

Sum of oscillator-strength moments and asymptotic behaviour of thermally induced broadening and shift of energy levels of Rydberg atom circular states

I.L. Glukhov, A.A. Kamenski, V.D. Ovsianikov

Abstract. Based on the rules for summing oscillator-strength moments, we derive analytical expressions for environmentally (thermally) induced energy-level shifts and broadenings of circular Rydberg states with maximum orbital (l) and magnetic (m) quantum numbers, $l = |m| = n - 1$. The formulae for the energy of interaction with blackbody radiation are presented in the form of series expansion in even powers of the small parameter $\eta = Z^2/(n^3 k_B T) \ll 1$ in the region of high temperatures T and principal quantum numbers n (Z is the charge of the residual ion). The expression for the thermally induced width contains a negative temperature-independent term coinciding in absolute value with the spontaneous width, so that the temperature-independent term is absent in the expression for the sum of the spontaneous and thermally induced widths. A similar expansion in powers of η for the thermally induced shift also contains a temperature-independent term proportional to $1/n^6$.

Keywords: atom, circular Rydberg states, sums of oscillator strengths, thermal radiation, energy level width, shift.

1. Introduction

The methods of multiphoton laser spectroscopy enable excitation of atoms and ions into circular Rydberg states $|nlm\rangle$ with large values of the principal (n), orbital (l), and magnetic (m) quantum numbers ($l = |m| = n - 1$) [1–4]. Spontaneous decay of such states is possible due to dipole-allowed radiative transitions to the states $|n'l'm'\rangle$ with principal, orbital, and magnetic quantum numbers, $n' = n - 1$, $l' = l - 1$, $|m'| = |m| - 1$. The matrix elements of such transitions rapidly decrease with increasing n and l . Therefore, the natural lifetime of Rydberg states increases in proportion to n^5 , in full agreement with the general dependence proportional to the product $n^3 l^2$ [5]. Using specially selected external conditions that exclude the possibility of spontaneous emission, the lifetime of Rydberg states can be increased by several orders of magnitude [1–4], significantly expanding the possibilities for manipulating highly excited atoms and their practical application. In the field of virtually inevitable thermal radiation, the lifetimes and frequencies of radiative transitions for Rydberg states can vary significantly. Therefore, for the properties of circular states to be successfully controlled, a detailed calculation of the dependences of the shifts and

broadenings of Rydberg energy levels on the ambient temperature T is needed.

The wave functions and energies of circular Rydberg states are close to hydrogen-like and identical for all atoms, in contrast to states with small orbital moments, which have a specific energy structure characteristic of atomic particles of each specific chemical element. The energy spectrum of states with an orbital momentum $l < 5$ is described by the Rydberg formula, which differs from the formula for the spectrum of a hydrogen-like atom by the fact that the principal quantum number n is replaced by the effective principal quantum number $v = n - \delta_l$ determined by the quantum defect δ_l of a series of states with a certain angular momentum l . For states with $l > 5$, the defect δ_l practically does not differ from zero in all many-electron atoms. Thus, the manyfold single-electron state with a principal quantum number n coincides with the corresponding manyfold of a hydrogen-like atom in which there are no states with small orbital momenta $l < 6$. Therefore, highly excited circular states are identical to the corresponding states of the hydrogen atom described by Coulomb wave functions. The use of these functions allows obtaining analytical expressions for the constants of the polarisation and dispersion long-range interactions of atoms in circular Rydberg states [6, 7], which are necessary to evaluate the possibility of using the blockade effect of resonant excitation of Rydberg states [8–10].

Along with the effects of interatomic interaction, environmental thermal radiation has an important effect on the structure of the energy levels of Rydberg states. The authors of Refs [11–13] obtained asymptotic expressions for the shift and broadening, the accuracy of which has so far been determined by comparing with the results of numerical calculations for specific states in a specific range of blackbody radiation temperatures. To analytically present the results of such calculations, the contributions to the thermally induced shift and broadening from ionisation [14–16] were separated from those of thermally induced decays and excitations to the states of a discrete spectrum [17, 18].

In the present paper, we have obtained analytical expressions for corrections to asymptotic formulae using the rules for summing the oscillator-strength moments. Section 2 presents the procedures for finding closed expressions for the sums of oscillator-strength moments. For circular states, we used the sum rules to obtain analytical expressions for summing the moments over an infinite set of highly excited states, including integrals over the continuous spectrum. Section 3 discusses the effect of environmental thermal radiation, referred to in the literature as blackbody radiation (BBR), on the lifetime described by the imaginary part of the energy of the level. Using the rules for summing the oscillator-strength moments,

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we have derived analytical formulae for corrections to the asymptotic expression for the thermally induced decay rate. In Section 4, analytical expressions are obtained for corrections to the asymptotic formula that describes the BBR-induced changes in the energy of circular Rydberg states.

Throughout the work, unless expressly stated otherwise, we use the atomic system of units $e = m = \hbar = 1$, the speed of light numerically coincides with the inverse fine structure constant $c = \alpha^{-1} = 137.036$, the temperature is expressed in kelvins, and the Boltzmann constant is determined by the ratio $k_B = 1/T_a$ of the atomic unit of energy to atomic unit of temperature $T_a = 315776$ K.

2. Sum of oscillator-strength moments

2.1. Oscillator-strength moments

The oscillator strengths $f_{n'n(\mu)} = 2\omega_{n'n} |\langle n' | r_\mu | n \rangle|^2$ of electric dipole transitions are important characteristics of atomic spectra. Here, the symbol $n(n')$ denotes a complete set of quantum numbers nlm ($n'l'm'$) of the stationary states of the atom, and r_μ is the coordinate of the Rydberg electron ($\mu = 0, \pm 1$ is the cyclic coordinate [19], and $r_0 = z$ is the projection onto the z axis directed along the polarisation vector of the emitted or absorbed photon during the transition between the states n and n'). In the one-electron approximation, the components of the dipole moment coincide in absolute value and are opposite in sign to the coordinates of the valence electron.

In calculating the probabilities of radiative transitions and the energy of interaction with external fields, there arise sums of the oscillator-strength moments over a complete set of atomic eigenstates, including the integral over the continuous spectrum [20, 21]

$$S_{nlm(\mu)}^{(q)} = \sum_{n'} \omega_{n'n}^q f_{n'n(\mu)}. \quad (1)$$

In particular, the dipole dynamic polarisability of an atom in the state $|nlm\rangle$ is determined by the expression

$$\alpha_{nlm}(\omega) = \sum_{n'l'm'} \frac{2\omega_{n'n} |\langle n'l'm' | z | nlm \rangle|^2}{\omega_{n'n}^2 - \omega^2} = \sum_{n'l'm'} \frac{f_{n'n(0)}}{\omega_{n'n}^2 - \omega^2} \quad (2)$$

and can be represented as a series expansion in powers of the square of the frequency ω^2 using the formula for the sum of the series of geometric progression. The coefficients of this expansion are the sum of the oscillator-strength moments (1). Depending on the relationship between ω^2 and the square of the atom eigenfrequency $\omega_{n'n}^2$, there are two types of expansions:

