DISPERSION FORMULA FOR THE HYDROGEN ATOM IN THE GROUND STATE

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Abstract

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M. I. CHIBISOV

DISPERSION FORMULA FOR THE HYDROGEN ATOM IN THE GROUND STATE

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1. According to quantum theory, the optical polarizability of the hydrogen atom in the ground state is equal to:

$$\alpha(\omega) = 2\sum_{n=2}^{\infty} \frac{\nu_n |z_{0n}|^2}{\nu_n^2 - \omega^2} + 2\int_0^{\infty} \frac{\nu |r_{0\nu}|^2}{\nu^2 - \omega^2}\, d\nu, \tag{1}$$

where ν_n are the transition frequencies from the ground state to the n-th excited state of the discrete spectrum; ν is the same for a transition into the continuous spectrum of the hydrogen atom; z_{0n} is the matrix element of the z-component of the dipole moment. The atomic system of units is used: $h = m = e^2 = 1$. With the aid of the apparatus of Green functions and the Laplace transform of the intermediate differential equation, the polarizability (1) can be represented in the form ([1,2])

$$\alpha(\omega) = -\frac{2}{3\omega}[f(\omega) - f(-\omega)]; \tag{2}$$

$$f(\omega) = \frac{96}{p_2^a p_1^{4-a}} \int_{p_1}^{2} \frac{(x-p_1)^{a-1}(x-p_2)^{3-a}}{x^5}\, dx; \tag{2’}$$

$$p_1 = 1 + \sqrt{1+2\omega}; \qquad p_2 = 2 - p_1; \qquad a = 2 - \frac{1}{p_1 - 1}; \qquad -\infty < a \leq 2. \tag{2”}$$

As is seen from the definition of the parameters P_1, P_2, and a, the integral (2) does not exist for $\omega \leq 0$ or $\omega \leq -\nu_1 = -3/8$. To extend the domain of definition of ($2'$) to the region $-\nu_n < \omega < \infty$, an n-fold integration of expression ($2'$) by parts is required ([1]).

Analysis of expression ($2'$) in the plane of the complex x makes it possible to obtain another integral representation for $\alpha(\omega)$, free of the indicated shortcoming, and in which the pole part is separated out as a simple analytic term.

2. The points p_1 and p_2 in the plane of the complex x are branch points of the integrand in formula $(2')$. The cut of the x-plane may be drawn along a segment of a curve connecting these points. For frequencies ω for which $a < -1$ and is not equal to an integer, p_1 is an essentially singular point. At the origin $x = 0$ there is a fifth-order pole whose residue is

$$\operatorname{Res} \left. \frac{(x-p_1)^{a-1}(x-p_2)^{3-a}}{x^5} \right|_{x=0} \equiv Q(\omega) = \frac{-2}{3p_1^4}\left(\frac{3-a}{1-a}\right)^a . \qquad (3)$$

The contour of integration in $(2')$ must be such that, in the limit $\omega \to 0$, expression $(2')$ gives the known value of the static polarizability $\alpha(0) = 4.5$. For this it is sufficient that, as $\omega \to 0$ $(p_1 \to 2)$, the contour, if it became closed, would not contain the point $x = 0$ inside it. Otherwise $f(\omega)$ would be proportional to the residue (3), which as $\omega \to 0$ diverges as ω^{-1}. For $a \geq 0$, as the contour of integra-

can be the segment of the real axis $(p_1, 2)$, which also gives $a(0) = 4.5$ (1).

Restricting ourselves for the time being to frequencies for which $a \geq 0$, we divide the integration contour in (2) into two parts. The first is the lower edge of the cut from p_1 to p_2, and the second is a certain curve satisfying the requirements given above and joining p_2 and 2. We denote the integral over the first contour by J_3, and over the second by J_2. The first integral can be evaluated exactly by expressing it in terms of the residue $Q(\omega)$, while the second is defined for any ω. Since on the upper edge of the cut the values of the integrand in (2) differ by the factor $e^{2\pi i a}$ from the values of the function on the lower edge, we have

$$(1 - e^{2\pi i a})J_3 = \int_C (x-p_1)^{a-1}(x-p_2)^{3-a}\frac{dx}{x^5}, \qquad (4)$$

where the contour C goes around the cut clockwise. This contour, together with an infinitely large circle (the integral over which tends to zero), bounds a region inside which the point $x = 0$ lies, and therefore the integral (4) is equal to $2\pi i Q(\omega)$. This gives

$$f(\omega) = -\frac{96}{p_2^a p_1^{4-a}}\left[(\pi i - \pi \operatorname{ctg} \pi a)Q(\omega) + J_2(\omega)\right], \qquad (5)$$

$$J_2(\omega) = \int_{p_2}^{2} (x-p_1)^{a-1}(x-p_2)^{3-a}\frac{dx}{x^5}, \qquad (6)$$

where the residue $Q(\omega)$ is defined by formula (3).

