Bound-bound two-photon transition matrix elements for the hydrogen atom in the dipole approximation

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(Received 6 July 1988)

By use of the linear-response-vectors method, the Kramers-Heisenberg matrix elements for arbitrary bound-bound transitions of a nonrelativistic hydrogenlike atom have been evaluated. To illustrate the discussion, Rayleigh and Raman scattering have been selected as relevant examples of second-order processes. We have derived, in a unitary manner, **A**- and ϕ-gauge compact analytic formulas, both for angular momentum and Stark states. Our results are expressed in terms of two new generalized hypergeometric functions with four variables, ${}_1F_E$ and ${}_2F_E$, which are finite sums of Gauss hypergeometric functions. Special attention is given to the two-photon transitions involving the atomic ground state. For angular momentum states, we mention the connection that we have established between our general results and earlier ones.

I. INTRODUCTION

In the last two decades, bound-bound two-photon transitions of nonrelativistic hydrogenic atoms have received considerable attention. Gavrilă's remarkable work on Rayleigh scattering from the ground state in the dipole approximation [1](DA) was the first to exploit one of the newly available compact forms of the Coulomb Green's function (CGF).[2] Since then many authors have used these powerful mathematical tools to investigate various transitions, especially involving low quantum numbers.[3] Nevertheless, in the case of the Stark states no attempt was made to establish general formulas, while for angular momentum states there are only two papers that do it. The former is a letter by Karule[4] which gives the radial parts of the N-photon bound-bound and bound-free DA transition matrix elements in the ϕ gauge ($N \geq 2$). Its starting point is Hostler's Sturmian-function expansion of the radial CGF,[5] which allows a straightforward integration and whose specific structure remains embedded in the resulting noncompact formulas. The latter is a group-theoretical work by Gazeau[6] that derives exact and DA **A**-gauge expressions of the two-photon transition amplitude between an arbitrary pair of angular momentum bound states.

More recently, applying the linear-response-vectors method,[7] the present author has obtained compact DA formulas describing the $1s \rightarrow ns$ and $1s \rightarrow nd$ two-photon transitions.[8] In this paper, we derive by the same *simple* method general closed-form DA expressions of the bound-bound two-photon transition amplitudes for angular momentum states, as well as for Stark states. Systematic use is made of our previous results concerning the linear-response vectors.[9,10] As a matter of fact, our preceding paper, Ref. 10, will be referred to in the following as I. Needless to say, we shall preserve in the present work the notations introduced in I.

In Sec. II, we recall the Kramers-Heisenberg (KH) matrix element for photon scattering by a bound electron.[11] The equivalent **A**- and ϕ-gauge expressions of the KH matrix element for a given transition $|N\rangle \rightarrow |N'\rangle$ are determined by two tensors denoted $\Pi_{N',N}$ and $\Xi_{N',N}$, respectively. These tensors, which characterize all the two-photon transitions between the bound states $|N\rangle$ and $|N'\rangle$, may be written as scalar products of a compact factor and a noncompact one: the noncompact factors involving a sum over the intermediate states are precisely our linear-response vectors $\mathbf{w}_N(\Omega;\mathbf{r})$ and, respectively, $\mathbf{v}_N(\Omega;\mathbf{r})$, defined in I. Section III is devoted to the evaluation of the tensors $\Pi^s_{n'l'm',nlm}$ and $\Xi^s_{n'l'm',nlm}$, associated to an arbitrary pair of angular-momentum states. The explicit form of the **A**-gauge tensor $\Pi^p_{n'_\xi n'_\eta m',n_\xi n_\eta m}$ describing the transition between two arbitrary Stark states is established in Sec. IV: we conclude this section with a comment on the similar ϕ-gauge tensor $\Xi^p_{n'_\xi n'_\eta m',n_\xi n_\eta m}$. Section V deals with the special case when either the initial or the final atomic state is the ground state. In Sec. VI, after deriving explicit Sturmian-function expansions of the tensors $\Xi^s_{n'l'm',nlm}$ and $\Pi^s_{n'l'm',nlm}$, we make brief remarks concerning the connection between our general formulas for angular momentum states and the earlier ones.[4,6] The importance and usefulness of our results are finally emphasized. In obtaining them we have repeatedly used two integrals given in the Appendix.

