of the system to the perturbation[2,3] $H_{T.D.}(t) = -\vec{T}(t)\cdot[\nabla\times\vec{H}^{ext}]_{\vec{x}=0,t} = -\vec{T}(t)[(4\pi/c)\vec{J}^{ext} + (1/c)d\vec{D}^{ext}/dt]_{\vec{x}=0,t}$, which appears in the multipole decomposition of the Hamiltonian.

In connection with the current interest in toroid moments[1-5] we present here the main technical points of a method which enabled us to calculate analytically $\gamma_{ij}(\omega)$ for a (nonrelativistic, spinless) hydrogen-like atom in its ground state.

Denoting $\Omega_1 \equiv E_0 + \hbar\omega + i\epsilon$, $\Omega_2 \equiv E_0 - \hbar\omega$, one may write

$$\gamma_{ij}(\omega) = \mathcal{J}_{ij}(\Omega_1) + \mathcal{J}_{ji}(\Omega_2), \qquad (3)$$

where

$$\mathcal{J}_{ij}(\Omega) = \sum_n \int \frac{d\vec{x}_1 d\vec{x}_2}{E_n - \Omega} u_0^*(\vec{x}_1) T_i(\vec{x}_1) u_n(\vec{x}_1) u_n^*(\vec{x}_2) T_j(\vec{x}_2) u_0(\vec{x}_2). \qquad (4)$$

$u_n(\vec{x})$ are the wave functions of the H-like atom,

$$u_0(\vec{x}) = \frac{1}{\sqrt{\pi}}\left(\frac{\lambda}{\hbar}\right)^{3/2} e^{-\lambda r/\hbar}, \quad r = |\vec{x}|, \quad \lambda = \alpha Z m c, \quad \alpha = \frac{e^2}{\hbar c} - \frac{1}{137,...},$$

and the one particle toroid dipole operator, by Eq.(2), is[2]

$$T_i(\vec{x}) = \frac{e}{10mc} \Sigma_k (-2\vec{x}^2 \delta_{ik} P_k + x_i x_k P_k), \quad P_k = -i\hbar \frac{\partial}{\partial x_k}, \qquad (5)$$

(e and m are the charge and mass of the electron, $Z|e|$ is the nucleus charge). The sum in Eq.(4) extends over the whole spectrum (the ground-state does not contribute). Using relations like

$$P_j u_0(\vec{x}) = i\lambda\left(\frac{x_j}{r}\right) u_0(\vec{x}), \quad x_i r u_0(\vec{x}) = \frac{(\lambda/\hbar)^{3/2}}{\sqrt{\pi}} i\hbar^2 \frac{\partial}{\partial\lambda}\frac{\partial}{\partial\kappa_i} e^{-(\lambda r - i\vec{\kappa}\vec{x})/\hbar}\Big|_{\vec{\kappa}=0} \qquad (6)$$

one may bring $\mathcal{J}_{ij}(\Omega)$ to the form

$$\mathcal{J}_{ij}(\Omega) = -\frac{1}{100}\left(\frac{e}{mc}\right)^2 \frac{\lambda^5 \hbar}{\pi}\left[\frac{\partial}{\partial\lambda''}\frac{\partial}{\partial\lambda'}\frac{\partial^2}{\partial\vec{\kappa}_{1i}\partial\vec{\kappa}_{2j}}\right] \times \qquad (7)$$

$$\times\{\int d\vec{x}_1 d\vec{x}_2\, e^{-(\lambda' r_1 - i\vec{\kappa}_1\vec{x}_1)/\hbar}\; e^{-(\lambda'' r_2 - i\vec{\kappa}_2\vec{x}_2)/\hbar} \times$$

$$\times \sum_n \frac{u_n(\vec{x}_1)u_n^*(\vec{x}_2)}{E_n - \Omega}\}|_{\substack{\lambda''=\lambda'=\lambda \\ \vec{\kappa}_2=\vec{\kappa}_1=0}} \quad . \tag{7}$$

