Calculation of the light-shifts in the \(ns\)-states of hydrogenic systems

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1 Introduction

Calculation of the light-shifts of both the ground and excited states of the atoms are mostly easily performed in the formalism of the so-called “dressed” atom (see e.g. [1]). Within the framework of this approach the shift, $\Delta \varepsilon_n$, of the level $n$ occurring due to the incident photon beam of the energy, $\omega$, and polarization, $e$, is defined as follows:

$$\Delta \varepsilon_n(\omega) = \frac{P}{2\varepsilon_0 \hbar^2 Sc} \Re \sum_{r} \left\{ \frac{\langle n|D\cdot e^*|r\rangle \langle r|D\cdot e|n\rangle}{\varepsilon_n + \omega - \varepsilon_r} + \frac{\langle n|D\cdot e|r\rangle \langle r|D\cdot e^*|n\rangle}{\varepsilon_n - \omega - \varepsilon_r} \right\}. \quad (1)$$

Here $D = e r$ is the dipole momentum operator of the electron; $P = \frac{1}{2} \varepsilon_0 ScE^2$ is the power of the photon beam with the cross section $S$ and the electric strength $E$; $\Re$ designates the real part. According to (1), the calculation of the shift, $\Delta \varepsilon_n$, reduces to that of the tensor of dynamical polarizability (DP), $\alpha_{ij}^n(\omega)$, of the state $n$. It is defined as (see e.g. [3])

$$\alpha_{ij}^n(\omega) = -\sum_{r} \left\{ \frac{\langle n|D_i|r\rangle \langle r|D_j|n\rangle}{\varepsilon_n + \omega - \varepsilon_r} + \frac{\langle n|D_j|r\rangle \langle r|D_i|n\rangle}{\varepsilon_n - \omega - \varepsilon_r} \right\}. \quad (2)$$

Here $D_i$ denotes the $i$th component of the vector of the dipole moment. An ab initio exact analytical calculation of DP is evidently possible for hydrogenic systems only and the corresponding results are known (in principle) for all states already for long time (see [4] and references herein). They are usually performed by means of the exact explicit expression for the non-relativistic Green’s function either in coordinate or momentum spaces. As a result, DP are expressed in terms of the special (Appel) functions whose complicated mathematical structure makes accurate numerical (and analytical) analysis of $\alpha_{ij}^n(\omega)$ hard to carry out. Especially this argument refers to the case when the photon energy, $\omega$, lies in the vicinity of the threshold: $\omega \sim I_n$, $I_n$ being the ionization potential of the state $n$. It is not surprising, therefore, that calculations of this type seem to be available for the hydrogenic 1s-state only (see [4]). In fact, provided that the principal quantum number, $n$, of the level is fixed, $\alpha_{ij}^n(\omega)$ has singularities when the photon energy, $\omega$, is in the resonance with the higher/lower discrete levels of the atom $\footnote{This singularities can be avoided if the finite widths of all atomic levels are taken into account.}$

2
\( \omega = |\varepsilon_i - \varepsilon_n|, \ i > n, i < n \). Beyond that, DP acquires also a non-zero imaginary part if \( \omega \geq I_n \). For such \( \omega \) the real part of DP, \( \Re \alpha^ij_n(\omega) \), describes (as for \( \omega < I_n \)) the shift of the level, whereas imaginary part, \( \Im \alpha^ij_n(\omega) \), allows for a decay probability (photoionization) of the atom under the action of the photon field. Namely, according to the optical theorem \([2]\): \( \sigma^{\gamma n}(\omega) = 4\pi \alpha \omega \Im \alpha^ij_n(\omega) \), where \( \sigma^{\gamma n}(\omega) \) is the total photoionization cross section of the state with the principal quantum number, \( n \), and \( \alpha = e^2/(\hbar c) = 1/137 \) is the fine structure constant. In mathematical terms, \( \alpha^ij_n(\omega) \) has unremovable singularity at the point \( \omega = I_n \), so that a great care must be taken to make numerical calculation within this region of \( \omega \) stable and highly accurate. The most efficient way of achieving that consists in combining numerical methods together with analytical ones. It is relevant to point out that the detailed description of the DP’s behavior of the mentioned type proves to be of particular importance, e.g. for the problem of the light-shifts’ calculation in muonium atom, denoted \((\mu^+ - e^-)^0\). This is due to the fact that in the highly accurate experimental measurements of the 1s – 2s energy splitting in this exotic system, which are in progress now, the energies, \( \omega_1 \) and \( \omega_2 \), of two incident photon beams are supposed to be in the resonance with the following transitions: 1s + \( \hbar \omega_1 \rightarrow 2s \) and 2s + \( \hbar \omega_2 \rightarrow \varepsilon p \) (see \([3]\) for more details). Therefore precise calculation of the corresponding light-shifts of 1s- and 2s-levels would be rather desirable.

In the current letter we present the results of analytical and numerical calculation of \( \alpha^ij_n(\omega) \) together with the corresponding light-shifts in the ns-states, \( n = 1, 2 \), of the muonium atom. It should be pointed out that the similar calculation by Beausoleil \([7]\) employing a pure numerical scheme proves to be incomplete. Besides, in the contrast to the usual technique (i.e. by means of the Green’s function) the current calculation is carried out in the fashion of Sternheimer \([8]\) where (exact and analytical) summation over the intermediate states \( r \) in \((2)\) is reduced to solution of a certain differential equation. Such an approach, which is applied to the problem under consideration for the first time, to our knowledge, seems to be rather instructive. Apart from its self-contained academic interest, it may also give certain advantages in treating the higher ns-states \( (n \geq 4) \) of the hydrogenic systems, as well as for exact calculation of the various \( \omega \)-dependent sums of the form:

\[
S^{(\mu)}_n(\omega) = \sum_r \left\{ \frac{\langle n||r||s\rangle \langle s||r^\mu||n\rangle}{\varepsilon_n + \omega - \varepsilon_s} + \frac{\langle n||r||s\rangle \langle s||r^\mu||n\rangle}{\varepsilon_n - \omega - \varepsilon_s} \right\}.
\]
Here $\mu$ is an arbitrary number, being not necessarily positive and integer; $\langle s||r^\mu||n \rangle$ denotes reduced matrix element. Such type of expressions make their appearance in numerous problems of atomic physics.

## 2 Calculation of the light-shifts

### 2.1 General consideration

For the $ns$-states under consideration Eq. (1) can be reduced to the following angular- and spin-independent form \[ \Delta \varepsilon_{ns}(\omega) = -\frac{P}{2\varepsilon_0 h^2 Sc} (e \cdot e^*) \Re \alpha_{ns}^S(\omega) \equiv -\frac{P}{2\varepsilon_0 h^2 Sc} \Re \alpha_{ns}^S(\omega). \] Here $\alpha_{ns}^S(\omega)$ denotes the so-called scalar DP (henceforth the atomic units, $e^2 = h = m = 1$ are used):

\[ \alpha_{ns}^S(\omega) = -\frac{1}{3} \sum_{kp} \left\{ \frac{\langle ns||r||kp \rangle \langle kp||r||ns \rangle}{\varepsilon_{ns} + \omega - \varepsilon_{kp} + i0} + \frac{\langle ns||r||kp \rangle \langle kp||r||ns \rangle}{\varepsilon_{ns} - \omega - \varepsilon_{kp}} \right\}, \]

which involves the radial integrals only. Summation is performed here over complete set of discrete and continuum $p$-states of the Coulomb field with the charge $Z$. The infinitesimal positive imaginary constant added in the denominator of the first term in the sum defines the sign of $\Im \alpha_{ns}^S(\omega)$ occurring if $\omega > |\varepsilon_{ns}|$, $|\varepsilon_{ns}| = Z^2/(2n^2)$ being the ionization potential of the $ns$-state. Calculation of $\alpha_{ns}^S(\omega)$, Eq. (4), is actually the final aim of our consideration.