II. KRAMERS-HEISENBERG MATRIX ELEMENT FOR RAYLEIGH AND RAMAN SCATTERING

Our choice is to discuss the scattering of photons by a nonrelativistic hydrogenlike atom in the rest frame of its nucleus. This has the atomic number Z and is taken as the origin of the coordinate axes. We denote by ω and $\boldsymbol{\varepsilon}$ the frequency and the polarization vector of the incident photon and by ω' and $\boldsymbol{\varepsilon}'$ those of the scattered one. Let N and N' stand for the sets of quantum numbers of the initial and, respectively, final atomic state. Only conservation of energy holds,

$$E_{n'}+\hbar\omega'=E_n+\hbar\omega \ , \quad (1)$$

but not that of momentum. We distinguish the inelastic (Raman) scattering (with $n'>n$, Stokes transition, or $n'<n$, anti-Stokes transition) from the elastic (Rayleigh) scattering, either coherent ($N'=N$), or incoherent ($n'=n$, $N'\neq N$).

The differential cross section of photon scattering in the DA,[12]

$$d\sigma=r_0^2\frac{\omega'}{\omega}|\mathfrak{M}_{N',N}|^2 d\Omega' \ , \quad (2)$$

with $r_0=e^2/m_e c^2$ the classical electron radius, is determined by the corresponding KH matrix element,

$$\mathfrak{M}_{N',N}=\sum_{\mu'}\sum_{\mu}\varepsilon'^{*\mu'}\varepsilon_{\mu}\mathcal{M}_{N',N;\mu'}{}^{\mu}(\omega) \ . \quad (3)$$

In Eq. (3), μ' and μ are spherical tensor indices, introduced in Eqs. (35) of I. When using the **A** gauge, the dimensionless KH tensor $\mathcal{M}_{N',N}(\omega)$ has the components

$$\mathcal{M}_{N',N;\mu'}{}^{\mu}(\omega)=\delta_{N',N}\delta_{\mu'}{}^{\mu}-\Pi_{N',N;\mu'}{}^{\mu}(\Omega_1) - \Pi_{N',N;}{}^{\mu}{}_{\mu'}(\Omega_2) \ , \quad (4)$$

where

$$\Pi_{N',N;\mu'}{}^{\mu}(\Omega)=\frac{1}{m_e}\langle u_{N'}|P_{\mu'}w_{N;}{}^{\mu}(\Omega)\rangle \quad (5)$$

and

$$\Omega_1=E_n+\hbar\omega+i0, \quad \Omega_2=E_{n'}-\hbar\omega \ . \quad (6)$$

In Eq. (5), **P** is the electron momentum operator and $\mathbf{w}_N(\Omega;\mathbf{r})$ the linear-response vector defined by its eigenfunction expansion in Eq. (11) of I. If we substitute this definition into Eq. (5) and then use repeatedly the identity (13) of I, we finally get the ϕ-gauge expression of the tensor (4),

$$\mathcal{M}_{N',N;\mu'}{}^{\mu}(\omega)=-\frac{\hbar\omega'\hbar\omega}{4|E_1|^2}[\Xi_{N',N;\mu'}{}^{\mu}(\Omega_1)+\Xi_{N',N;}{}^{\mu}{}_{\mu'}(\Omega_2)] \ , \quad (7)$$

where

$$\Xi_{N',N;\mu'}{}^{\mu}(\Omega)=\frac{4|E_1|^2}{e^2a_0}\langle u_{N'}|x_{\mu'}v_{N;}{}^{\mu}(\Omega)\rangle \ . \quad (8)$$

In Eq. (8), a_0 is the Bohr radius, while the ϕ-gauge linear-response vector $\mathbf{v}_N(\Omega;\mathbf{r})$ is defined by Eq. (10) of I.

We shall evaluate the scalar products (5) and (8) first for angular momentum states, $|N\rangle=|nlm\rangle$, and then for Stark states, $|N\rangle=|n_\xi n_\eta m\rangle$. We shall occasionally use also the Cartesian components of the tensor (5),

$$\Pi_{N',N;ij}(\Omega)=\tfrac{1}{3}\sum_{\mu'}\sum_{\mu}C^*_{1\mu',i}C_{1\mu,j}\Pi_{N',N;\mu'}{}^{\mu}(\Omega) \ . \quad (9)$$

The coefficients $C_{1\mu,j}$ in Eq. (9) are those of the polynomials of degree one in the Cartesian coordinates, belonging to the class of the homogeneous harmonic polynomials

$$(4\pi)^{1/2}r^lY_{lm}(\theta,\varphi)=\sum_{(j=1,2,3)}C_{lm,j_1\cdots j_l}x_{j_1}\cdots x_{j_l} \ ,$$
$$(l=1,2,3,\ldots;m=-l,-l+1,\ldots,l) \ . \quad (10)$$