1) for $\omega^2 < \omega_{n'n}^2$, the series contains only positive powers of ω^2 , and the coefficients are the sums of moments (1) with even negative exponents q , starting from $q = -2$, corresponding to static polarisability, $S_{nlm}^{(-2)} = \alpha_{nlm}(0)$:

$$\alpha_{nlm}(\omega) = \sum_{p=0}^{\infty} S_{nlm(0)}^{(-2p-2)} \omega^{2p} = \alpha_{nlm}(0) + S_{nlm(0)}^{(-4)} \omega^2 + S_{nlm(0)}^{(-6)} \omega^4 + \dots; \quad (3)$$

2) the opposite inequality $\omega^2 > \omega_{n'n}^2$ is formally valid for bound states provided that the frequency exceeds the level ionisation potential, $\omega > |E_{nl}|$. If in this case the contribution of the states of the continuous spectrum and the contribution

of the lower bound states with $n' < n$, which do not satisfy the condition $\omega^2 > \omega_{n'n}^2$, can be neglected, then we can use the series expansion in negative powers of ω^2 . The coefficients of this expansion are the sums of moments (1) with even positive exponents $q \geq 0$, and $S_{nlm}^{(0)} = 1$:

$$\alpha_{nlm}(\omega) = - \sum_{p=0}^{\infty} S_{nlm(0)}^{(2p)} \omega^{-2-2p} = - \frac{1}{\omega^2} - \frac{S_{nlm(0)}^{(2)}}{\omega^4} - \frac{S_{nlm(0)}^{(4)}}{\omega^6} - \dots \quad (4)$$

Along with $S_{nlm}^{(0)}$, one can immediately obtain a closed expression for $S_{nlm(0)}^{(-1)} = 2 \langle nlm | z^2 | nlm \rangle$ [20, 21], which for arbitrary values of the orbital and magnetic quantum numbers can be represented as the product of the angular and radial matrix elements:

$$S_{nlm(0)}^{(-1)} = 2 \langle lm | \cos^2 \theta | lm \rangle \langle nl | r^2 | nl \rangle = \frac{2}{2l+3} \times \left(1 + 2 \frac{l^2 - m^2}{2l-1} \right) \langle nl | r^2 | nl \rangle. \quad (5)$$

For the circular state of a hydrogen-like atom, this expression takes the form

$$S_{nlm(0)}^{(-1)} = 2 \langle nl | r^2 | nl \rangle / (2n+1) = n^2(n+1)/Z^2,$$

where Z is the charge of the atomic core. Similarly, one can obtain fairly simple analytical expressions for sums (1) with other exponents q . Below we present the rules for sums (1) for negative and positive values of q .

2.2. Analytical expressions for the sums of oscillator-strength moments with negative q

Strictly speaking, the sum rules (1) can be expressed in closed form if analytical expressions for the wave functions and energies of single-electron stationary states are known. The simplest solution to this problem can be obtained for circular Rydberg states described for all atoms using the wave functions of a hydrogen-like atom. After integration over the angular variables of the matrix element, the expression for sums (1) with a negative exponent $q = -p$ determining the low-frequency expansion of polarisability (3) can be represented as

$$S_{nlm(0)}^{(-p)} = \frac{2}{2n+1} \langle nl = n-1 | r [g_{l'=n}^{(n)}(r; r')]^{p-1} r' | nl \rangle, \quad (6)$$

where the exponentiation, $[g_{l'=n}^{(n)}(r; r')]^{p-1}$, is the $(p-2)$ -fold integration of the product $p-1$ of the radial Green's functions,

$$[g_{l'}^{(n)}(r; r')]^{p-1} = \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 \dots \int_0^\infty r_{p-2}^2 dr_{p-2} g_{l'}^{(n)}(r; r_1) \times g_{l'}^{(n)}(r_1; r_2) \dots g_{l'}^{(n)}(r_{p-2}; r'). \quad (7)$$

For the function $g_{l'}^{(n)}(r; r')$, one can use the spectral expansion

$$g_{l'}^{(n)}(r, r') = \sum_{n'} \frac{R_{n'l'}(r) R_{n'l'}(r')}{E_{n'} - E_n} + \int_0^\infty \frac{R_{\varepsilon l'}(r) R_{\varepsilon l'}(r')}{\varepsilon - E_n} d\varepsilon, \quad (8)$$

where $R_{n'l'}(r)$ is the radial wave function of the bound state; $R_{\epsilon l'}(r)$ is the radial function of the stationary state of the continuum with positive energy, $\epsilon > 0$; and E_n is the energy of the level. The orbital momentum of intermediate states in (6)–(8) is $l' = l + 1 = n$, since the result of integration in the matrix element with respect to angular variables

$$\begin{aligned} |\langle n'l'm'|z|nlm\rangle|^2 &= \frac{l_{>}^2 - m^2}{(2l'+1)(2l+1)} |\langle n'l'|r|nl\rangle|^2 \delta_{m'm} \\ &= \frac{|\langle n'l'|r|nl\rangle|^2}{2n+1} \delta_{l'l+1} \delta_{m'm} \end{aligned} \quad (9)$$

vanishes for $l' = l - 1$. Here $l_{>} = \max(l', l)$.

The orthogonality of radial wave functions makes it possible to write the relation

$$\begin{aligned} [g_{l'}^{(n)}(r, r')]^{2p+1} &= \sum_{n'} \frac{R_{n'l'}(r) R_{n'l'}(r')}{(E_{n'} - E_n)^{2p+1}} \\ &+ \int_0^\infty \frac{R_{\epsilon l'}(r) R_{\epsilon l'}(r')}{(\epsilon - E_n)^{2p+1}} d\epsilon. \end{aligned} \quad (10)$$

The use of expressions (8) and (10) does not allow us to calculate the matrix element (6) in a closed analytical form. Therefore, the expansion of the Green's function in terms of the Sturm functions [22] $F_{kl'}(x) = x^l \exp(-x/2) L_k^{2l'+1}(x)$, where $L_k^{2l'+1}(x)$ is the associated Laguerre polynomial [23]:

$$\begin{aligned} g_{l'=n}^{(n)}(r, r') &= \frac{4Z}{(2n+1)!n} \sum_{k=0}^\infty \frac{k!}{(2n+2)_k (k+1)} \\ &\times F_{kn}\left(\frac{2Zr}{n}\right) F_{kn}\left(\frac{2Zr'}{n}\right), \end{aligned} \quad (11)$$

where $(a)_k = \Gamma(a+k)/\Gamma(a) = a(a+1)\dots(a+k-1)$ is the Pochhammer symbol [23].