Let us introduce auxiliary function $\psi_n(r; E)$ by the equation:

\[ \psi_n(r; E) = \sum_{kp} \frac{\langle kp||r|| ns \rangle}{E - \varepsilon_{kp}}, \]

$E = \varepsilon_{ns} \pm \omega + i0$ being a parameter. In terms of $\psi_n(r; E)$ DP, $\alpha_{ns}^S(\omega)$, is expressed as:

\[ \alpha_{ns}^S(\omega) = -\frac{1}{3} \left[ \langle ns||r||\psi_n(\varepsilon_{ns} + \omega + i0) \rangle + \langle ns||r||\psi_n(\varepsilon_{ns} - \omega) \rangle \right]. \]

By acting on $\psi_n(r)$ of Eq. (3) with the operator,

\[ E - \widehat{H}^{(l=1)} \equiv E + \frac{1}{2r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{1}{r^2} + \frac{Z}{r}, \]

\[ E = \varepsilon_{ns} \pm \omega + i0 \]

...
and by virtue of completeness of the set $|kp⟩$ one immediately obtains the following inhomogeneous differential equation obeyed by the function $ψ_n(r)$:

$$\frac{1}{r^2} \frac{∂}{∂r} \left( r^2 \frac{∂ψ_n}{∂r} \right) + 2 \left( E - \frac{1}{r^2} + \frac{Z}{r} \right) ψ_n = 2rR_{ns}(r). \quad (8)$$

Here $R_{ns}(r)$ denotes the radial non-relativistic coulomb s-function. In terms of the new parameters,

$$ν = \frac{Z}{\sqrt{-2E}}, \quad ρ = \frac{2Zr}{ν}, \quad (9)$$

Eq.(8) takes the form:

$$\frac{1}{ρ^2} \frac{∂}{∂ρ} \left( ρ^2 \frac{∂ψ_n}{∂ρ} \right) + \left( -\frac{1}{4} - \frac{2}{ρ^2} + \frac{ν}{ρ} \right) ψ_n = \frac{1}{4} \left( \frac{ν}{Z} \right)^3 ρR_{ns} \left( \frac{νρ}{2Z} \right).$$

Finally, on introducing the new auxiliary function $ζ(ρ)$ as

$$ψ_n(r) = ρe^{-ρ/2}ζ(ρ), \quad (10)$$

we result in the equation of the hypergeometric type,

$$ρζ''(ρ) + (4 - ρ)ζ'(ρ) + (ν - 2)ζ(ρ) = \frac{1}{4} \left( \frac{ν}{Z} \right)^3 ρe^{ρ/2}R_{ns} \left( \frac{νρ}{2Z} \right). \quad (11)$$

Its solution, $ζ(ρ)$, is supposed to be subject for $ℜν > -n$ ($n$ is fixed) to conditions:

$$ζ(ρ) = O(1), \text{ as } ρ → 0, \quad ζ(ρ) = o \left( \exp \left( \frac{n + ν}{2n} ρ \right) \right), \text{ as } ρ → ∞. \quad (12)$$

These follow directly from the definitions, Eqs.(3),(10), since (see [3]): $R_{ns}(r) ≍ e^{-Zr/n}$, as $r → ∞$, and $R_{ns}(r) = O(1)$, $R_{kp}(r) = O(r)$, as $r → 0$. It should be emphasized that Eqs.(12) are consistent with the “orthogonality-condition”,

$$⟨2p|ψ_1⟩ = \frac{(2p||r||1s)}{E - ε_{2p}}, \text{ if } n = 1, \quad ⟨np|ψ_n⟩ = \frac{(np||r||ns)}{E - ε_{np}}, \text{ if } n ≥ 2, \quad (13)$$

which follows from the Eq.(8) and by virtue of the orthogonality of the $kp$-functions:

$$⟨kp||r||k'p⟩ = δ_{k,k'}. \quad (14)$$
Relations (13) may be used as an additional check of correctness of the function $\psi_n(r)$.

The general solution of (11) has the form:

$$\zeta(\rho) = D_1 \Phi(2 - \nu, 4; \rho) + D_2 \Psi(2 - \nu, 4; \rho) + \zeta_0(\rho).$$  \hspace{1cm} (14)

Here $\Phi(2 - \nu, 4; \rho)$, $\Psi(2 - \nu, 4; \rho)$ are the regular and irregular solutions of homogeneous hypergeometric equation [10]; $D_1, D_2$ are some arbitrary constants which will finally be chosen to comply with (12); $\zeta_0(\rho)$ is some particular solution of Eq.(11). For the distinguished case: $\nu = 2$, explicit general solution of Eq.(11) reads:

$$\zeta_{\nu=2}(\rho) = -\frac{1}{6\rho^3}D_1 \left(2e^\rho + \rho e^\rho + \rho^2 e^\rho + \rho^3 \text{Ei}(-\rho)\right) + D_2 + \zeta_0(\rho).$$

Here $\text{Ei}(-\rho)$ stands for the integral exponential function.

Let us seek $\zeta_0(\rho)$ in the form:

$$\zeta_0(\rho) = \frac{1}{2\pi i} \oint_\gamma e^{\rho t} \xi(t) dt.$$  \hspace{1cm} (15)

Here the integral is taken along some contour $\gamma$ in the complex plane of $t$.

Figure 1: The contours of integration in Eqs.(20),(21) and (24).

It has to be chosen to comply both with (12) and the form of the contour $\gamma_1$ (see below) in the integral representation of the right-hand side of (11). Besides, after passing along $\gamma$ the integrand of (15) should return back to its
initial value. To find $\xi(t)$ and establish $\gamma$ we can write first (see e.g. [3]):

$$\frac{1}{4} \left( \frac{\nu}{Z} \right)^3 e^{\rho/2} R_{ns} \left( \frac{\nu \rho}{2Z} \right) \equiv \frac{1}{2} \left( \frac{\nu}{\sqrt{nZ}} \right)^3 \rho \exp \left( \frac{n - \nu}{2n} \rho \right) \Phi(-n + 1, 2; \nu \rho/n).$$

Then, we use the well-known integral representation [10] of the confluent hypergeometric function, $\Phi(-n + 1, 2; \nu \rho/n)$:

$$\Phi(-n + 1, 2; \nu \rho/n) = -\frac{1}{\pi in} \oint_{\gamma_0} e^{\nu \rho t/n} (-t)^{-n}(1-t)^n dt,$$

where the contour $\gamma_0$, shown in the Figure 1(a), is passed in the counterclockwise sense along the circle of an arbitrary radius, $\varepsilon$. By means of Eq.(16) and after two variable changes the right-hand side of (11) can be finally express as

$$\frac{1}{4} \left( \frac{\nu}{Z} \right)^3 e^{\rho/2} R_{ns} \left( \frac{\nu \rho}{2Z} \right) = \frac{1}{4\pi i} \left( \frac{\nu}{\sqrt{nZ}} \right)^3 \oint_{\gamma_1} e^{\rho t} \left( t - \frac{n - \nu}{2n} \right)^{-n-1} \left( t - \frac{n + \nu}{2n} \right)^{-n-1} dt.$$

It has thereby the form similar to Eq.(15). Here the contour $\gamma_1$, drawn in the Figure 1(b), is passed in the counterclockwise sense around the point $(n - \nu)/(2n)$ along a circle of an arbitrary radius. A substitution of (15) and (17) in Eq.(11) yields:

$$t(1-t)\xi'(t) + (2t+\nu-1)\xi(t) = \frac{1}{2} \left( \frac{\nu}{\sqrt{nZ}} \right)^3 \left( t - \frac{n - \nu}{2n} \right)^{-n-1} \left( t - \frac{n + \nu}{2n} \right)^{-n-1}.$$

The general solution of this equation can be written as

$$\xi(t) = C_0 t^{1-\nu}(1-t)^{1+\nu} - \frac{1}{2} \left( \frac{\nu}{\sqrt{nZ}} \right)^3 t^{1-\nu}(1-t)^{1+\nu} \int_t^\infty t^{\nu-2}(1-t)^{-\nu-2} \left( \frac{t - \frac{n + \nu}{2n}}{t - \frac{n - \nu}{2n}} \right)^{n-1} dt.$$

Here $C_0$ is the arbitrary constant which can be set to 0 for convenience. The integral is assumed to be taken along any path in the complex $t$-plane which does not pass through the points: $\{0, 1, (n - \nu)/(2n)\}$.