III. THE TENSORS $\Pi^s_{n'l'mm',nlm}(\Omega)$ AND $\Xi^s_{n'l'm',nlm}(\Omega)$

Substituting in Eq. (5) the expressions of the vectors $\mathbf{w}_{nlm}(\Omega;r,\theta,\varphi)$ and $\mathbf{P}u_{n'l'm'}(r,\theta,\varphi)$ in terms of spherical harmonics, which are given by Eq. (9) of Ref. 9 and Eq. (A4) of I, we get

$$\Pi^s_{n'l'm',nlm;\mu'}{}^{\mu}(\Omega)=\delta_{m'-\mu',m-\mu}\sum_{q'=1,-1}\sum_{q=1,-1}\delta_{l'+q',l+q}q'q\left[\frac{|\lambda_{l'+q',l'}\lambda_{l+q,l}|}{(2l'+1)(2l+1)}\right]^{1/2} \times\langle l+q\ m-\mu,1\mu'|l+q\ 1,l'm'\rangle\langle l+q\ m-\mu,1\mu|l+q\ 1,lm\rangle b^{(q',q)}_{n'l',nl}(\tau) \ . \quad (11)$$

The superscript s on the letter Π on the left-hand side of Eq. (11) means *spherical.* The symbol $\lambda_{l+q,l}$ is defined by Eq. (A5) of I and the standard notation is used for the Clebsch-Gordan coefficients. The Kronecker symbols in Eq. (11) express the DA selection rules for the angular momentum quantum numbers in two-photon transitions, while $b^{(q',q)}_{n'l',nl}(\tau)$ are four dimensionless scalar amplitudes,

$$b^{(q',q)}_{n'l',nl}(\tau)=-\int_0^\infty dr\, r^2\left[\left[\frac{d}{dr}+\frac{1+\lambda_{l'+q',l'}}{r}\right]R_{n'l'}(r)\right] \times\mathcal{B}_{n\,l\,l+q}(\Omega;r) \quad (l'=l+q-q') \ , \quad (12)$$

depending on the parameter τ, defined by Eq. (24) of I.

The expansion of the function $\mathcal{B}_{n\,l\,l+q}(\Omega;r)$ in terms of Coulomb radial eigenfunctions is

$$\mathcal{B}_{n\,l\,l+q}(\Omega;r)=-e^2a_0\,\sum\!\!\!\!\!\!\int_{n''}\frac{Q^{n''l+q}_{nl}}{E_{n''}-\Omega}R_{n''\,l+q}(r) \ , \quad (13)$$

where the summation is extended over the Bohr levels $E_{n''}$ with $n''>l+q$ and over the whole continuous part of the energy spectrum. For $E>0$, the radial eigenfunctions are normalized in the energy scale. We have denoted

$$Q_{nl}^{n''l+q} \equiv \int_0^\infty dr\, r^2 R_{n''\,l+q}(r) \left[\frac{d}{dr} + \frac{1+\lambda_{l+q,l}}{r} \right] \times R_{nl}(r) \ . \tag{14}$$

In fact, the radial integral (14) is proportional to the more familiar one $R_{nl}^{n''l+q}$, defined by Eq. (21) of I,

$$Q_{nl}^{n''l+q} = -\frac{1}{e^2 a_0}(E_{n''}-E_n) R_{nl}^{n''l+q} \ . \tag{15}$$

Equations (13) and (14) yield the spectral expansion of an amplitude (12),

$$b_{n'l',nl}^{(q';q)}(\tau) = e^2 a_0 \sum\!\!\!\!\!\!\int_{n''} \frac{Q_{n'l'}^{n''l+q} Q_{nl}^{n''l+q}}{E_{n''}-\Omega} \quad (l'=l+q-q') \ . \tag{16}$$

In order to get an explicit expression of the scalar amplitudes (12), we use our integral representation of the radial function $\mathcal{B}_{n\,l\,l+q}(\Omega;r)$ (Ref. 13) together with the expansion formula (A7) of I. Then, the radial integration is performed simply by applying Eq. (A2). We finally obtain

$$b_{n'l',nl}^{(q';q)}(\tau) = \frac{1}{[2(l+q)+1]!} \left[\frac{(n'+l')!(n+l)!}{(n'-l'-1)!(n-l-1)!} \right]^{1/2} \frac{\tau}{4n'n} (\beta_{n',n})^{l+q+1}$$
$$\times \sum_{s'=-1,1} \sum_{s=-1,1} d_{n',l'}^{(q',s')} d_{n,l}^{(q,s)} \left[\frac{n'-\tau}{n'+\tau} \right]^{n'-s'} \left[\frac{n-\tau}{n+\tau} \right]^{n-s} \frac{1}{l+q+1-\tau}$$
$$\times {}_1F_E(l+q+1-\tau; n'+n-s'-s, l+q+1+s'-n', l+q+1+s-n\ ,$$
$$2(l+q)+2; l+q+2-\tau; \zeta_{n',n}, \zeta_{-n',n}, \zeta_{n',-n}, \beta_{n',n}) \quad (l'=l+q-q') \ . \tag{17}$$