The radial wave function can also be expressed through the Sturm function:

$$R_{n'l'}(r) = \frac{2Z^{3/2}}{(n')^2} \sqrt{\frac{n_r!}{(n'+l')!}} F_{n_r, l'}\left(\frac{2Zr}{n}\right), \quad (12)$$

where $n_r = n' - l' - 1$ is the radial quantum number. In particular, for the circular state $|nlm\rangle$ we have $|m| = l = n - 1$, so that $n_r = 0$, the Laguerre polynomial $L_0^{2l'+1}(x) = 1$, and the wave function has the form

$$R_{nl=n-1}(r) = \frac{2Z^{3/2}}{n^2 \sqrt{(2n-1)!}} \left(\frac{2Zr}{n}\right)^{n-1} \exp(-Zr/n). \quad (13)$$

Using expressions (7), (11), (13) and the orthogonality property of the Laguerre polynomials, we obtain the analytical expressions of the sums for (6) for circular states:

$$\begin{aligned} S_{nlm(0)}^{(-2)} &= \alpha_{nlm}(0) = \sum_{n'l'm'} \frac{2|\langle n'l'm'|z|nlm\rangle|^2}{\omega_{n'n}} \\ &= \frac{n^4(n+1)(4n+5)}{4Z^4}, \\ S_{nlm(0)}^{(-3)} &= \sum_{n'l'm'} \frac{2|\langle n'l'm'|z|nlm\rangle|^2}{\omega_{n'n}^2} \end{aligned} \quad (14)$$

$$= \frac{n^6(n+1)(8n^2+21n+14)}{8Z^6},$$

$$\begin{aligned} S_{nlm(0)}^{(-4)} &= \sum_{n'l'm'} \frac{2|\langle n'l'm'|z|nlm\rangle|^2}{\omega_{n'n}^3} = \frac{n^8(n+1)}{48Z^8} \\ &\times (48n^3 + 195n^2 + 269n + 126), \dots \end{aligned}$$

These expressions are applicable not only for Rydberg, but also for any circular states of hydrogen-like atoms with quantum numbers $l = |m| = n - 1$. For example, for the 1s state we have well-known values of matrix elements with the Green's function in the first, second, and third degrees, determining the susceptibility of an atom in static electric and magnetic fields [24]:

$$S_{1s}^{(-2)} = \alpha_{1s}(0) = 9/(2Z^4),$$

$$S_{1s}^{(-3)} = 43/(8Z^6),$$

$$S_{1s}^{(-4)} = 319/(12Z^8).$$

Expressions (14) determine, in particular, the region of applicability of expansion (3) for the dynamic polarisabilities of circular Rydberg states by the inequality $\omega \ll Z^2/n^3$. Obviously, on the right-hand side of this inequality is the frequency of the transition between neighbouring Rydberg states. For states with $n \approx 30$, this value is approximately 200 GHz; therefore, expansion (3) is applicable in the vicinity of these values of n for the microwave frequency not exceeding 20 GHz.

2.3. Analytical expressions for the sums of oscillator-strength moments with positive q

Polarisability expansions (3) and (4) make use of oscillator strengths with fixed directions of the photon polarisation vector along the z axis and the atomic orbital vector of the atom determined by the magnetic quantum number m . In a number of problems, the directions of the polarisation vectors and/or orbital momentum can be arbitrary. In particular, the distribution of all possible directions of the polarisation vectors of photons acting on the atom of thermal radiation (BBR) can be considered equally probable. In the case of free orientation of atoms, the directions of the vector of the orbital momentum (numerical values of the magnetic quantum number) can also be considered equally probable. The general relations of the quantum theory of angular momentum [19] make it possible to demonstrate the complete equivalence of the results of averaging over the directions of the polarisation vector for a fixed magnetic quantum number m and averaging over the directions of the vector of orbital momentum (over m) for a fixed projection of the electric dipole moment μ :

$$\overline{S_{nlm}^{(q)}} = \frac{1}{2l+1} \sum_m S_{nlm(\mu)}^{(q)} = \frac{1}{3} \sum_\mu S_{nlm(\mu)}^{(q)}, \quad (15)$$

where $S_{nlm(\mu)}^{(q)}$ is defined in (1). Both sums in (15) yield the same result, which depends neither on m nor on μ .

Further, when calculating sums (1) with $q > 0$, along with the fixed directions of the vectors [as in expressions (3)–(6)], we will use averaging over the projections of the photon

polarisation vector, which reduces to additional summation over the projections of the operator of the dipole electric moment and to division by 3. Averaging over the projections of the dipole moment is necessary when calculating the interaction energy of an atom with randomly polarised radiation, in particular with environmental thermal radiation. Note that these averagings do not affect the basic summation rule for $q = 0$ (Thomas–Reiche–Kuhn rule), so that $S_{nlm(0)}^{(0)} = \overline{S_{nlm}^{(0)}} = 1$. It should also be noted that in the calculations of the sums of moments (1) for $q \neq 0$, averaging is usually performed over projections of the dipole moment [20, 21].

In calculating averaged sums (15), the following operator identities can be used:

$$\begin{aligned} i[\hat{p}, r] &= 3, \quad i[\hat{H}, r] = \hat{p}, \\ i[\hat{H}, \hat{p}] &= -\nabla V(r) = \frac{Zr}{r^3}, \end{aligned} \quad (16)$$

$$[\hat{p}, [\hat{H}, \hat{p}]] = \Delta V(r) = 4\pi Z\delta(r),$$

with the Hamiltonian \hat{H} , the internal atomic potential $V(r)$, the radius vector r , and the momentum operator \hat{p} of the optical electron. These relations yield the identities for matrix elements [20]:

$$\omega_{n'n} \langle n'l'm' | x_\mu | nlm \rangle = i \langle n'l'm' | \hat{p}_\mu | nlm \rangle, \quad (17)$$

$$\omega_{n'n} \langle n'l'm' | \hat{p} | nlm \rangle = i \langle n'l'm' | \nabla V(r) | nlm \rangle,$$

transforming frequency factors into corresponding operators inside the matrix element. After such transformations, it suffices to use the condition of completeness of the set of eigenstates of the valence electron

$$\sum_{n'l'm'} \langle r | n'l'm' \rangle \langle n'l'm' | r' \rangle = \delta(r - r'), \quad (18)$$

to express sums (15) as the average value of the function of the radial variable, similarly to expression (5). Using relation (15) for averaged values, as well as averaging the matrix element from angular variables

$$\begin{aligned} \frac{1}{2l+1} \sum_{m=-l}^l \langle lm | \cos^2 \theta | lm \rangle &= \frac{1}{2l+1} \sum_{m=-l}^l \frac{1}{2l+3} \\ &\times \left(1 + 2 \frac{l^2 - m^2}{2l-1} \right) = \frac{1}{3}, \end{aligned} \quad (19)$$

we obtain the expressions

$$\begin{aligned} S_{nlm(0)}^{(1)} &= 2 \langle nl | \frac{Z}{r} | nl \rangle \langle lm | \cos^2 \theta | lm \rangle, \\ \overline{S_{nlm}^{(1)}} &= \frac{2}{3} \langle nl | \hat{p}^2 | nl \rangle = \frac{2}{3} \langle nl | \frac{Z}{r} | nl \rangle = \frac{2Z^2}{3n^2}, \\ S_{nlm(0)}^{(2)} &= \langle nl | \frac{Z}{r^3} | nl \rangle (1 - 3 \langle lm | \cos^2 \theta | lm \rangle), \\ \overline{S_{nlm}^{(2)}} &= \frac{Z}{3} |R_{nl}(0)|^2 = \frac{4Z^4}{3n^3} \delta_{l0}, \end{aligned} \quad (20)$$

where δ_{l0} is the Kronecker delta.

