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Abstract

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AN INTEGRAL REPRESENTATION OF THE DISPERSION FORMULA FOR THE HYDROGEN ATOM IN THE GROUND STATE

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Quantum theory leads to the following expression for the optical polarizability $\alpha(\omega)$ of the hydrogen atom or a hydrogen-like ion in the ground state:

$$\alpha(\omega) = -2 \int \psi(r)[\chi(\mathbf{r};\omega) + \chi(\mathbf{r};-\omega)] z \, d\tau \tag{1}$$

(in atomic units), where $\psi = \sqrt{Z^3/\pi}\, e^{-Zr}$; $\mathbf{r}$ is the radius vector of the electron; Z is the nuclear charge; the function $\chi(\mathbf{r};\omega)$ satisfies the equation

$$(H_0 + \tfrac{1}{2}Z^2 + \omega)\chi(\mathbf{r};\omega) = -\tfrac{1}{2} z\psi; \tag{2}$$

here

$$H = -\tfrac{1}{2}\Delta - \frac{Z}{r};$$

ω is the angular frequency of the oscillations of an electric field directed along the Oz axis. Using the expansion of the function $\chi(\mathbf{r};\omega)$ in the eigenfunctions of the operator H_0, one obtains the usual dispersion formula:

$$\alpha(\omega) = 2\sum_{n=2}^{\infty} \frac{(E_n - E_1)\langle 1,0,0|z|n,1,0\rangle^2}{(E_n - E_1)^2 - \omega^2} + 2\int_0^{\infty} \frac{(E - E_1)\langle 1,0,0|z|E,1,0\rangle^2 \, dE}{(E - E_1)^2 - \omega^2}. \tag{3}$$

Calculations by formula (3) are difficult because of the slow convergence of the series (especially at frequencies ω not very close to one of the eigenfrequencies $\omega_n = E_n - E_1$). Below it will be shown that one can construct an integral representation of $\alpha(\omega)$ convenient for calculations.

Put

$$\chi(\mathbf{r};\omega) = r^{-2}\psi(r)V(r;\omega)\cos\vartheta \tag{4}$$

under the condition

$$V(0;\omega) = V'(0;\omega) = 0. \tag{5}$$

Substituting (4) into (2), we find that the function $V(r;\omega)$ must satisfy the equation

$$\left[r\frac{d^2}{dr^2} - 2(Zr+1)\frac{d}{dr} + 4Z - 2\omega r\right] V(r,\omega) = r^4. \tag{6}$$

Now apply the Laplace transform

$$W(p;\omega) = \int_0^\infty e^{-Zpr} V(r;\omega)\, dr \tag{7}$$

and note that, according to (1), (4), (7),

$$\alpha(\omega) = \frac{8}{3}Z^2 \left|W'(2;\omega) + W'(2;-\omega)\right|. \tag{8}$$

For the Laplace image of the function $V(r;\omega)$ we obtain the equation

$$\left[\left(2p - p^2 + \frac{2\omega}{Z^2}\right)\frac{d}{dp} + 6 - 4p\right] W(p;\omega) = \frac{24}{Z^6 p^5}. \tag{9}$$

We write the solution of equation (9) in the form

$$W(p) = \frac{24}{Z^6}\frac{(p-p_2)^b}{(p_1-p)^a}\, I(p), \tag{10}$$

$$I(p) = \int_{p_1}^{p} \frac{(p_1-p)^{a-1}\, dp}{p^5(p-p_2)^{b+1}}, \tag{11}$$

where

$$p_1(\omega) = 1 + \gamma(\omega), \qquad p_2(\omega) = 1 - \gamma(\omega), \qquad a(\omega) = 2 - \frac{1}{\gamma(\omega)},$$

$$b(\omega) = -2 - \frac{1}{\gamma(\omega)}, \qquad \gamma(\omega) = \sqrt{1 + \frac{2\omega}{Z^2}}.$$