If combined with (15), Eq.(18) defines desired particular solution, $\zeta_0(\rho)$, of Eq.(14):

$$\zeta_0(\rho) = -\frac{1}{2\pi i} \frac{1}{2} \left( \frac{\nu}{\sqrt{nZ}} \right)^3 \oint_{\gamma} e^{\rho t} t^{1-\nu}(1-t)^{1+\nu} \int_t^\infty t^{\nu-2}(1-t)^{-\nu-2} \left( \frac{t - \frac{n + \nu}{2n}}{t - \frac{n - \nu}{2n}} \right)^{n-1} dt.$$
In view of the given above argument, the contour $\gamma$ in (19), is still a free “parameter”, provided that it is deformable into $\gamma_1$. Let us show how we can fix it. In fact, the integrand in Eq.(19) is analytical function in the $t$-plane cut along any path with the ends at $t = \infty$, $t_0 = (n - \nu)/(2n)$, the latter being its logarithmic branching point and the pole of the $n$th order at the same time. Owing to that, we can choose $\gamma$ to be a curve which starts at $-\infty$ at the lower edge of the cut, runs along the real axis, encircles the point $t_0$ in the counterclockwise sense and runs back to $-\infty$ along the upper edge of the cut (see Figure 1(c)). Such a contour is topologically equivalent to $\gamma_1$ in the Figure 1(b). Moreover, after passing along $\gamma$ the integrand returns back to its initial value, since it decreases exponentially as $t \to -\infty$. Here we have temporary assumed that $\Re(\nu) > n$, $\Im\nu = 0$. This restriction will however be released later by means of the analytical continuation in $\nu$. For the contour $\gamma$ under consideration the integral (19) can be split into two (independent) parts: (i) along two edges of the cut and (ii) along the circle centered at $t_0$. The part (i) is reduced in its turn to the integral of the jump at the cut of the integrand of Eq.(19). It has the form:

$$
\int_{\text{cut}} \ldots dt = -\frac{1}{2\pi i} \left( \frac{\nu}{\sqrt{nZ}} \right)^3 \int_{-\infty}^{\nu} e^{-\rho x} (-x)^{1-\nu}(1+x)^{1+\nu} \times
$$

$$
\times \left\{ \int_t^\infty t^{\nu-2}(1-t)^{-\nu-2} \left( t - \frac{n+\nu}{2n} \right)^{n-1} dt \right|_{t=-x+i0}^{t=-x-i0} - (\ldots) \right\} dx
$$

$$(20)$$

Conversely, the part (ii) is expressed as a residue of the integrand at $t = t_0$:

$$
- \frac{1}{2} \left( \frac{\nu}{\sqrt{nZ}} \right)^3 \text{res}_{t=t_0} \left[ e^{\rho t} t^{1-\nu}(1-t)^{1+\nu} \int_t^\infty t^{\nu-2}(1-t)^{-\nu-2} \left( t - \frac{n+\nu}{2n} \right)^{n-1} dt \right].
$$

$$(21)$$

Combining Eqs.(20) and (21) together we get:

$$
\zeta_0(\rho) = -\frac{1}{2} \left( \frac{\nu}{\sqrt{nZ}} \right)^3 \left\{ \frac{1}{n!} \frac{d^n}{dt^n} \left[ t^{\nu-2}(1-t)^{-\nu-2} \left( t - \frac{n+\nu}{2n} \right)^{n-1} \right] \right\}_{t=t_0} \times
$$

8
\[
\times \int_{\nu-n}^{\infty} e^{-\rho x} (-x)^{1-\nu} (1+x)^{1+\nu} dx + \\
+ \text{res}_{t=t_0} \left[ e^{\rho t} t^{1-\nu} (1-t)^{1+\nu} \int_{t}^{\infty} t^{\nu-2} (1-t)^{-\nu-2} \frac{\left( t - \frac{n+\nu}{2n} \right)^{n-1}}{\left( t - \frac{n-\nu}{2n} \right)^{n+1}} dt \right]. \tag{22}
\]

By virtue of the integral representation \[10\] of the function \( \Psi(\alpha, \gamma; z) \), entering Eq.(14),

\[
\Psi(\alpha, \gamma; z) = \frac{1}{\Gamma(\alpha)} \int_{0}^{\infty} e^{-zt} t^{\alpha-1} (1+t)^{-\alpha-1} dt, \quad \Re \alpha > 0, \tag{23}
\]

we can finally write:

\[
\psi_n(r) = \rho e^{-\rho/2} \left( D_1 \Phi(2 - \nu, 4; \rho) + D_2 \Psi(2 - \nu, 4; \rho) + \tilde{\zeta}_0(\rho) \right). \tag{24}
\]

Here we have redefined the constant \( D_2 \) without changing its notation; \( \tilde{\zeta}_0(\rho) \) is obtained from \( \zeta_0(\rho) \) of Eq. (22) by means of the substitution:

\[
\int_{\nu-n}^{\infty} \ldots dt \to - \int_{0}^{\nu-n} \ldots dt. \tag{25}
\]

It it clear now that for \( \nu : 2 - \nu \neq 0, -1, -2, \ldots \) the function \( \psi_n(r) \) of Eqs.(22), (23) will satisfy conditions (12) if we set:\( D_1 = D_2 = 0, \) since \[10\]

\[
\Phi(2 - \nu, 4; \rho) \sim \begin{cases} \frac{1}{(2-\nu)} \rho^{-2-\nu} e^\rho, & \text{as } \rho \to \infty \\ 1, & \text{as } \rho \to 0 \end{cases},
\]

\[
\Psi(2 - \nu, 4; \rho) \sim \begin{cases} \rho^{\nu-2}, & \text{as } \rho \to \infty \\ \frac{1}{(2-\nu)} \rho^{-3}, & \text{as } \rho \to 0 \end{cases}.
\]

We can adopt the same choice of \( D_1 \) also for \( \nu = 2, 3, 4, \ldots \), being of no physical interest. Whence, one finally obtains:

\[
\psi_n(r) = \frac{1}{2} \left( \frac{\nu}{\sqrt{nZ}} \right)^3 \rho e^{-\rho/2} \left\{ \frac{1}{n!} \frac{d^n}{dt^n} \left[ t^{\nu-2} (1-t)^{-\nu-2} \left( t - \frac{n+\nu}{2n} \right)^{n-1} \left( t - \frac{n-\nu}{2n} \right)^{n+1} dt \right] \right\}_{t=t_0}
\times \int_{0}^{\nu-n} e^{-\rho x} (-x)^{1-\nu} (1+x)^{1+\nu} dx - \\
- \text{res}_{t=t_0} \left[ e^{\rho t} t^{1-\nu} (1-t)^{1+\nu} \int_{t}^{\infty} t^{\nu-2} (1-t)^{-\nu-2} \frac{\left( t - \frac{n+\nu}{2n} \right)^{n-1}}{\left( t - \frac{n-\nu}{2n} \right)^{n+1}} dt \right]. \tag{26}
\]
In the given derivation we assumed that parameter $\nu$ is subject to condition: $n < \Re(\nu) < 2, \Im\nu = 0$. Analytical continuation of (26) on all $\nu$ is achieved by means of the substitution:

$$\int_{0}^{\frac{\nu-n}{2n}} e^{-\rho x} (-x)^{1-\nu} (1+x)^{1+\nu} dx \to \left(1 - e^{-2\pi \nu i}\right)^{-1} \int_{0+}^{\frac{\nu-n}{2n}} e^{-\rho x} (-x)^{1-\nu} (1+x)^{1+\nu} dx.$$