In Eq. (17), we have denoted

$$\beta_{n',n} \equiv \frac{2^4 n' n \tau^2}{(n'-\tau)(n'+\tau)(n-\tau)(n+\tau)} \ , \tag{18}$$

and

$$\zeta_{n',n} \equiv \frac{(n'-\tau)(n-\tau)}{(n'+\tau)(n+\tau)} \ . \tag{19}$$

The coefficients $d_{n,l}^{(q,s)}$ are listed in Table VI of I. We have introduced a new generalized hypergeometric function, ${}_1F_E$, with six parameters and four variables, defined by the contour integral

$${}_1F_E(a;b,a_1,b_1,c_1;c;x,x',x'',z) \equiv \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \frac{-ie^{-i\pi a}}{2\sin(\pi a)}$$
$$\times \int_1^{(0+)} d\rho\, \rho^{a-1}(1-\rho)^{c-a-1}(1-x\rho)^{-b}(1-x'\rho)^{-a_1}$$
$$\times (1-x''\rho)^{-b_1} {}_2F_1\left[a_1, b_1; c_1; \frac{z\rho}{(1-x'\rho)(1-x''\rho)} \right] , \tag{20}$$

where $a \neq 1,2,3,\ldots$, $\mathrm{Re}(c-a)>0$, and $c_1 \neq 0,-1,-2,\ldots$. In this paper we are interested in the special case when both a_1 and b_1 are *nonpositive integers.* Then, according to Eqs. (A3) and (A4), ${}_1F_E$ is a *finite* sum of Gauss hypergeometric functions ${}_2F_1$,

$${}_1F_E(a;b,a_1,b_1,c_1;c;x,x',x'',z) = \sum_{\nu_1=0}^{\infty} \sum_{\nu'=0}^{\infty} \sum_{\nu''=0}^{\infty} \frac{(a)_{\nu_1+\nu'+\nu''}}{(c)_{\nu_1+\nu'+\nu''}} \frac{(a_1)_{\nu_1+\nu'}(b_1)_{\nu_1+\nu''}}{(c_1)_{\nu_1}\nu_1!\nu'!\nu''!} z^{\nu_1}(x')^{\nu'}(x'')^{\nu''}$$
$$\times {}_2F_1(a+\nu_1+\nu'+\nu'', b; c+\nu_1+\nu'+\nu''; x)$$
$$\text{for } x' \neq x'',\ x' \neq 1,\ x'' \neq 1 \tag{21}$$

and

$${}_1F_E(a;b,a_1,b_1,c_1;c;x,x',x'',z) = \sum_{\nu_1=0}^{\infty} \frac{(a)_{\nu_1}(c-a)_{-a_1-b_1-2\nu_1}}{(c)_{-a_1-b_1-\nu_1}} \frac{(a_1)_{\nu_1}(b_1)_{\nu_1}}{(c_1)_{\nu_1}\nu_1!} z^{\nu_1}$$
$$\times {}_2F_1(a+\nu_1, b; c-a_1-b_1-\nu_1; x) \quad \text{for } x'=x''=1 \ . \tag{22}$$

The function (20) is not modified by a simultaneous interchange $a_1 \leftrightarrow b_1$ and $x' \leftrightarrow x''$. It is obvious that each function ${}_1F_E$ included in the tensor (11) has only four parameters and three variables which are independent. In the case of Raman scattering, $\zeta_{-n',n}=(\zeta_{n',-n})^{-1}\neq 1$, so that one has to use the finite sum (21), while for Rayleigh scattering, $\zeta_{-n,n}=\zeta_{n,-n}=1$, and, therefore, the simpler expansion (22) is valid.