It should be noted that the sums $S_{nlm}^{(0)}$ and $\overline{S_{nlm}^{(1)}}$ were used to derive asymptotic formulae for the shift and broadening of Rydberg energy levels by thermal radiation [11–13]. For states with a nonzero orbital momentum $S_{nlm}^{(2)} = 0$, which means mutual reduction of the negative contribution $\overline{S_{nlm}^{(2-)}}$ of the finite number of terms with $n' < n$ from the sum on the right-hand side of expression (1) with the positive contribution $\overline{S_{nlm}^{(2+)}}$ of an infinite number of terms of the sums over the states of the discrete spectrum and the integral over the continuous spectrum: $\overline{S_{nlm}^{(2-)}} = -\overline{S_{nlm}^{(2+)}}$. The negative contribution is proportional to the rate of spontaneous decay: $\overline{S_{nlm}^{(2-)}} = -(c^3/2)\Gamma_{nl}^{\text{sp}}$ (see Section 3.1 below). Therefore, for an infinite sum over $n' > n$ and an integral over the continuous spectrum from the right-hand side of expression (1), we can also write a closed analytic expression $\overline{S_{nlm}^{(2+)}} = (c^3/2)\Gamma_{nl}^{\text{sp}}$. Using the analytic expression for Γ_{nl}^{sp} in the case of circular states [7], we find the relation

$$\begin{aligned} -\overline{S_{nlm}^{(2-)}} &= \overline{S_{nlm}^{(2+)}} = \frac{2}{3} \sum_{(n'>n)l'm'\mu} \omega_{n'n}^3 |\langle n'l'm' | r_\mu | nlm \rangle|^2 \\ &= \frac{Z^4}{3n^3(n-1/2)(n-1)} \left[1 - \frac{1}{(2n-1)^2} \right]^{2n-1}. \end{aligned} \quad (21)$$

Similarly, one can also obtain closed expressions for infinite sums and integrals resulting from closed expressions for the rules of summation of higher-order oscillator-strength moments. Obviously, with an increase in q , additional commutators appear in terms of sums (15), which are expressed in by the kinetic and potential energy operators and their derivatives. For circular states, we have the expressions

$$\begin{aligned} S_{nlm(0)}^{(3)} &= 2 \langle nl | \frac{Z^2}{r^4} | nl \rangle \langle lm | \cos^2 \theta | lm \rangle, \\ \overline{S_{nlm}^{(3)}} &= \frac{2}{3} \langle nl | \frac{Z^2}{r^4} | nl \rangle = \frac{16Z^6}{3n^5(2n-3)_3}, \\ S_{nlm(0)}^{(4)} &= \langle nl | \frac{Z^2}{r^6} | nl \rangle (1 + 3 \langle lm | \cos^2 \theta | lm \rangle), \\ \overline{S_{nlm}^{(4)}} &= 2 \langle nl | \frac{Z^2}{r^6} | nl \rangle = \frac{64Z^8}{n^7(2n-5)_5}, \\ \overline{S_{nlm}^{(5)}} &= \frac{2}{3} n(n-1) \langle nl | \frac{Z^2}{r^8} | nl \rangle - \frac{8Z^2}{3} \langle nl | \left(\frac{1}{r^3} \frac{\partial}{\partial r} \right)^2 | nl \rangle \\ &+ \frac{8Z^2}{3} \langle nl | \frac{1}{r^7} \frac{\partial}{\partial r} | nl \rangle = \frac{Z}{6} \left(\frac{2Z}{n} \right)^9 \frac{n^2 + n + 18}{(2n-7)_7}. \end{aligned} \quad (22)$$

As can be seen from expressions (20)–(23) for the sums of oscillator-strength moments, with increasing q , the quantities $S_{nlm}^{(q)}$ quickly decrease with increasing principal quantum number n . Moreover, $S_{nlm}^{(q)} \propto Z^{2q}/n^{3q}$ for even $q = 2k$ and $S_{nlm}^{(q)} \propto Z^{2q}/n^{3q-1}$ for odd $q = 2k-1$ ($k = 0, 1, 2, \dots$ are natural numbers). These asymptotics take into account the first non-vanishing terms of the expansions of the exact values of the sums (20)–(23), which we will use below to calculate the corrections to the asymptotic formulae for induced broadenings and shifts of energy levels of circular Rydberg states.

3. Natural and BBR-induced widths of the circular-state energy level

3.1. Natural width

The spontaneous energy width of the level of the circular state $|nlm\rangle$ represents the rate of dipole radiative decay to the nearest state $|n' = n - 1, l' = l - 1\rangle$. For this probability, one can obtain a closed analytical expression [7] in a form convenient for simplified estimates:

$$\Gamma_n^{\text{sp}} = -\frac{2}{c^3} S_{nlm}^{(2-)} = 1704.554 \frac{Z^4}{n^5} \gamma_n \text{ (in MHz)}, \quad (24)$$

where the factor

$$\gamma_n = \frac{1}{(1 - 1/n)[1 - 1/(2n)]} \left\{ \frac{1 - 1/n}{[1 - 1/(2n)]^2} \right\}^{2n-1} \quad (25)$$

slowly decreases with increasing n ($\gamma_2 = 1.873$, $\gamma_{20} = 1.052$, $\gamma_n \xrightarrow{n \rightarrow \infty} 1$). From (24) we obtain a simple formula for estimating the natural lifetime of a circular state:

$$\tau_n^{\text{sp}} = \frac{1}{\Gamma_n^{\text{sp}}} = 9.337 \frac{(n/10)^5}{\gamma_n Z^4} \text{ (in } \mu\text{s)}. \quad (26)$$

The spontaneous energy width of states with arbitrary orbital momenta $1 < l < n - 1$ can be represented as $\Gamma_{nl}^{\text{sp}} \approx [855.4/(n^3 l^2)] f(n, l) Z^4$ (in MHz). Here $f(n, l)$ is a dimensionless factor that smoothly depends on l and almost coincides with unity for small l and slowly increases with increasing l , so that for large values of the orbital momentum $f(n, l = n - 1) \approx 2$ [5, 7, 20]. This shows that the natural width of the circular state is approximately n^2 times smaller than the width of the highly excited hydrogen-like state with a small angular momentum $l \ll n$. This circumstance contributes to 'survival', increasing the possibility of the practical use of states with maximum orbital moments from a hydrogen-like energy shell with a fixed n .

3.2. BBR-induced broadening

It can be seen from expression (26) that the natural lifetime of the circular Rydberg-shell state with $n = 100$ is approximately 1 s. For $n = 200$, the lifetime will be about 30 s. However, in practice, the ubiquitous thermal radiation of the environment can significantly reduce the lifetime of an atom in a highly excited state and even turn an atom into an ion due to photo-ionisation [14–16].