(27)

Depending on the cases: $\Re\nu > n$ or $\Re\nu < n$, the integral on the right-hand side here is taken along the paths shown in the Figure 2(a),(b). Each of them starts at the point $(-t_0) = (\nu-n)/(2n)$ lying on the lower edge of the corresponding cut, encircles the origin in the clockwise (counterclockwise) sense, and ends up at $(-t_0)$ lying on the upper edge of the same cut. In the following we shall use for simplicity a sign of the ordinary integral but imply, whenever necessary, the substitution (27). Alternatively, the same analytical continuation can be achieved by means of the identity:

$$\int_{0}^{\frac{\nu-n}{2n}} e^{-\rho x} (-x)^{1-\nu} (1+x)^{1+\nu} dx =$$

$$= \frac{(-1)^{1-\nu}}{2-\nu} \left(\frac{\nu-n}{2n}\right)^{2-\nu} \Phi_1 \left(2 - \nu, -1 - \nu, 3 - \nu, \frac{n - \nu}{2n}, \frac{n - \nu}{2n} \rho\right), \quad \Re\nu < 2. \quad (28)$$

Here $\Phi_1(\ldots)$ denotes degenerate hypergeometric function of two variables defined by the following series [11]:

$$\Phi_1(\alpha, \beta, \gamma, x, y) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(\alpha)_{m+n}(\beta)_{m+n}}{(\gamma)_{m+n}} \frac{x^m y^n}{m! n!}, \quad |x| < 1. \quad (29)$$

In particular cases, $n = 1, 2, 3$, explicit expressions for the functions $\psi_n(r)$ are combined below.

\begin{align*}
\text{n = 1} \\
\psi_1(r) &= -\frac{32\nu^4}{Z^{3/2}(\nu^2 - 1)^3} \left(\frac{\nu - 1}{\nu + 1}\right)^{\nu} \rho e^{-\rho/2} \int_{0}^{\nu - 1} e^{-\rho x} x^{1-\nu} (1+x)^{1+\nu} dx + \\
&\quad + \frac{2\nu^3}{Z^{3/2}(\nu^2 - 1)^3} \rho e^{-\nu \rho/2} \quad (30)
\end{align*}

\begin{align*}
\text{n = 2} \\
\psi_2(r) &= -\frac{32\nu^4}{Z^{3/2}(\nu^2 - 1)^3} \left(\frac{\nu - 1}{\nu + 1}\right)^{\nu} \rho e^{-\rho/2} \int_{0}^{\nu - 1} e^{-\rho x} x^{1-\nu} (1+x)^{1+\nu} dx + \\
&\quad + \frac{2\nu^3}{Z^{3/2}(\nu^2 - 1)^3} \rho e^{-\nu \rho/2} \quad (30)
\end{align*}
\[ \psi_2(r) = -\frac{512\sqrt{2}\nu^4}{Z^{3/2}(\nu^2 - 4)^3} \left( \frac{\nu - 2}{\nu + 2} \right)^{\nu} \rho e^{-\rho/2} \int_0^{\nu=2} e^{-\rho x} x^{1-\nu} (1 + x)^{1+\nu} dx - \frac{\sqrt{2}\nu^3}{2Z^{3/2}(\nu^2 - 4)^2} \rho e^{-\nu\rho/4} \left[ \nu(\nu^2 - 4)\rho + 4(\nu^2 + 4) \right] \quad (31) \]

\[ \psi_3(r) = -\frac{864\sqrt{3}\nu^4 (7\nu^2 - 27)}{Z^{3/2}(\nu^2 - 9)^4} \left( \frac{\nu - 3}{\nu + 3} \right)^{\nu} \rho e^{-\rho/2} \int_0^{\nu=3} e^{-\rho x} x^{1-\nu} (1 + x)^{1+\nu} dx + \frac{\sqrt{3}\nu^3}{27Z^{3/2}(\nu^2 - 9)^2} \rho e^{-\nu\rho/6} \left[ \nu^2(\nu^2 - 9)\rho^2 - 6\nu(\nu^2 - 27)\rho - (306\nu^2 + 486) \right] \quad (32) \]

It can be proved (see Appendix A) that Eqs. (30)-(32) satisfy orthogonality condition of Eq. (13).

Let us also give for reference explicit expression for the leading term in the expansion of \( \psi_n(r) \) in the small parameter \( \nu/n \ll 1 \):

\[ \psi_n(r) \approx -2 \left( \frac{\nu}{\sqrt{n}Z} \right)^3 \rho \left[ 16\nu \int_0^{1/2} e^{-\rho t} \left( \frac{1}{2} - t \right)^{1-\nu} \left( \frac{1}{2} + t \right)^{1+\nu} dt + 1 \right] , \Re \nu < 2. \quad (33) \]

This identity follows directly from Eq. (26).

### 2.2 Calculation of the light-shifts in particular cases

Now we are in a position of calculating the matrix elements entering Eq. (7) for \( n = 1, 2 \), being of particular interest. Integration, using Eqs. (30)-(31), yields the following equivalent forms of \( \langle 1s||r||\psi_1 \rangle \), \( \langle 2s||r||\psi_2 \rangle \) (see Appendix B):

\[ \frac{1}{3} \langle 1s||r||\psi_1 \rangle = -\frac{512\nu^9}{Z^4(\nu^2 - 1)^2(\nu + 1)^8} \int_0^{1} \frac{t^{1-\nu}}{1 - \left( \frac{\nu - 1}{\nu + 1} \right)^2 t^2} dt + \frac{2\nu^2 (2\nu^2 - 1)}{Z^4(\nu^2 - 1)^2} \quad (34) \]