The curl bracket in Eq.(7), by Fourier transforming, may be written as

$$\{...\} = \int d\vec{p}_1 d\vec{p}_2 \Phi(\vec{p}_1, \lambda', \vec{\kappa}_1)\Phi(-\vec{p}_2, \lambda'', \vec{\kappa}_2) G(\vec{p}_2, \vec{p}_1; \Omega) , \tag{8}$$

with

$$\Phi(\vec{p}, \lambda, \vec{\kappa}) = -\frac{2\hbar^2}{\sqrt{2\pi\hbar}} \frac{\partial}{\partial\lambda} \frac{1}{(\vec{p}-\vec{\kappa})^2 + \lambda^2} , \tag{9}$$

and

$$\sum_n \frac{u_n(\vec{x}_1)u_n^*(\vec{x}_2)}{E_n - \Omega} \equiv \frac{1}{(2\pi\hbar)^3} \int d\vec{p}_1 d\vec{p}_2 G(\vec{p}_2, \vec{p}_1; \Omega) e^{i(\vec{p}_2\vec{x}_2 - \vec{p}_1\vec{x}_1)/\hbar} . \tag{10}$$

Using now the integral representation of the nonrelativistic Coulomb Green's function in the form found by Schwinger[6]

$$G(\vec{p}, \vec{p}\,'; \Omega) = \frac{mX^3}{2\pi^2} \cdot \frac{ie^{i\pi\tau}}{2\sin\pi\tau} \int_1^{(0+)} d\rho\, \rho^{-\tau} \times$$

$$\times \frac{d}{d\rho}\{\frac{1-\rho^2}{\rho} \frac{1}{[X^2(\vec{p}-\vec{p}\,')^2 + (\vec{p}^{\,2} + X^2)(\vec{p}\,'^2 + X^2)\frac{(1-\rho)^2}{4\rho}]^2}\} \tag{11}$$

(where $X^2 = -2m\Omega$, $\mathrm{Re}X > 0$, $\tau \equiv \lambda/X$ and the integration contour starts at 1, encircles the origin in the counterclockwise sense and returns to 1), Eq.(7) becomes

$$\mathcal{T}_{ij}(\Omega) = C\frac{mX^3}{2\pi^2} \frac{ie^{i\pi\tau}}{2\sin\pi\tau} [\frac{\partial^2}{\partial\lambda''^2} \frac{\partial^2}{\partial\lambda'^2} \frac{\partial^2}{\partial\vec{\kappa}_{1i}\partial\vec{\kappa}_{2j}}] \times$$

$$\times \{\int_1^{(0+)} d\rho\, \rho^{-\tau} \frac{d}{d\rho}[\frac{1-\rho^2}{\rho} J(\lambda', \lambda'', \vec{\kappa}_1, \vec{\kappa}_2; X^2)]\}|_{\substack{\lambda''=\lambda'=\lambda \\ \vec{\kappa}_2=\vec{\kappa}_1=0}} \quad ; \tag{12}$$

$C = (\lambda^5\hbar^4/50\pi^2)(e/mc)^2$ and $J(\lambda', \lambda'', \vec{\kappa}_1, \vec{\kappa}_2; X^2)$ denotes the "basic integral"

$$\int \frac{d\vec{p}_1 d\vec{p}_2}{[(\vec{p}_1-\vec{\kappa}_1)^2 + \lambda'^2][X^2(\vec{p}_1-\vec{p}_2)^2 + (\vec{p}_1^{\,2}+X^2)(\vec{p}_2^{\,2}+X^2)\frac{(1-\rho)^2}{4\rho}][(\vec{p}_2-\vec{\kappa}_2)^2 + \lambda''^2]} \tag{13}$$

introduced and calculated in refs.7. There it has been found that

$$\frac{d}{d\rho}\left[\frac{1-\rho^2}{\rho} J(\lambda',\lambda'',\vec{\kappa}_1,\vec{\kappa}_2; X^2)\right] =$$

$$= \frac{16\pi^4}{X^2} \frac{(1-s\rho + p\rho^2)^{-1}}{[(X+\lambda')^2+\vec{\kappa}_1^2][(X+\lambda'')^2+\vec{\kappa}_2^2]}, \tag{14}$$

where

$$s = 2\frac{(\lambda''^2 - X^2)(\lambda'^2 - X^2) + 4X^2\vec{\kappa}_1\vec{\kappa}_2}{(X+\lambda'')^2(X+\lambda')^2}, \quad p = \frac{(X-\lambda'')^2(X-\lambda')^2}{(X+\lambda'')^2(X+\lambda')^2}. \tag{15}$$