Interaction of the BBR with the electromagnetic field leads to broadening of atomic levels, which is equal to the sum of probabilities of induced transitions

$$\begin{aligned} \Gamma_{nlm}^{\text{BBR}}(T) &= \frac{4}{3c^3} \sum_{n'l'm'\mu} \frac{|\omega_{n'n}|^3 |\langle n'l'm' | r_\mu | nlm \rangle|^2}{\exp[|\omega_{n'n}|/(k_B T)] - 1} \\ &= \frac{2}{3c^3} \sum_{n'} \frac{\omega_{n'n}^2 |f_{n'n(\mu)}|}{\exp[|\omega_{n'n}|/(k_B T)] - 1}, \end{aligned} \quad (27)$$

where the summation is performed over the projections μ of the dipole moment, as well as over the complete set of states with fixed orbital l' and magnetic m' quantum numbers, including states of the continuum. The term corresponding to the single possible radiative decay of the circular state $|nlm\rangle$

with the transition to the state with quantum numbers $n' = n - 1$, $l' = l - 1$, $|m'| = |m| - 1$, is the probability of thermally induced decay

$$\Gamma_{nl}^{\text{d}} = \Gamma_{nl}^{\text{sp}} \bar{n}(\omega_{nn-1}, T), \quad (28)$$

different from the probability of spontaneous decay (24) by a factor

$$\bar{n}(\omega_{nn-1}, T) = \frac{1}{\exp[\omega_{nn-1}/(k_B T)] - 1}. \quad (29)$$

Function (29) determines the number of thermal photons (occupation number or population) from the Planck distribution at a frequency $\omega_{nn-1} = Z^2[1 - 1/(2n)]/[n^3(1 - 1/n)^2]$. This function can be considered as the relative (compared to the spontaneous) rate of stimulated radiative decay $\bar{n}(\omega_{nn-1}, T) = \Gamma_{nl}^{\text{d}}(T)/\Gamma_{nl}^{\text{sp}}$ of the circular state of an atom under the influence of thermal radiation. It should be noted that, for a small parameter $\eta = Z^2/(n^3 k_B T) \ll 1$, the value of $\bar{n}(\omega_{nn-1}, T) \approx n^3 k_B T / Z^2$ grows rapidly with the product $n^3 T$, and in this case it is Z^2 times smaller for ions as compared to $\bar{n}(\omega_{nn-1}, T)$ for neutral atoms. Such an estimate of the number of photons corresponds to taking into account only the main term ($1/x$) in the expansion in powers of the exponent in the fraction on the right-hand side of (29)

$$\begin{aligned} \frac{1}{\exp(x) - 1} &= -\frac{1}{2} + \frac{1}{2} \coth\left(\frac{x}{2}\right) = \frac{1}{x} - \frac{1}{2} + \frac{x}{12} - \frac{x^3}{720} \\ &+ \frac{x^5}{30240} - o((x/6)^7). \end{aligned} \quad (30)$$

Replacing the factor $\{\exp[|\omega_{n'n}|/(k_B T)] - 1\}^{-1}$ by the first term of expansion (30) and using the summation rule for $S_{nlm}^{(1)}$ from expressions (20) gives a well-known asymptotic result for the probability of the BBR-induced decay of the Rydberg state [11, 12]:

$$\Gamma_{nlm}^{\text{BBR}}(T) \approx \Gamma_n^{(0)}(T) = \frac{2k_B T S_n^{(1)}}{c^3} = \frac{4Z^2 k_B T}{3c^3 n^2}. \quad (31)$$

For $x < 1$, the terms of the sign-alternating series on the right-hand side of expression (30) quickly decrease, so that the first three terms provide an approximation of the function $\{\exp[|\omega_{n'n}|/(k_B T)] - 1\}^{-1}$ with a relative error not exceeding 0.2%, and the account of the fourth term reduces the error by additional two orders of magnitude. Note that at room temperature ($T \approx 300$ K) the argument of the exponent in (27) and (29) takes values below unity for $n \geq 11Z^{2/3}$.

Of interest from the point of view of numerical calculation and determination of the region of applicability of the expression for the thermally induced width (27) is the x independent constant term in expansion (30), equal to $-1/2$. This term, taking into account the equality of the contributions of states with $n' < n$ and with $n' > n$ in sum (27), gives a negative correction to the asymptotic expression for the thermally induced width (31), which exactly coincides in absolute value with the spontaneous width (24). Thus, in the expansion in powers of the parameter η of the total probability $\Gamma_n^{\text{tot}}(T) = \Gamma_n^{\text{sp}} + \Gamma_n^{\text{BBR}}(T)$ of the Rydberg state decay, there is no temperature-independent component, and the first nonvanishing correction to $\Gamma_n^{(0)}(T)$ is proportional to η^2 . Therefore, the asymptotic formula for $\Gamma_n^{\text{tot}}(T)$ can be expressed as

$$\Gamma_n^{\text{tot}}(T) = \Gamma_n^{(0)}(T)[1 + a_1\eta^2 - a_2\eta^4 + o(\eta^6)]. \quad (32)$$

The coefficients of this expansion a_k are determined by the coefficients of series (30) and the sum rules for the moments $S_{nlm}^{(q)}$ with odd exponents $q = 2k + 1$:

$$\begin{aligned} a_1 &= \frac{n^6 \overline{S_{nlm}^{(3)}}}{12Z^4 \overline{S_{nlm}^{(1)}}} = \frac{2n^3}{3(2n-3)_3}, \\ a_2 &= \frac{n^{12} \overline{S_{nlm}^{(5)}}}{720Z^8 \overline{S_{nlm}^{(1)}}} = \frac{8n^5(n^2+n+18)}{45(2n-7)_7}. \end{aligned} \quad (33)$$

The opposite signs of the corrections $a_1\eta^2$ and $-a_2\eta^4$ correspond to the signs of the corresponding terms $x/12$ and $-x^3/720$ in expansion (30). Note that the coefficient η^2 in [7] is written as an expansion in powers of the small parameter $1/n$, which exactly coincides with the expansion of the closed expression for a_1 from (33).

Thus, for $\eta \leq 1$, the total width (32) (spontaneous plus thermally induced) of the energy level of the circular state coincides with the asymptotic expression (31) for the thermally induced width with a relative error on the order $a_1\eta^2 \approx \eta^2/12$. The higher-order corrections for $\eta \leq 1$ are negligible, since the coefficient a_2 is 12 times smaller than a_1 for $n = 10$, and with increasing n this ratio gradually decreases, so that $a_2/a_1 \rightarrow 1/60$ for $n \rightarrow \infty$, as can be seen from explicit expressions (33). At $T = 100$ K and $n = 15$, the parameter $\eta \approx Z^2$ and the correction to $\Gamma_n^{(0)}(T)$ for a neutral atom ($Z = 1$) do not exceed 10% (40% for a singly ionised atom, $Z = 2$).

A comparison of $\Gamma_n^{(0)}(T)$ with the spontaneous width (24) shows that at room temperature the total width (32) exceeds the spontaneous one for all circular Rydberg states of atoms and ions with principal quantum numbers $n > 8$. The dependence on the core charge and temperatures for this inequality can be supplemented by the expression $n > 8(Z^2 300/T)^{1/3}$. Note that this dependence is smoother than a similar dependence in the inequality $n > bZ^2 300/T$ for states with small orbital moments, where the coefficient b takes different values for Rydberg states of different series of multielectron atoms: $2 < b < 20$ [17, 25].