\[ \equiv \frac{512\nu^9}{Z^4(\nu^2 - 1)^2(\nu + 1)^8(\nu - 2)} {}_2F_1 \left( 4, 2 - \nu, 3 - \nu; \left( \frac{\nu - 1}{\nu + 1} \right)^2 \right) + \frac{2\nu^2 (2\nu^2 - 1)}{Z^4(\nu^2 - 1)^2} \quad (35) \]
\[
\frac{1}{3} \langle 2s || r || \psi_2 \rangle = -\frac{2^{18} \nu^9}{Z^4(\nu^2 - 4)^2(\nu + 2)^8} \int_0^1 \frac{t^{1-\nu}}{\left(1 - \left(\frac{\nu - 2}{\nu + 2}\right)^2 t\right)} dt + \\
\frac{e^{2}}{2^{20} \nu^9 / Z^4(\nu^2 - 4)(\nu + 2)^{11}} \int_0^1 \frac{t^{2-\nu}}{\left(1 - \left(\frac{\nu - 2}{\nu + 2}\right)^2 t\right)} dt + \\
\frac{2^{18} \nu^9 (\nu + 1)}{Z^4(\nu + 2)^{12}(\nu - 2)(\nu - 3)} \, _2F_1 \left(4, 3 - \nu, 4 - \nu; \left(\frac{\nu - 2}{\nu + 2}\right)^2 \right) + \\
\frac{e^{2}}{2^{20} \nu^9 / Z^4(\nu^2 - 4)(\nu + 2)^{11}} \int_0^1 \frac{t^{2-\nu}}{\left(1 - \left(\frac{\nu - 2}{\nu + 2}\right)^2 t\right)} dt + \\
\frac{2^{18} \nu^9 (\nu + 1)}{Z^4(\nu + 2)^{12}(\nu - 2)(\nu - 3)} \, _2F_1 \left(4, 3 - \nu, 4 - \nu; \left(\frac{\nu - 2}{\nu + 2}\right)^2 \right) + \\
\frac{e^{2}}{2^{20} \nu^9 / Z^4(\nu^2 - 4)(\nu + 2)^{11}} \int_0^1 \frac{t^{2-\nu}}{\left(1 - \left(\frac{\nu - 2}{\nu + 2}\right)^2 t\right)} dt + \\
\frac{2^{18} \nu^9 (\nu + 1)}{Z^4(\nu + 2)^{12}(\nu - 2)(\nu - 3)} \, _2F_1 \left(4, 3 - \nu, 4 - \nu; \left(\frac{\nu - 2}{\nu + 2}\right)^2 \right) + \\
\frac{e^{2}}{2^{20} \nu^9 / Z^4(\nu^2 - 4)(\nu + 2)^{11}} \int_0^1 \frac{t^{2-\nu}}{\left(1 - \left(\frac{\nu - 2}{\nu + 2}\right)^2 t\right)} dt + \\
\frac{2^{18} \nu^9 (\nu + 1)}{Z^4(\nu + 2)^{12}(\nu - 2)(\nu - 3)} \, _2F_1 \left(4, 3 - \nu, 4 - \nu; \left(\frac{\nu - 2}{\nu + 2}\right)^2 \right) + \\
\frac{e^{2}}{2^{20} \nu^9 / Z^4(\nu^2 - 4)(\nu + 2)^{11}} \int_0^1 \frac{t^{2-\nu}}{\left(1 - \left(\frac{\nu - 2}{\nu + 2}\right)^2 t\right)} dt + \\
\frac{2^{18} \nu^9 (\nu + 1)}{Z^4(\nu + 2)^{12}(\nu - 2)(\nu - 3)} \, _2F_1 \left(4, 3 - \nu, 4 - \nu; \left(\frac{\nu - 2}{\nu + 2}\right)^2 \right) + \\
\frac{e^{2}}{2^{20} \nu^9 / Z^4(\nu^2 - 4)(\nu + 2)^{11}} \int_0^1 \frac{t^{2-\nu}}{\left(1 - \left(\frac{\nu - 2}{\nu + 2}\right)^2 t\right)} dt + \\
\frac{2^{18} \nu^9 (\nu + 1)}{Z^4(\nu + 2)^{12}(\nu - 2)(\nu - 3)} \, _2F_1 \left(4, 3 - \nu, 4 - \nu; \left(\frac{\nu - 2}{\nu + 2}\right)^2 \right) + \\
\frac{e^{2}}{2^{20} \nu^9 / Z^4(\nu^2 - 4)(\nu + 2)^{11}} \int_0^1 \frac{t^{2-\nu}}{\left(1 - \left(\frac{\nu - 2}{\nu + 2}\right)^2 t\right)} dt.
\]

Eqs. (34), (36) prove to be convenient for an analysis of the DP’s behavior when \( \omega \gg Z^2 / (2n^2) \equiv I_n \) and \( \omega \approx 0 \), as well as for calculation of the DP’s imaginary part; Eq. (37) is suitable for numerical calculation of the light-shift of the 2s-level; Eqs. (35), (38), and (39) define the matrix elements in terms of the hypergeometric function \( \, _2F_1(\ldots) \). In this form they easily admit analytical continuation in \( \nu \).

By means of Eqs. (34), (36) we can explicitly express now DP, \( \alpha_{1s}^S(\omega), \alpha_{2s}^S(\omega) \), as:

\[
\alpha_{1s}^S(\omega) = -\frac{1}{3} \left( \langle 1s || r || \psi_1 \rangle \big|_{\nu = \nu_{11}} + \langle 1s || r || \psi_1 \rangle \big|_{\nu = \nu_{12}} \right), \\
\alpha_{2s}^S(\omega) = -\frac{1}{3} \left( \langle 2s || r || \psi_2 \rangle \big|_{\nu = \nu_{21}} + \langle 2s || r || \psi_2 \rangle \big|_{\nu = \nu_{22}} \right).
\]

Here we have introduced the following notations:

\[
\nu_{11} = \frac{Z}{\sqrt{-2(\varepsilon_{1s} + \omega + i0)}}, \quad \nu_{12} = \frac{Z}{\sqrt{-2(\varepsilon_{1s} - \omega)}}
\]
\[ \nu_{21} = \frac{Z}{\sqrt{-2(\varepsilon_{2s} + \omega + i0)}} \], \quad \nu_{22} = \frac{Z}{\sqrt{-2(\varepsilon_{2s} - \omega)}} \] (43)

so that the following identities hold true:

\[ \omega^2 = \frac{Z^4(1 - \nu_{1m}^2)^2}{4\nu_{1m}^4} = \frac{Z^4(4 - \nu_{2m}^2)^2}{64\nu_{2m}^2}, \quad m = 1, 2. \] (43)

Here \( \varepsilon_{1s} = -Z^2/2, \varepsilon_{2s} = -Z^2/8 \) are the energies of the 1s- and 2s-levels. We assume, according to the standard rule of analytical continuation of the square root (see [3]), that

\[ \frac{Z}{\sqrt{-2(E + i0)}} = \begin{cases} \frac{Z}{\sqrt{-2E}} > 0 & \text{if } E < 0 \\ \frac{iZ}{\sqrt{2E}} & \text{if } E > 0 \end{cases}. \] (44)

Hence, by choosing the matrix elements \( \langle 1s||r||\psi_1 \rangle, \langle 2s||r||\psi_2 \rangle \) in the forms of Eqs.(35),(38), DP can be expressed as:

\[ \alpha_{1s}^S(\omega) = -\frac{1}{\omega^2} - \sum_{m=1}^{2} \frac{512\nu_{1m}^9}{Z^4(\nu_{1m}^2 - 1)^2(\nu_{1m} + 1)^8(\nu_{1m}^2 - 2)} \times \\
\times \binom{\nu_{1m} - 1}{\nu_{1m} + 1}^2 \binom{4, 2 - \nu_{1m}, 3 - \nu_{1m}}{2} \binom{\nu_{1m} - 1}{\nu_{1m} + 1}^2, \] (45)

\[ \alpha_{2s}^S(\omega) = -\frac{1}{\omega^2} - \sum_{m=1}^{2} \frac{2^{18}\nu_{2m}^9}{Z^4(\nu_{2m}^2 + 2)^7(\nu_{2m}^2 - 4)^3} \binom{4, 2 - \nu_{2m}, 3 - \nu_{2m}}{2} \binom{\nu_{2m} - 2}{\nu_{2m} + 2}^2 \] (46)

Eq.(45) is in agreement with the well known result of Gavrila [3], as it should. Eqs.(45)-(46) are rather inconvenient, however, for numerical calculation of DP for energies lying above the threshold of the levels, i.e. when parameters \( \nu_{11}, \nu_{21} \) become purely imaginary (cf Eq.(44)). Besides, they are also unsuitable for obtaining various asymptotics of these quantities. As was already mentioned above, for these purposes the integral forms of the matrix elements, Eqs.(34),(36),(37), prove to be more convenient. Below we combine various most important results of such calculations (see Appendix for details).

1. **The case: \( \omega/Z^2 \ll 1. \)**

\[ \alpha_{1s}^S(\omega) \approx \frac{9}{2} \frac{1}{Z^4} + \frac{319}{12} \left( \frac{\omega}{Z^4} \right)^2 + \ldots \] (47)
\( \alpha_{2s}^S(\omega) \propto 120 \frac{1}{Z^4} + 21120 \left( \frac{\omega}{Z^4} \right)^2 + \ldots \) (48)

2. The case: \( \omega/Z^2 \gg 1 \).

\[
\alpha_{1s}^S(\omega) \approx \frac{1}{\omega^2} - \frac{4}{3 \omega^4} \left( 1 + i \right) \frac{Z^5}{\omega^9/2} - \frac{4\pi Z^6}{3 \omega^5} - \frac{\sqrt{2}}{144} \left( -336i - 35i\pi^2 + 336 + 32\pi^2 - 3(1 + i)\pi \ln(8Z^2/\omega) \right) \frac{Z^7}{\omega^{11/2}} + \ldots
\]