We shall show that for real ω formula (5) defines a real function $f(\omega)$. To this end, consider the following contour of integration in (6): departure from p_2 parallel to the imaginary axis to infinity and return from infinity along the real axis to the point $x = 2$. The second part of the contour gives a purely real contribution. When integrating along the first branch of the contour, note that the integrand in (6) satisfies the relation $\varphi(x^*) = \varphi^*(x)$, which means that the required imaginary part of the integral (6) is equal to one half of the imaginary part of the same integral taken along the entire straight line $(p_2 - i\infty;\ p_2 + i\infty)$. The latter integral is equal to $-2\pi i Q(\omega)$ (we are considering the frequencies $-\nu_1 < \omega < 0$, for which $p_2 > 0$ and $a > 0$). Thus, instead of (5), for real ω one may write

$$f(\omega) = -\frac{96}{p_2^a p_1^{4-a}}\left[-\pi \operatorname{ctg}(\pi a) \cdot Q(\omega) + \operatorname{Re} J_2(\omega)\right]. \tag{7}$$

For integral a, $\operatorname{ctg} \pi a$ becomes infinite, and $f(\omega)$ has poles. Indeed, $a = 2$ for $\omega = +\infty$, $a = 1$ for $\omega = 0$, and $a = -n$ for

$$\omega = -\frac{1}{2}(1 - 1/n^2) = -\nu_n. \tag{8}$$

As is seen from formula (3), $Q(\omega)$ does not vanish at these points. Consequently, the polarizability $\alpha(\omega)$ has poles at $\omega = \nu_n$, as it should. There are no other poles of $\alpha(\omega)$.

Expressions (7) and (6) exist for all ω, which makes it possible to define $f(\omega)$ in the entire ω-plane as the analytic continuation of expression (7), since (7) has poles only at isolated points.

For positive values of ω, it is convenient to retain representation (2′) for $f(\omega)$, and to use (7) for $f(-\omega)$. Thus we obtain the polarizability of the hydrogen atom in the ground state:

$$\alpha(\omega) = \frac{64}{\omega}\left\{\frac{1}{q_2^b q_1^{4-b}}\left[\pi Q(\omega) \operatorname{ctg} \pi a - \operatorname{Re} J_2(-\omega)\right] - \frac{J_1(\omega)}{p_2 p_1^{4-a}}\right\}, \tag{9}$$

$$J_1 = \int_{p_1}^{2} (x - p_1)^{a-1}(x - p_2)^{3-a}\frac{dx}{x^5}, \tag{10}$$

$$J_2 = \int_{p_2}^{2} (x - q_1)^{b-1}(x - q_2)^{3-b}\frac{dx}{x^5}, \qquad b = a(-\omega), \qquad q_{1,2} = p_{1,2}(-\omega). \tag{11}$$

To study J_2, we consider the contour defined above, consisting of two segments: the first X from p_2 to $p_2 - i\infty$, and the second $2 < x < +\infty$. For the first segment we make the change of variable $x = p_2 - iy$, and for the second $x = 2 + y$, and obtain

$$\operatorname{Re} J_2 = j_1 + j_2,$$

$$j_1 = -\operatorname{Re} \int_0^\infty \frac{[i(p_2 - p_1) + y]^{a-1} y^{3-a}}{(y + ip_2)^5}\, dy, \tag{12}$$

$$j_2 = -\int_0^\infty \frac{(y + p_2)^{a-1} (y + p_1)^{3-a}}{(y + 2)^5}\, dy. \tag{13}$$

For $\omega \to 0$, from formulas (6) and (3) we obtain

$$\operatorname{Re} J_2 \to \frac{1}{12\omega^2}, \qquad Q(\omega) \to -\frac{1}{12\omega^2}. \tag{14}$$

For $\omega \to -\frac{1}{2}$, $a \to -\infty$, and the integrals (12), (13) are transformed to the form

$$\operatorname{Re} J_2 \left(-\frac{1}{2}\right) = -\operatorname{Re} \int_0^\infty \frac{e^{2it} t\, dt}{(1 + it)^5} - \int_0^1 \frac{e^{2t} t\, dt}{(t + 1)^5} \simeq -0.190,$$

$$Q\left(-\frac{1}{2}\right) = \frac{2}{3} e^{-2} = 0.0905. \tag{15}$$

For intermediate values of ω, the integrals J_1 and J_2 were obtained by numerical integration and are given in Table 1.