4. Thermally induced energy level shift of the circular state

The shift of the energy level of the circular state under the action of the BBR electric field can be represented in the form [13]

$$\varepsilon_{nlm}^{\text{BBR}}(T) = -\frac{\alpha_{nlm}(\omega_{\text{max}})}{2} \overline{E^2}(T), \quad (34)$$

where $\alpha_{nlm}(\omega_{\text{max}})$ is the dynamic polarisability at the frequency $\omega_{\text{max}} \approx 2.82k_B T$ corresponding to the maximum of the frequency-dependent distribution $E^2(\omega, T) = [8\omega^3/(\pi c^3)] \times \{\exp[\omega/(k_B T)] - 1\}^{-1}$ of the BBR electric field squared; and

$$\overline{E^2}(T) = \int_0^\infty \frac{E^2(\omega, T)}{2} d\omega = \frac{4\pi^3}{15c^3} (k_B T)^4 \quad (35)$$

is the average of the BBR electric field squared. For low ambient temperatures, that is, for $1/\eta = (n^3 k_B T)/Z^2 \ll 1$, the frequency ω_{max} is also small, so that the dynamic polarisability in (34) can be replaced by the static one (14), $\alpha_{nlm}(\omega_{\text{max}}) \approx$

$\alpha_{nlm}(0)$. Then, taking into account (14), expression (34) for the circular state can be rewritten in the form

$$\varepsilon_{nlm}^{\text{BBR}}(T) = -2.1528 \frac{n^4(n+1)(4n+5)}{4Z^4} \left(\frac{T}{300}\right)^4 \text{ (mHz)}. \quad (36)$$

In particular, for $n = 5$ at a temperature $T < 300Z^2$ (in K) satisfying the condition $\eta \gg 1$, the thermally induced shift is $\varepsilon_{nlm}^{\text{BBR}}(T) \approx -[T/(300Z)]^4 \times 247.86$ (in Hz). The dynamic correction taking into account the quadratic term in the expansion of polarisability in frequency (3) is below $[T/(300Z^2)]^2 \times 0.05\%$ of this value.

In the case of the opposite inequality, for the ratio of the transition energy to thermal energy, $\eta \ll 1$, one could use the expansion of the real part of polarisability (4) over even powers of the reciprocal frequency. However, integration over the BBR frequency of the product of series (4) and the distribution $E^2(\omega, T)$ is possible only for the first term of this series, which is independent of the principal quantum number n . The result of this integration gives the well-known asymptotic expression [11–13]

$$\varepsilon_0(T) = \frac{\pi(k_B T)^2}{3c^3} = 2416.65(T/300)^2 \text{ (Hz)}. \quad (37)$$

The integrals over the BBR frequencies with the higher-order terms of series (4) diverge in the lower limit, $\omega = 0$. Therefore, to obtain corrections to $\varepsilon_0(T)$ in analytical form, one can use the function [13]

$$F(y) = -2yP \int_0^\infty \frac{x^3 dx}{(x^2 - y^2)[\exp(x) - 1]}, \quad (38)$$

where P is the notation for the principal value of the integral, which effectively takes into account the frequency dependence of the real part of the dynamic polarisability in the integral determining the BBR-induced shift of the atomic energy level [26]:

$$\begin{aligned} \varepsilon_{nl}^{\text{BBR}}(T) &= -\frac{2}{3\pi c^3} P \int_0^\infty \left[\sum_{n'l'm'\mu} \frac{2\omega_{n'n} |\langle n'l'm'|r_\mu|nlm\rangle|^2}{\omega_{n'n}^2 - \omega^2} \right. \\ &+ \left. \int_0^\infty \frac{2(\varepsilon + |E_{nl}|) |\langle \varepsilon l'm'|r_\mu|nlm\rangle|^2 d\varepsilon}{(\varepsilon + |E_{nl}|)^2 - \omega^2} \right] \frac{\omega^3 d\omega}{\exp[\omega/(k_B T)] - 1} \\ &= -\frac{2(k_B T)^3}{3\pi c^3} \left\{ \sum_{n'l'm'\mu} [|\langle n'l'm'|r_\mu|nlm\rangle|^2 F\left(\frac{\omega_{n'n}}{k_B T}\right)] \right. \\ &+ \left. \int_0^\infty |\langle \varepsilon l'm'|r_\mu|nlm\rangle|^2 F\left(\frac{\varepsilon + |E_{nl}|}{k_B T}\right) d\varepsilon \right\}. \end{aligned} \quad (39)$$

Here, the summation over the projections of the dipole moment corresponds to taking into account all possible polarisations of the BBR photons. Function (38) can be transformed to a form that allows obtaining a closed analytical expression [7] $F(y) = -\pi^2 y/3 - 2y^3 \text{Re}\{\Phi(iy)\}$, where [27]

$$\begin{aligned} \Phi(z) &= \int_0^\infty \frac{xdx}{(x^2 + z^2)[\exp(x) - 1]} \\ &= \frac{1}{2} \left[\ln\left(\frac{z}{2\pi}\right) - \frac{\pi}{z} - \psi\left(\frac{z}{2\pi}\right) \right], \quad \text{Re } z > 0. \end{aligned} \quad (40)$$

The function $\psi(x) = d\{\ln\Gamma(x)\}/dx$ is the logarithmic derivative of the gamma function. Using the analytic continuation for the right-hand side of expression (40) and setting $z = \pm i|y| + \delta$, we obtain for $\delta \rightarrow 0$

$$F(y) = -\frac{\pi^2}{3}y - \left\{ \ln\left(\frac{|y|}{2\pi}\right) - \operatorname{Re}\left[\psi\left(i\frac{|y|}{2\pi}\right)\right] \right\} y^3. \quad (41)$$

To determine the real part of the ψ -function in this expression, we can use the expansion in series [28]

$$\operatorname{Re}\left[\psi\left(i\frac{|y|}{2\pi}\right)\right] = -\gamma + \frac{y^2}{4\pi^2} \sum_{k=1}^{\infty} \frac{1}{k[k^2 + y^2/(4\pi^2)]},$$

where $\gamma = 0.5772156649$ is the Euler constant. Using the expansion of the terms of the series in powers of the ratio $y^2/(4\pi^2k^2)$ and performing the summation over k , we obtain a formal expansion of function (38) in series of odd powers of the argument [7]:

$$F(y) = -\frac{\pi^2}{3}y - \left[\ln\left(\frac{|y|}{2\pi}\right) + \gamma + \sum_{p=1}^{\infty} (-1)^p \times \zeta(2p+1) \left(\frac{y}{2\pi}\right)^{2p} \right] y^3, \quad (42)$$

where

$$\zeta(s) = \sum_{k=1}^{\infty} k^{-s}$$

is the Riemann zeta function [27, 28]. The term proportional to y^3 must be taken into account in the region $|y| > 0.01$, and to achieve accuracy in the sixth decimal place in the region $0.1 < |y| < 1$, one should also take into account the first term of the sum from the factor (in square brackets) at y^3 . Detailed discussions of the properties of expression (42) are given in [7].

For a shift, as well as for broadening the energy level of the Rydberg circular state, it is possible to propose a polynomial approximation that significantly expands the range of use of the asymptotic approximation (37), identical for all Rydberg states and is independent of n and Z , which corresponds to taking into account only the first (linear) term in expansion (42). Such an approximation determines the shift (39) with a relative error of the order of 10^{-3} under the condition $n^3k_B T > 100Z^2$, which corresponds to the numerical values of the principal quantum number $n > 47\sqrt[3]{300Z^2/T}$.