(49)

\[
\alpha_{2s}^S(\omega) \approx \frac{1}{\omega^2} - \frac{1}{6 \omega^4} + \frac{\sqrt{2}}{6} (1 + i) \frac{Z^5}{\omega^9/2} - \frac{\pi Z^6}{6 \omega^5} - \frac{1}{2304} \sqrt{2} \left( -504i - 61i\pi^2 + 504 + 64\pi^2 + 3(1 + i)\pi \ln(2Z^2/\omega) \right) \frac{Z^7}{\omega^{11/2}} + \ldots
\]

(50)

3. Calculation of \( \Im \alpha_n^S(\omega) \), \( \omega > I_n \equiv Z^2/(2n^2) \).

\[
\Im \alpha_{1s}^S(\omega) = \frac{64\pi}{3\omega^3} \frac{\eta^6 e^{-4\eta\arctan(1/\eta)}}{(1 + \eta^2)^3 \left( 1 - e^{-2\pi\eta} \right)}, \quad \eta = |\nu_{11}|,
\]

(51)

\[
\Im \alpha_{2s}^S(\omega) = \frac{2048\pi}{3\omega^3} \frac{\eta^6 (1 + \eta^2) e^{-4\eta\arctan(2/\eta)}}{(4 + \eta^2)^4 \left( 1 - e^{-2\pi\eta} \right)}, \quad \eta = |\nu_{21}|.
\]

(52)

Accordingly, the photoionization cross sections, \( \sigma_{ns}^{(\gamma)}(\omega) = 4\pi \alpha \omega \Im \alpha_n^S(\omega) \), are defined as:

\[
\sigma_{1s}^{(\gamma)}(\omega) = \frac{2^9 \pi^2}{3Z^2} \alpha \left( \frac{I_{1s}}{\omega} \right)^4 \frac{e^{-4\eta\arctan(1/\eta)}}{1 - e^{-2\pi\eta}}, \quad \eta = \sqrt{\frac{I_{1s}}{\omega - I_{1s}}} > 0,
\]

(53)

\[
\sigma_{2s}^{(\gamma)}(\omega) = \frac{2^{14} \pi^2}{3Z^2} \alpha \left( 1 + 3 \frac{I_{2s}}{\omega} \right) \left( \frac{I_{2s}}{\omega} \right)^4 \frac{e^{-4\eta\arctan(2/\eta)}}{1 - e^{-2\pi\eta}}, \quad \eta = \sqrt{\frac{4I_{2s}}{\omega - I_{2s}}}
\]

(54)

4. The case: \( \omega/I_n \to 1 + 0 \).

\[
\frac{1}{3} \langle 1s | r | \psi_1 \rangle \approx \frac{88}{3Z^4} - \frac{256}{3Z^4} e^{-4Ei(4)(1 - i)} - \frac{1}{9Z^4} \left( 1016 - 2816e^{-4Ei(4)(1 - i)} \right) \frac{1}{\eta^2} + \ldots
\]

(55)

\[
\frac{1}{3} \langle 2s | r | \psi_2 \rangle \approx \frac{18896}{3Z^4} - \frac{131072}{3Z^4} e^{-8Ei(8)(1 - i)} - \frac{1}{9Z^4} \left( 709952 - 4849664e^{-8Ei(8)(1 - i)} \right) \frac{1}{\eta^2} + \ldots
\]

(56)
Here parameters $\eta$ are defined by Eqs.(53),(54); $e = 2.71828\ldots$; $\text{Ei}(\ldots)$ stands for the integral exponential function; condition $\eta \gg 1$ is assumed in either case.

5. The case: $Z^2/(2\omega n^2) \ll 1$; $Z, \omega$ are fixed.

By means of Eq.(33) and in view of the evident relations,

$$\nu_{m,2} \propto \frac{Z}{n \sqrt{2\omega}} \equiv \nu_0 > 0, \quad \nu_{m,1} \propto \frac{iZ}{n \sqrt{2\omega}} \equiv i\nu_0,$$

the leading term of the expansion of DP in the small parameter, $\nu_0/n \ll 1$, can be expressed as

$$\alpha_n^S(\omega) \propto \frac{32\nu^8}{Z^4} \frac{1}{n^3} \left\{ \Gamma(1 - \nu_0)e^{-2\nu_0} [4\Psi(-\nu_0, 1; 4\nu_0) - (2\nu_0 + 1)\Psi(-\nu_0, 0; 4\nu_0)] + (\ldots)|_{\nu_0 \to i\nu_0} \right\} . \quad (57)$$

Here $\Psi(\ldots)$ denotes irregular degenerate hypergeometric function (cf (14)), whereas $\Gamma(\ldots)$ stands for the $\Gamma$-function [10].

| $1s$ – level | $2s$ – level |
|--------------|--------------|
| $\omega_1 = 3/16$ | $\omega_1 = 3/16$ | $\omega_2 = 1/8$ | $\omega_2 = 1/8$ |
| $\nu_{i1}$ | $\nu_{i2}$ | $\nu_{i1}$ | $\nu_{i2}$ | $\nu_{21}$ | $\nu_{22}$ | $\nu_{21}$ | $\nu_{22}$ |
| $\sqrt{8/5}$ | $\sqrt{8/11}$ | $2/\sqrt{3}$ | $2/\sqrt{5}$ | $i\sqrt{8}$ | $\sqrt{8/5}$ | $+\infty$ | $\sqrt{2}$ |

Table 1: The values of parameters $\nu_{ij}$, $i, j = 1, 2$.

Let us apply the results obtained to particular photon energies adopted in the above-mentioned 1S-2S experiment in muonium atom ($Z = 1$). The latter is carried in the presence of two laser beams with the energies $\omega_1 = 3/16$ a.u. ($\lambda_1 = 244$ nm) and $\omega_1 = 1/8$ a.u. ($\lambda_2 = 366$ nm). The corresponding values of $\nu_{ij}$, $i, j = 1, 2$ [12], [13] and $\alpha_n^S(\omega)$ are compiled in the Tables [14]. In obtaining $\alpha_{2s}^S(\omega_2)$ we used the value,

$$\frac{1}{3} \langle 2s|v||\psi_2 \rangle \bigg|_{\nu \to +\infty} = 155.799140 - 46.045022i,$$

15
Table 2: The values of $\alpha_{ns}^S(\omega)$.

| $\omega_1$ | $\omega_2$ | $\omega_1$ | $\omega_2$ |
|------------|------------|------------|------------|
| $-5.714105$ | $-4.962372$ | $29.853542 - 12.823175i$ | $89.818540 - 46.045022i$ |

being equal to the leading ($\eta$-independent) term in Eq. (56). Its imaginary part coincides, as it should, with $3\alpha_2^S(I_2s)$ of Eq. (52), whereas the real part defines the level shift at the photoionization threshold. According to Eq. (4), the numbers displayed enable to obtain, e.g. the following important dimensionless ratio:

$$R_{\omega_1\omega_2} \equiv \frac{\Delta \varepsilon_{2s}(\omega_2) - \Delta \varepsilon_{1s}(\omega_2)}{\Delta \varepsilon_{2s}(\omega_1) - \Delta \varepsilon_{1s}(\omega_1)} = \frac{I_{\omega_2}}{I_{\omega_1}} \frac{\Re \alpha_{2s}^S(\omega_2) - \Re \alpha_{1s}^S(\omega_2)}{\Re \alpha_{2s}^S(\omega_1) - \Re \alpha_{1s}^S(\omega_1)} = 2.664 \frac{I_{\omega_2}}{I_{\omega_1}}.$$  

Here $I_{\omega_1} \equiv P_{\omega_1}/S_1$, $I_{\omega_2} \equiv P_{\omega_2}/S_2$ are the beam intensities, $P_{\omega_1,\omega_2}$, $S_{1,2}$ being the corresponding powers and cross sections. The absolute value of the light-shift of the $ns$-level due to (one) photon beam of the field strength, $E_\omega$, is defined as (henceforth in this section the ordinary units are used)

$$\Delta \varepsilon_{ns}(\omega) = \frac{1}{4} E_\omega^2 \Re \alpha_{ns}^S(\omega), \quad E_\omega \equiv \sqrt{\frac{2I_\omega}{c \varepsilon_0}} = 5.338 \cdot 10^{-5} \sqrt{\frac{A_p^\omega}{S_\omega \tau_\omega}} E_0 \text{ mm} \cdot \text{ns}^{-1/2} \cdot \text{mJ}^{-1/2}.$$  