Since for $\omega \to \frac{1}{2}$ the integrals J_1 and J_2 tend to constant values, near the ionization threshold (practically for frequencies ω greater than the second eigenfrequency) the polarizability is close to the expression

$$\alpha(\omega) = -4.96 \operatorname{ctg} \left(\pi / \sqrt{1 - 2\omega}\right) + 1.80, \tag{16}$$

which differs, in the last term, from the analogous expression obtained in work (3) using the asymptotic representation of the coordinate Green' s function near the ionization threshold.

Table 1

$-\omega$	$-Q(\omega)$	$\operatorname{Re} J_2$	$f(2,\omega)$	$-\omega$	$-Q(\omega)$	$\operatorname{Re} J_2$	$f(2,\omega)$	ω	$f(2,\omega)$	$\alpha(\omega)$
0.500	0.0904	−0.190		0.297	0.177	0.090	5.49	0.00	1.50	4.50
0.443	0.105	−0.155	51.23	0.269	0.201	0.206	4.24	0.05	1.35	4.57
0.435	0.108	−0.151	3.68	0.262	0.208	0.239	4.04	0.10	1.23	4.77
0.430	0.110	−0.147	0.915	0.255	0.214	0.276	3.86	0.15	1.12	5.12
0.424	0.112	−0.142	−1.025	0.241	0.230	0.357	3.52	0.20	1.03	6.00
0.418	0.114	−0.136	−2.80	0.234	0.240	0.423	3.36	0.25	0.965	7.95

$-\omega$	$-Q(\omega)$	$\operatorname{Re} J_2$	$f(2,\omega)$	$-\omega$	$-Q(\omega)$	$\operatorname{Re} J_2$	$f(2,\omega)$	ω	$f(2,\omega)$	$\alpha(\omega)$
0.411	0.117	−0.129	−4.85	0.226	0.250	0.490	3.21	0.30	0.912	10.6
0.403	0.120	−0.121	−7.82	0.208	0.276	0.653	2.94	0.35	0.861	26.1
0.394	0.123	−0.110	−13.6	0.190	0.309	0.916	2.70	0.40	0.810	−14.7
0.383	0.128	−0.097	−34.9	0.169	0.355	1.31	2.47	0.45	0.768	+9.12
0.371	0.133	−0.072	+83.7	0.147	0.421	1.98	2.27	0.50	0.730	–
0.357	0.140	−0.056	19.4	0.135	0.466	2.51	2.17			
0.340	0.149	−0.025	10.9	0.122	0.524	3.26	2.08			
0.321	0.161	+0.020	7.41	0.063	1.11	15.6	1.752			

We now obtain a series for $\alpha(\omega)$ in positive powers of ω and determine the coefficients of this expansion. The function $f(\omega)$ appearing in formulas (2) satisfies the differential equation ([1,2])

$$[p(p-2)-2\omega]f'_p(p,\omega)+(4p-6)f=\frac{96}{p^5}. \tag{17}$$

Expanding $f(p,\omega)$ in powers of ω and substituting this expansion into (17), for the coefficients of the expansion we obtain:

$$p(p-2)f'_0+(4p-6)f_0=\frac{96}{p^5}, \qquad f(p,\omega)=\sum_{n=0}^{\infty} f_n(p)\omega^n, \tag{18}$$

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$$p(p-2)f'_n+(4p-6)f_n=2f_{n-1}, \qquad f_0=12/p^4+24/p^5. \tag{18'}$$

From (18′) we obtain:

$$f_n(p)=\frac{2}{p^3(p-2)}\int_2^p f'_{n-1}(z)z^2\,dz, \quad \to f_n(p)\bigg|_{p=2}=f'_{n-1}(2)=\frac{d^n}{dp^n}f_0(p)\bigg|_{p=2}. \tag{19}$$

Substituting (19) into (18), after differentiating $f_0(p)$ n times, we obtain an expansion (in the form of an asymptotic series) for $\alpha(\omega)$ and for the sums $S(k)$ important in spectroscopy:

$$\alpha(\omega)=\frac{1}{48}\sum_{n=0}^{\infty}\frac{(2n+9)(2n+4)!}{2^{2n}}\omega^{2n}\simeq\frac{9}{2}+\frac{165}{4}\omega^2+\frac{1365}{2}\omega^4+\cdots; \tag{20}$$

$$S(k) \equiv 2\sum_n \frac{|z_{0n}|^2}{\nu_{0n}^k} = \frac{(k+8)(k+3)!}{3 \cdot 2^{k+3}}, \qquad k = 0, 1, 2, ... \tag{21}$$

The last equality (21) follows from comparing (20) with expansion (1) in powers of ω^2.

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