The expression for the corrections to $\varepsilon_0(T)$, improving precision of $\varepsilon_n^{\text{BBR}}(T)$ for lower values of the principal quantum number n and temperature T , can be obtained by taking into account the term proportional to y^3 from the right-hand side of expression (42). To this end, we substitute (42) into (39) and rewrite the expression for $\varepsilon_n^{\text{BBR}}(T)$ using definition (14) for the averaged oscillator strengths:

$$\varepsilon_{nl}^{\text{BBR}}(T) = \frac{1}{\pi c^3} \left[\frac{(\pi k_B T)^2}{3} \overline{S_{nlm}^{(0)}} + \tilde{S}_{nlm}^{(2)} + \gamma \overline{S_n^{(2)}} + \sum_{p=1}^{\infty} \frac{(-1)^p \zeta(2p+1)}{(2\pi k_B T)^{2p}} \overline{S_n^{(2p+2)}} \right]. \quad (43)$$

A special notation is introduced here for the oscillator strengths with a logarithmic factor

$$\tilde{S}_{nlm}^{(2)} = \frac{2}{3} \sum_{n'l'm'} \omega_{n'n}^3 |\langle n'l'm' | r_{\mu} | nlm \rangle|^2 \ln\left(\frac{|\omega_{n'n}|}{2\pi k_B T}\right). \quad (44)$$

Because $\overline{S_n^{(2)}} = 0$, the third term (Euler constant γ) in square brackets on the right-hand side of (42) can be omitted, and the term $\ln(2\pi/\eta)$ independent of n' can be added to the logarithm. Then expression (44) transforms to the form

$$\tilde{S}_{nlm}^{(2)} = \frac{2}{3} \sum_{n'l'm'} \omega_{n'n}^3 |\langle n'l'm' | r_{\mu} | nlm \rangle|^2 \ln\left(\frac{n^3 |\omega_{n'n}|}{Z^2}\right), \quad (45)$$

clearly showing that the thermally induced shift (43) contains a temperature-independent term. It is not possible to obtain an analytical expression for sum (45) in closed form. Therefore, to estimate $\tilde{S}_{nlm}^{(2)}$, one can use the series expansion in powers of the small parameter $|p/n| \ll 1$, where $p = n' - n$, for each of the three factors of the product summed over n' from the right-hand side of expression (45). Since the argument of the logarithm in (45) is close to unity, the expansion for it has the form

$$\ln\left(\frac{n^3 |\omega_{n'n}|}{Z^2}\right) = \ln|p| - \frac{3p}{2n} + \frac{7p^2}{8n^2} - \frac{5p^3}{8n^3} + \dots \quad (46)$$

Substituting the expansions [similar to (46)] for $\omega_{n'n}^3$ and the radial matrix elements $|\langle n'l' | r | nl \rangle|^2$ into (45) (after integration over the angular variables of the matrix elements $\langle n'l'm' | r_{\mu} | nlm \rangle$ [7]), we obtain a series of terms representing the quantity $\tilde{S}_{nlm}^{(2)}$ in the form of an expansion in powers of the small parameter $1/n \ll 1$. Confining ourselves to terms of the order of $1/n^3$, we can write

$$\tilde{S}_{nlm}^{(2)} = -A_1 \pi c^3 \varepsilon_0(T) \eta^2 B_1(n) = -\frac{\pi^2 Z^4}{3n^6} A_1 B_1(n), \quad (47)$$

where $A_1 = [3 - 4\ln(2)]/\pi^2 = 0.0230416$ is a constant; and $B_1(n) = 1 + b_1/n + b_2/n^2 + b_3/n^3$ is the cubic polynomial with coefficients

$$b_1 = \frac{9[32\ln(2) - 27\ln(3) + 8]}{8[3 - 4\ln(2)]} \approx 2.56342, \\ b_2 = -\frac{42496\ln(2) - 25515\ln(3) - 1464}{48[3 - 4\ln(2)]} \approx 3.58290, \\ b_3 = \frac{7819264\ln(2) - 2123577\ln(3) - 1953125\ln(5) + 56880}{384[3 - 4\ln(2)]} \\ \approx 4.11773. \quad (48)$$

Thus, by analogy with the formula for thermally induced broadening (32), the expression for shift (43) can be written as an expansion in even powers of the parameter η :

$$\varepsilon_{nl}^{\text{app}}(T) = \varepsilon_0(T) [1 - \eta^2 A_1 B_1(n) - \eta^4 A_2 B_2(n) + o(\eta^6)], \quad (49)$$

where the constant $A_2 = 3\zeta(3)/(2\pi^4) \approx 0.0185104$ and the factor $B_2(n) = (2n)^5/(2n-5)_5$ is determined from the explicit expression in (22) for the sum of the angular moments of the oscillator strengths $S_{nlm}^{(4)}$. The second term in (49) corresponds to the second term in square brackets in expression (43) and determines the temperature-independent component of the thermally induced shift

Table 1. Numerical values of the parameter η , η^2 proportional corrections to $\varepsilon_0(T)$, corrections to broadening $\Delta\Gamma_n^{\text{app}}(T) = a_1\eta^2/Z^4 - a_2\eta^4/Z^8$ and $\Delta\Gamma_n^{\text{BBR}}(T) = [\Gamma_n^{\text{BBR}}(T) - \Gamma_n^{(0)}(T)]/\Gamma_n^{(0)}(T)$; as well as to the shifts $\Delta\varepsilon_{nl}^{\text{app}}(T) = -\eta^2 A_1 B_1(n) - \eta^4 A_2 B_2(n)$ and $\Delta\varepsilon_{nl}^{\text{BBR}}(T) = [\varepsilon_{nl}^{\text{BBR}}(T) - \varepsilon_0(T)]/\varepsilon_0(T)$ for circular states with principal quantum numbers n for neutral atoms ($Z = 1$) at $T = 300$ K.

n	η/Z^2	$-\eta^2 A_1 B_1(n)/Z^4$	$\Delta\Gamma_n^{\text{app}}$	$\Delta\Gamma_n^{\text{BBR}}$	$\Delta\varepsilon_{nl}^{\text{app}}(T)$	$\Delta\varepsilon_{nl}^{\text{BBR}}(T)$
10	1.0526	-3.3093×10^{-2}	1.1604×10^{-1}	1.2040×10^{-1}	-8.3791×10^{-2}	-6.2326×10^{-2}
15	0.3119	-2.6626×10^{-3}	9.9404×10^{-3}	9.9114×10^{-3}	-2.9594×10^{-3}	-2.9631×10^{-3}
20	0.1316	-4.5379×10^{-4}	1.6828×10^{-3}	1.6765×10^{-3}	-4.6199×10^{-4}	-4.7189×10^{-4}
30	0.0390	-3.8156×10^{-5}	1.4025×10^{-4}	1.4006×10^{-4}	-3.8211×10^{-5}	-3.8588×10^{-5}
50	0.0084	-1.7200×10^{-6}	6.2789×10^{-6}	6.2784×10^{-6}	-1.7201×10^{-6}	-1.7213×10^{-6}

$$\tilde{\varepsilon} = \frac{\tilde{S}_n^{(2)}}{\pi c^3} = -\frac{\pi Z^4}{3c^3 n^6} A_1 B_1(n). \quad (50)$$