Here $A_p^\omega$ and $\tau_\omega$ stand for the energy of the beam within one pulse (in $\text{mJ}$) and the pulse duration (in $\text{ns}$); the beam cross section, $S_\omega$, is measured in $\text{mm}^2$; $E_0 = m_e^2 e^5/\hbar^4 = 5.142 \cdot 10^{11}$ Volts/m denotes the atomic unit of electric field strength. For the typical values of these parameters adopted in the experiment ($S_\omega = 2 \times 3 \text{ mm}^2$, $\tau_\omega = 28 \text{ ns}$, $A_p^\omega = 6 \text{ mJ}$) one obtains: $E_\omega \simeq 1.0 \cdot 10^{-5} E_0$, i.e. the electric field employed happens to be rather weak. Accordingly, the average intensity within a pulse equals: to $I_\omega = A_p^\omega/(S_\omega \tau_\omega) \simeq 3.57 \cdot 10^6 \text{ W/cm}^2$. In the presence of two counterpropagating beams\(^\dagger\) having the intensities, $I_\omega$, $I'_\omega$, and the same frequency, $\omega$, the shift

\(^\dagger\)The presence of two counterpropagating beams of the same frequency enables to avoid both the Doppler-broadening and the Doppler-shift of the line.\(^\dagger\)
of the level (at the frequency $\omega$) can be expressed in the form:

$$\Delta \varepsilon_{ns}(\omega) = \frac{1}{4} \left( E_{\omega}^2 + E_{\omega}'^2 \right) \Re \alpha_{ns}^S(\omega) \equiv 4.6875(I_{\omega} + I_{\omega}') \Re \alpha_{ns}^S(\omega)$$

$$\equiv 4.6875 \left( \frac{A^\omega}{S_{\omega} \tau_{\omega}} + \frac{A'^\omega}{S'_{\omega} \tau'_\omega} \right) \Re \alpha_{ns}^S(\omega) a_0^{-3} \text{ mm}^2 \cdot \text{ns}^{-1} \cdot \text{mJ}^{-1} \cdot \text{MHz}. $$

Here it is taken into account that $\alpha_{ns}^S(\omega)$, whose values are displayed in the Table (2), is measured in the units of $a_0^3$, $a_0 = \hbar^2/(m_e e^2) = 0.529 \cdot 10^{-8} \text{ cm}$ being the Bohr radius. As a result, the total energy shift between $ns$- and $ms$-levels caused by two counterpropagating beams of the same frequency $\omega$ is, then, given by

$$\Delta \mathcal{E}_{nm}(\omega) \equiv \Delta \varepsilon_{ns}(\omega) - \Delta \varepsilon_{ms}(\omega)$$

$$= 4.6875 \left( \frac{A^\omega}{S_{\omega} \tau_{\omega}} + \frac{A'^\omega}{S'_{\omega} \tau'_\omega} \right) \left( \Re \alpha_{ns}^S(\omega) - \Re \alpha_{ms}^S(\omega) \right) a_0^{-3} \text{ mm}^2 \cdot \text{ns}^{-1} \cdot \text{mJ}^{-1} \cdot \text{MHz}. $$

An application of this formula to the case of $1S$-$2S$ experiment, assuming that parameters of the counterpropagating beams are identical ($S_{\omega_1} = S'_{\omega_1} = S_{\omega_2} = S'_{\omega_2} = 2 \times 3 \text{ mm}^2$, $\tau_{\omega_1} = \tau'_{\omega_1} = \tau_{\omega_2} = \tau'_{\omega_2} = 28 \text{ ns}$, $A^\omega_{\omega_1} = A'^\omega_{\omega_1} = A^\omega_{\omega_2} = A'^\omega_{\omega_2} = 6 \text{ mJ}$), yields:

$$\Delta \mathcal{E}_{21}(\omega_1) = 11.9 \text{ MHz}$$

$$\Delta \mathcal{E}_{21}(\omega_2) = R_{\omega_1 \omega_2} \Delta \mathcal{E}_{21}(\omega_1) = 31.7 \text{ MHz}. $$

### 3 Conclusion

The numbers of Eqs. (59), (60) may serve as a good illustration of the method employed. They are, however, of independent significance. The value of $\Delta \mathcal{E}_{21}(\omega_1)$ is in fair agreement with the result [7]. One has to stress that in obtaining these energy shifts we used the average intensities. As it shown in [7], an account for a space-inhomogeneity of a laser field may increase each of these numbers by a factor of 10. It is relevant to point out here that the results obtained for $n = 1, 2$ can be extended on the case of arbitrary $n$. Such type of calculation can be mostly efficiently performed on the basis of Eq.(26) valid for all $n$, e.g. with the help of Maple [12], being an easy-to-use computer algebra program. Hence, in the contrast to a pure numerical scheme (say,
in a fashion of Beausoleil \[7\]), one obtains analytical, rather than numerical, result which is already well adapted for further numerical calculation (one-fold integration). Such an integration is performed only at the very last stage of calculation and usually carried out in no time. Furthermore, by that means one considerably reduces numerical errors. Beyond that, analytical formulae admit straightforward computation of the various asymptotics with respect to all parameters encountered in them. As an example we can mention the result of Eqs.\((55)-(56)\) when the photon energy, \(\omega\), tends to the threshold, \(I_{ns}\), being of particular importance for the problem under consideration. This argument may be considered as additional advantage of the method employed. Besides, as was already mentioned in the Introduction, the formula \((2k)\), as well as its particular cases, Eqs.\((30)-(32)\), enable a straightforward calculation of the sums, Eq.\((3)\). In fact, \(S_n^{(\mu)}(\omega)\) can be defined, in analogy with \((7)\), as

\[
S_n^{(\mu)}(\omega) = \langle ns||r^{\mu}||\psi_n(\varepsilon_{ns} + \omega + i0)\rangle + \langle ns||r^{\mu}||\psi_n(\varepsilon_{ns} - \omega)\rangle.
\]

The analysis, whose details will be given elsewhere, shows that for low \(n\) it can be expressed in a closed form for any \(\mu\). The corresponding calculations prove to be simpler than those where the Green function is employed. We would interpret this circumstance, thereby, as a self-contained importance of the current method when it is applied to the problem under consideration. One would expect that this advantage will even be enhanced if the states with \(n \geq 4\) are taken into consideration. It is interesting to emphasize here that one we can easily estimate the speed of the DP’s decrease, as \(n \to \infty\). Namely, according to Eq.\((57)\), \(\alpha_n S_n(\omega) \approx C/n^3, n/\nu_0 \gg 1\). So that the threshold itself \((E = 0)\), being the limit: \(\varepsilon_{ns} \to 0\), as \(n \to \infty\), is not affected by the laser field. This is in agreement with the well known result due to Ritus \[13\] stating that the DP vanishes for continuum states. The \(ns\)–levels with \(n \geq 4\) prove to be of particular importance owing to extensive experimental, as well as theoretical, investigation of the spectroscopic properties of the few-body systems, being carried out at present. In particular, we consider the light-shift calculation in the \(3s\)–, \(4s\)–, \(5s\)–levels as a subject of future publications.
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5 Appendix