Taking then the derivatives with respect to $\vec{\kappa}_{1i}$, $\vec{\kappa}_{2j}$, λ'' and using formulas for the Gauss hypergeometric functions of the type

$$F(a,b,a+1;z) = -ia\left(\frac{e^{-i\pi a}}{2\sin\pi a}\right)\int_1^{(o+)} \rho^{a-1}(1-z\rho)^{-b}\,d\rho, \tag{16}$$

one arrives at

$$\mathcal{J}_{ij}(\Omega) = \delta_{ij} D \frac{\partial^2}{\partial\lambda'^2}\left[\frac{Q(\lambda')}{(\lambda'+X)^4}\right]_{\lambda'=\lambda}; \quad D = C\cdot\frac{1280\, m\pi^2 X^3}{(\lambda+X)^6};$$

$$Q(\lambda') = \frac{F(2-\tau,6,3-\tau;\zeta(\lambda'))}{2-\tau} - \frac{2\zeta_1(\lambda')F(3-\tau,6,4-\tau;\zeta(\lambda'))}{3-\tau} + \tag{17}$$

$$+\frac{\zeta_1^2(\lambda')F(4-\tau,6,5-\tau;\zeta(\lambda'))}{4-\tau}; \quad \zeta_1(\lambda') = \frac{\lambda'-X}{\lambda'+X}, \quad \zeta(\lambda') = \frac{\lambda-X}{\lambda+X}\zeta_1(\lambda').$$

Next, the machinery of hypergeometric functions is put at work to take economically the last two derivatives with respect to λ'. The final result is $\gamma_{ij}(\omega) = \gamma(\omega)\delta_{ij}$ with

$$\gamma(\omega) = \frac{\alpha^2}{20}\frac{a_o^5}{Z^4}\sum_{i=1,2}\frac{\tau_i^2}{(\tau_i+1)^4}\frac{1}{2-\tau_i}\frac{1}{3-\tau_i}\cdot$$

$$\cdot\left[\frac{8\tau_i^2(\tau_i^2+1)^2}{(\tau_i+1)^2(4-\tau_i)}F(1,-1-\tau_i,5-\tau_i;\zeta_i) - 15\tau_i^4 + 7\tau_i^3 + 53\tau_i^2 + 57\tau_i + 18\right]. \tag{18}$$

$F(a,b,c;z)$ is the Gauss hypergeometric function with the series expansion

$$F(a,b,c;z) = 1 + \frac{ab}{c}\frac{z}{1!} + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{z^2}{2!} + \ldots$$

and

$$\tau_1 = (1-\omega_o)^{-1/2}, \quad \tau_2 = (1+\omega_o)^{-1/2}, \quad \zeta_i = \left(\frac{\tau_i - 1}{\tau_i + 1}\right)^2, \quad (i=1,2), \tag{19}$$

$$\omega_0 = \frac{\hbar\omega}{|E_0|} = \frac{2\hbar\omega}{\alpha^2 Z^2 mc^2} = \frac{2}{\alpha Z} \cdot \frac{a_0}{Z} \cdot \frac{\omega}{c}; \tag{19}$$

$$a_0 = \frac{\hbar}{\alpha mc} = 0.53\times 10^{-8}\ \text{cm}; \quad \alpha = \frac{e^2}{\hbar c} \simeq \frac{1}{137...}.$$

$\gamma(\omega)$ is an even analytic function of ω in the complex ω - plane with simple poles at $\omega = (E_n - E_0)/\hbar$, n = 2,3,4,... ($E_n = E_0/n^2$ is the discrete spectrum of the H-like atom), and a branch cut along the real ω -axis for $\omega > |E_0|$, i.e., above the ionization threshold $|E_0|$. The static result (which is the toroid analog of the static electric dipole polarizability $\alpha(\omega = 0) = (9/2)a_0^3 Z^{-4}$ found in 1926 by Epstein and by Waller [8]) looks very simple

$$\gamma(\omega = 0) = \frac{23}{60}\alpha^2 \frac{a_0^5}{Z^4} \simeq Z^{-4}\times 0.86\times 10^{-46}\ \text{cm}^5. \tag{20}$$

Some applications [9] as well as a more detailed presentation of this research will be published elsewhere.

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