For clarity, Table 1 lists the numerical values of the parameter η/Z^2 and the values of $-\eta^2 A_1 B_1(n)/Z^4$ at room temperature $T = 300$ K and various values of the principal quantum number n . The fourth and fifth columns of Table 1 show the numerical values of the relative corrections to the asymptotic value of $\Gamma_n^{(0)}(T)$ for the total broadening (32) in a neutral atom ($Z = 1$)

$$\Delta\Gamma_n^{\text{app}}(T) = [\Gamma_n^{\text{tot}}(T) - \Gamma_n^{(0)}(T)]/\Gamma_n^{(0)}(T) \approx a_1\eta^2 - a_2\eta^4$$

and corrections to $\Gamma_n^{(0)}(T)$ for the exact value of width (27)

$$\Delta\Gamma_n^{\text{BBR}}(T) = [\Gamma_n^{\text{BBR}}(T) - \Gamma_n^{(0)}(T)]/\Gamma_n^{(0)}(T).$$

The sixth and seventh columns give numerical values of the relative corrections to $\varepsilon_0(T)$ for the approximate value (49)

$$\Delta\varepsilon_{nl}^{\text{app}}(T) = [\varepsilon_{nl}^{\text{app}}(T) - \varepsilon_0(T)]/\varepsilon_0(T)$$

$$= -\eta^2 A_1 B_1(n) - \eta^4 A_2 B_2(n)$$

and corrections to $\varepsilon_0(T)$ for the exact value (39)

$$\Delta\varepsilon_{nl}^{\text{BBR}}(T) = [\varepsilon_{nl}^{\text{BBR}}(T) - \varepsilon_0(T)]/\varepsilon_0(T).$$

5. Conclusions

The results of analytical calculations obtained in this work provide important information about the accuracy and range of applicability of asymptotic expression (31) for thermally induced (27) and total (32) broadening, as well as expression (37) for the shift of the energy levels of circular states of atoms in the BBR field. The choice of circular orbits is justified not only by their presence in highly excited atoms of almost all elements of the periodic system, but also by the possibility of analytical calculations, since circular Rydberg states have zero quantum defects and are described by hydrogen-like wave functions. In an analytical form, the cancellation of the temperature-independent spontaneous component Γ_n^{sp} in the total width $\Gamma_n^{\text{tot}}(T) = \Gamma_n^{\text{sp}} + \Gamma_n^{\text{BBR}}(T)$, as well as the presence of the temperature-independent component $\tilde{\varepsilon}$ (50) in the expression for the shift of the Rydberg energy level are demonstrated. Note that the corrections to the asymptotic broad-

ening value are positive, as follows from (32) and (33), and the corrections to the shift asymptotics are negative, as can be seen from (49) and the data in Table 1.

For $n > 15$ and a fixed temperature $T = 300$ K, the main contribution to the deviations of $\Delta\Gamma_n^{\text{app}}(T)$ and $\Delta\varepsilon_{nl}^{\text{app}}(T)$ from the asymptotic values of $\Gamma_n^{(0)}(T)$ and $\varepsilon_0(T)$ of the thermally induced broadening and shift of the circular states of the neutral atom yield corrections proportional to η^2 : $a_1\eta^2$ and $-A_1 B_1(n)\eta^2$, respectively.

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References

1. Kleppner D. *Phys. Rev. Lett.*, **47**, 233 (1981).
2. Hulet R.G., Kleppner D. *Phys. Rev. Lett.*, **51**, 1430 (1983).
3. Hulet R.G., Hilfer E.S., Kleppner D. *Phys. Rev. Lett.*, **55**, 2137 (1985).
4. Nguen T.L., Raimond J.M., Sayrin C., et al. *Phys. Rev. X*, **8**, 011032 (2018).
5. Glukhov I.L., Mokhnenko S.N., Nikitina E.A., Ovsiannikov V.D. *Eur. Phys. J. D*, **69**, 1 (2015).
6. Kamenski A.A., Manakov N.L., Mokhnenko S.N., Ovsiannikov V.D., Zenischeva A.A. *Eur. Phys. J. D*, **72**, 174 (2018).
7. Kamenski A.A., Ovsiannikov V.D., Glukhov I.L. *Quantum Electron.*, **49**, 464 (2019) [*Kvantovaya Elektron.*, **49**, 464 (2019)].
8. Walker T.G., Saffman M. *Phys. Rev. A*, **77**, 032723 (2008).
9. Saffman M., Walker T.G., Mølmer K. *Rev. Mod. Phys.*, **82**, 2313 (2010).
10. Ryabtsev I.I., Beterov I.I., Tretyakov D.B., Yakshina E.A., Entin V.M. *Quantum Electron.*, **49**, 455 (2019) [*Kvantovaya Elektron.*, **49**, 455 (2019)].
11. Gallagher T.F., Cooke W.E. *Phys. Rev. Lett.*, **42**, 835 (1979).
12. Cooke W.E., Gallagher T.F. *Phys. Rev. A*, **21**, 588 (1980).
13. Farley J.W., Wing W.H. *Phys. Rev. A*, **23**, 2397 (1981).
14. Spencer W.P., Vaidyanathan A.G., Kleppner D., Ducas T.W. *Phys. Rev. A*, **26**, 1490 (1982).
15. Beterov I.I., Tretyakov D.B., Ryabtsev I.I., Ekers A., Bezuglov N.N. *Phys. Rev. A*, **75**, 052720 (2007).
16. Glukhov I.L., Ovsiannikov V.D. *J. Phys. B*, **42**, 075001 (2009).
17. Glukhov I.L., Nekipelov E.A., Ovsiannikov V.D. *J. Phys. B*, **43**, 125002 (2010).
18. Ovsiannikov V.D., Glukhov I.L., Nekipelov E.A. *J. Phys. B*, **44**, 195010 (2011).
19. Varshalovich D.A., Moskalev A.N., Khersonsky V.K. *Quantum Theory of Angular Momentum* (Singapore: World Scientific; Leningrad: Nauka, 1975).
20. Bethe H.A., Salpeter E.E. *Quantum Mechanics of One- and Two-Electron Atoms* (Berlin: Springer Verlag, 1957; Moscow: GIFFL, 1960).
21. Fano U., Cooper J.W. *Rev. Mod. Phys.*, **40**, 441 (1968).
22. Manakov N.L., Ovsiannikov V.D., Rapoport L.P. *Phys. Rep.*, **141**, 319 (1986).

23. Bateman H., Erdélyi A. *Higher Transcendental Functions* (New York: McGraw-Hill Book Co., 1953; Moscow: Nauka, 1973) Vols 1, 2.
24. Marmo S.I., Ovsianikov V.D. *Phys. Lett. A*, **202**, 201 (1995).
25. Ovsianikov V.D., Glukhov I.L. *Vestnik VGU. Ser. Fiz. Mat.*, (2), 99 (2006).
26. Glukhov I.L., Nikitina E.A., Ovsianikov V.D. *J. Phys. B*, **49**, 035003 (2016).
27. Gradshteyn I.S., Ryzhik I.M. *Tables of Integrals, Series and Products* (New York: Acad. Press, 1966; Moscow: Fizmatgiz, 1963).
28. Prudnikov A.P., Brychkov Yu.A., Marichev O.I. *Integrals and Series. Vol. 1: Elementary Functions* (New York: Gordon and Breach, 1986; Moscow: Nauka, 1981).