The choice of the lower limit in $I(p)$ makes it possible to remove the singularity of the function $W(p;\omega)$ at $p = p_1$ and thereby to ensure fulfillment of the condition $\chi(r;\omega) \to 0$ as $r \to \infty$. Further we find that

$$W'(p;\omega) = \frac{24}{Z^6}\left[\frac{1}{p^5(2\omega/Z^2 + 2p - p^2)} + \frac{(4p-6)(p-p_2)^{b-1}}{(p_1 - p)^{a+1}}\, I(p)\right], \tag{12}$$

$$W'(2;\omega) = \frac{24}{Z^6}\left[\frac{Z^2}{64\omega} + \frac{2p_1^{b-1}}{(p_1-2)^{a+1}}\, I(2)\right]. \tag{13}$$

According to (8) and (13):

$$\alpha(\omega) = \frac{128}{Z^4}\,[f(\omega) + f(-\omega)], \tag{14}$$

where

$$f(\omega) = \frac{p_1^{b-1}}{(p_1-2)^{a+1}}\, I(2) = \frac{p_1^{b-1}}{|p_2|^{a+1}} \int_{p_1}^{2} \frac{|p-p_1|^{a-1}}{p^5(p-p_2)^{b+1}}\, dp. \tag{15}$$

The integral in (15) has meaning only for $a > 0$, and, consequently, $f(-\omega)$ is defined so far only for $\omega < \frac{3}{8}Z^2$. However, by means of integration by parts one can obtain an analytic continuation of the function $f(\omega)$ which has meaning also for $a > -1$, thereby defining $f(-\omega)$ for $\omega < \frac{4}{9}Z^2$.

After a single integration by parts the function $f(\omega)$ takes the form:

$$f(\omega) = \frac{1}{ap_1}\left[\frac{p_1^b}{p_2|p_2|^a} \int_{p_1}^{2} |p-p_1|^a \left(\frac{(b+6)p - 5p_2}{p^6(p-p_2)^{b+1}} - \frac{Z^2}{64\omega}\right)\right]. \tag{16}$$

Carrying out successive integrations by parts, one can arrive at such an expression for $f(\omega)$ for which $f(-\omega)$ will have meaning for any $\omega < \omega_n$, where

$$\omega_n = \frac{1}{2}Z^2\left[1 - \frac{1}{(n+2)^2}\right]. \tag{17}$$

We note that ω_n is the frequency of the spectral lines of the Lyman series. It is easy to find the value of the static polarizability $\alpha(0)$. If $\omega = 0$,

then $p_1 = 2,\ p_2 = 0,\ a = 1,\ b = -3,$

$$W(p) = -\frac{3(p+2)}{p^5 Z^6}, \qquad W'(2) = \frac{27}{32Z^6}, \qquad \alpha(0) = \frac{16}{3}Z^2 W'(2) = \frac{4.5}{Z^4}.$$

For calculating $\alpha(\omega)$ at very low frequencies, it is convenient, according to (3), to use the expansion of $W'(2)$ in a series in powers of the small quantity $(2-p_1)$

$$W'(2) = W'(p_1) + W''(p_1)(2-p_1) + \frac{1}{2}W'''(p_1)(2-p_1)^2 + \dots \qquad (18)$$

The coefficients of the expansion (18) can be found by means of the following recurrence formula, which follows from equation (9):

$$2\left[n+3-(n+2)p_1\right]W^{(n)}(p_1) = \frac{(-1)^n(n+4)!}{Z^6 p_1^{n+5}} + n(n+3)W^{(n-1)}(p_1). \qquad (19)$$

Moreover, according to (19) or (9):

$$W(p_1) = \frac{12}{Z^6 p_1^5 (3-2p_1)}. \qquad (20)$$

The dispersion formula in closed form can be obtained not only for the ground state of the hydrogen atom, but also for excited states. In the latter case, however, complications arise due to the presence of degeneracy with respect to the azimuthal quantum number.

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Note: Figure translations are in progress. See original paper for figures.

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