A Orthogonality-relations

Let us prove, say for \( n = 1, 2 \), that the functions (31)-(32) satisfy “orthogonality relation”, Eq.(13). Namely, on calculating the integral,

\[
\langle \psi_n | 2p \rangle \equiv \frac{Z^{3/2}}{2\sqrt{6}} \int_0^\infty r^3 e^{-Zr/2} \psi_n(r) dr, \ n = 1, 2,
\]

we obtain:

\[
\langle \psi_1 | 2p \rangle = -\frac{4\sqrt{6}\nu^8}{Z^3(\nu^2 - 1)^3} (\nu - 1)^\nu \int_0^{\nu - 1} \frac{x^{1-\nu}(1 + x)^{1+\nu}}{(x + \frac{\nu+2}{4})^5} dx + \frac{256 \sqrt{6}\nu^2}{243 Z^3 (\nu^2 - 1)}, \quad (A.1)
\]

\[
\langle \psi_2 | 2p \rangle = -\frac{128\sqrt{3}\nu^8}{Z^3(\nu^2 - 4)^3} (\nu - 2)^\nu \int_0^{\nu - 2} \frac{x^{1-\nu}(1 + x)^{1+\nu}}{(x + \frac{\nu+2}{4})^5} dx - \frac{8 \sqrt{3}\nu^2 (7\nu^2 - 12)}{Z^3 (\nu^2 - 4)^2}, \quad (A.2)
\]

After the variable changes, \( x/(x + 1) = t(\nu - 1)/(\nu + 1), \ x/(x + 1) = t(\nu - 2)/(\nu + 2) \), Eqs.(A.1), (A.2) take the final form:

\[
\langle \psi_1 | 2p \rangle = -\frac{2^{12} \sqrt{6}\nu^8}{Z^3(\nu - 1)(\nu + 1)^5(\nu + 2)^5} \int_0^1 \frac{t^{1-\nu} \left( 1 - \frac{\nu-1}{\nu+1} t \right)}{(1 - \frac{(\nu-1)(\nu-2)}{(\nu+1)(\nu+2)})^5} dt + \frac{256 \sqrt{6}\nu^2}{243 Z^3 (\nu^2 - 1)} \quad (A.3)
\]

\[
\langle \psi_2 | 2p \rangle = -\frac{2^{17} \sqrt{3}\nu^8}{Z^3(\nu - 2)(\nu + 2)^{10}} \int_0^1 \frac{t^{1-\nu} \left( 1 - \frac{\nu-2}{\nu+2} t \right)}{(1 - \left( \frac{\nu-2}{\nu+2} \right)^2 t)} dt - \frac{8 \sqrt{3}\nu^2 (7\nu^2 - 12)}{Z^3 (\nu^2 - 4)^2} \quad (A.4)
\]

Here we have used the integrals:

\[
\int_0^1 \frac{t^{1-\nu} \left( 1 - \frac{\nu-1}{\nu+1} t \right)}{(1 - \frac{(\nu-1)(\nu-2)}{(\nu+1)(\nu+2)})^5} dt = -\frac{1}{1296} \frac{(1 + \nu)^4(\nu + 2)^4}{\nu^4(\nu - 2)}, \quad (A.5)
\]

\[
\int_0^1 \frac{t^{1-\nu} \left( 1 - \frac{\nu-2}{\nu+2} t \right)}{(1 - \left( \frac{\nu-2}{\nu+2} \right)^2 t)} dt = -\frac{1}{4096} \frac{(2 + \nu)^8}{\nu^4(\nu - 2)}, \quad (A.6)
\]
These can be calculated by means of the following elementary relation:
\[
\int_0^1 t^{1-\nu}(1-\nu t) dt = \frac{1}{4} b - a + \frac{4a + (2 + \nu)(b-a)}{4b} \int_0^1 t^{1-\nu} dt. \quad (A.7)
\]
Eqs. \[(A.3),(A.4)\] imply that \(\psi_1(r), \psi_2(r)\) satisfy Eqs.\[(13),\] as they should. The case of arbitrary \(n\) can be treated accordingly.

**B Matrix elements of \(\psi_n(r)\)**

Let us give here some details of a derivation of Eqs.\[(34)-(38)\]. On calculating the integrals, \(\langle ns||r||\psi_1\rangle, \ n = 1, 2, \) using Eqs.\[(30),(31)\] and explicit expressions [3],

\[
R_{1s}(r) = 2Z^{3/2}e^{-Zr}, \quad R_{2s}(r) = \frac{Z^{3/2}}{\sqrt{2}} \left(1 - \frac{Zr}{2}\right) e^{-Zr/2}, \quad (B.1)
\]
we get:

\[
\frac{1}{3} \langle 1s||r||\psi_1\rangle = -32Z^4(\nu^2 - 1)^3 \left(\frac{\nu - 1}{\nu + 1}\right) \nu \int_0^{\nu+1} x^{1-\nu}(1+x)^{1+\nu} \left(\frac{x + \nu}{2}\right)^5 dx + \frac{2\nu^2}{Z^4(\nu^2 - 1)}, \quad (B.2)
\]

\[
\frac{1}{3} \langle 2s||r||\psi_2\rangle = -256Z^4(\nu^2 - 4)^3 \left(\frac{\nu - 2}{\nu + 2}\right) \nu \int_0^{\nu+2} x^{1-\nu}(1+x)^{1+\nu} \left(\frac{x + \nu+2}{4}\right)^5 dx +
\]

\[
+320Z^4(\nu^2 - 4)^3 \left(\frac{\nu - 2}{\nu + 2}\right) \nu \int_0^{\nu+2} x^{1-\nu}(1+x)^{1+\nu} \left(\frac{x + \nu+2}{4}\right)^5 dx - 16\nu^2(28 - 13\nu^2)\]
\[
\quad (B.3)
\]

After making the variable changes, \(x/(x+1) = t(\nu - 1)/(\nu + 1), \ x/(x+1) = t(\nu - 2)/(\nu + 2),\) Eqs.\[(B.2),(B.3)\] take the form:

\[
\frac{1}{3} \langle 1s||r||\psi_1\rangle = -\frac{2^{10} \nu^8}{Z^4(\nu^2 - 1)(\nu + 1)^9} \int_0^1 t^{1-\nu} \left(1 - \frac{\nu - 1}{\nu + 1} t\right)^2 \left(t - \frac{\nu - 1}{\nu + 1} t\right)^5 dt + \frac{2\nu^2}{Z^4(\nu^2 - 1)}, \quad (B.4)
\]

\[
\frac{1}{3} \langle 2s||r||\psi_2\rangle = -\frac{2^{18} \nu^8}{Z^4(\nu^2 - 4)(\nu + 2)^9} \int_0^1 t^{1-\nu} \left(1 - \frac{\nu - 2}{\nu + 2} t\right)^2 \left(t - \frac{\nu - 2}{\nu + 2} t\right)^5 dt +
\]

\[
+\frac{2^{17} \nu^9}{Z^4(\nu^2 - 4)(\nu + 2)^9} \int_0^1 t^{1-\nu} \left(1 - \frac{\nu - 2}{\nu + 2} t\right)^2 \left(t - \frac{\nu - 2}{\nu + 2} t\right)^6 dt - 16\nu^2(28 - 13\nu^2)\]
\[
\quad (B.5)
\]
Finally, on applying successfully recurrence relations,

$$\int_0^1 \frac{t^{1-\nu}(1-at)^2}{(1-bt)^6} \, dt = \frac{(b-a)^2}{b^2} \int_0^1 \frac{t^{1-\nu}}{(1-bt)^6} \, dt + \frac{a(b-a)}{b^2} \int_0^1 \frac{t^{1-\nu}}{(1-bt)^5} \, dt + \frac{a^2}{b^2} \int_0^1 \frac{t^{1-\nu}}{(1-bt)^4} \, dt$$ \hspace{1cm} (B.6)

$$\int_0^1 \frac{t^{1-\nu}}{(1-bt)^{n+1}} \, dt = \frac{1}{n(1-b)^n} - \frac{2-\nu-n}{n} \int_0^1 \frac{t^{1-\nu}}{(1-bt)^n} \, dt,$$ \hspace{1cm} (B.7)

together with (A.7) to Eqs. (B.4), (B.5), we retrieve identities (34), (36).
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Figure 2: The contour of integration in Eq. (32).