Now, we proceed in a similar manner in order to get the tensor $\Xi^s_{n'l'm',nlm}(\Omega)$. First, we substitute in Eq. (8) the expressions of the vectors $\mathbf{v}_{nlm}(\Omega;r,\theta,\varphi)$ and $\mathbf{r}u_{n'l'm'}(r,\theta,\varphi)$, given, respectively, by Eqs. (18) and (A3) of I,

$$\Xi^s_{n'l'm',nlm;\mu'}{}^{\mu}(\Omega)=\delta_{m'-\mu',m-\mu}\sum_{q'=1,-1}\sum_{q=1,-1}\delta_{l'+q',l+q}q'q\left[\frac{|\lambda_{l'+q',l'}\lambda_{l+q,l}|}{(2l'+1)(2l+1)}\right]^{1/2}$$
$$\times\langle l+q\ m-\mu,1\mu'|l+q\ 1,l'm'\rangle\times\langle l+q\ m-\mu,1\mu|l+q\ 1,lm\rangle a^{(q',q)}_{n'l',nl}(\tau)\ . \tag{23}$$

The four dimensionless scalar amplitudes

$$a^{(q',q)}_{n'l',nl}(\tau)=\frac{4|E_1|^2}{e^2a_0}\int_0^\infty dr\, r^3R_{n'l'}(r)\mathcal{A}_{n\,l\,l+q}(\Omega;r)\quad (l'=l+q-q') \tag{24}$$

have, by virtue of Eq. (20) in I, the following spectral expansion:

$$a^{(q',q)}_{n'l',nl}(\tau)=\frac{4|E_1|^2}{e^2a_0}\sum\!\!\!\!\!\!\int_{n''}\frac{R^{n''l+q}_{n'l'}R^{n''l+q}_{nl}}{E_{n''}-\Omega}\quad (l'=l+q-q')\ . \tag{25}$$

By using Eqs. (22) and (A6) of I and then applying Eq. (A2), we get the explicit formula

$$a^{(q',q)}_{n'l',nl}(\tau)=\frac{1}{[2(l+q)+1]!}\left[\frac{(n'+l')!(n+l)!}{(n'-l'-1)!(n-l-1)!}\right]^{1/2}\frac{1}{4}\tau n'n(\beta_{n',n})^{l+q+1}$$
$$\times\sum_{s'=-2}^{2}\sum_{s=-2}^{2}c^{(q',s')}_{n',l'}c^{(q,s)}_{n,l}\left[\frac{n'-\tau}{n'+\tau}\right]^{n'-s'}\left[\frac{n-\tau}{n+\tau}\right]^{n-s}\frac{1}{l+q+1-\tau}$$
$$\times{}_1F_E(l+q+1-\tau;n'+n-s'-s,l+q+1+s'-n',l+q+1+s-n\ ,$$
$$2(l+q)+2;l+q+2-\tau;\zeta_{n'n},\zeta_{-n',n},\zeta_{n',-n},\beta_{n',n})\quad (l'=l+q-q')\ . \tag{26}$$

Note that the tensors $\Pi^s_{n'l'm',nlm}(\Omega)$ and $\Xi^s_{n'l'm',nlm}(\Omega)$ have identical expansions, Eqs. (11) and (23), in terms of scalar amplitudes with similar structure. Indeed, one may convert *formally* Eq. (17) into Eq. (26) by means of the change

$$\sum_{s'=-1,1}\sum_{s=-1,1}d^{(q',s')}_{n',l'}d^{(q,s)}_{n,l}\to\sum_{s'=-2}^{2}\sum_{s=-2}^{2}n'^2n^2c^{(q',s')}_{n',l'}c^{(q,s)}_{n,l}\ . \tag{27}$$

However, while the **A**-gauge tensor $\Pi^s_{n'l'm',nlm}(\Omega)$ involves only eight different functions ${}_1F_E$, the ϕ-gauge tensor $\Xi^s_{n'l'm',nlm}(\Omega)$ is composed of 50 such functions. This is due to the considerably larger number of coefficients c in Eq. (26) as compared to that of the coefficients d present in Eq. (17).

IV. THE TENSORS $\Pi^p_{n'_\xi n'_\eta m',n_\xi n_\eta m}(\Omega)$ AND $\Xi^p_{n'_\xi n'_\eta m',n_\xi n_\eta m}(\Omega)$

In order to evaluate the tensor $\Pi^p_{n'_\xi n'_\eta m',n_\xi n_\eta m}(\Omega)$, where the superscript p means parabolic, we substitute in Eq. (5) the expressions of the vectors $\mathbf{w}_{n_\xi n_\eta m}(\Omega;\xi,\eta,\varphi)$ and $\mathbf{P}u_{n'_\xi n'_\eta m'}(\xi,\eta,\varphi)$, given, respectively, by Eqs. (37) and (A13) of I. Then we carry out the integration over the parabolic coordinates by applying Eq. (A2) and get the result

$$\Pi^{p}_{n'_\xi n'_\eta m', n_\xi n_\eta m;\mu'}{}^{\mu}(\Omega)$$
$$=\delta_{m'-\mu',m-\mu}(-1)^{(1/2)(\mu'+|\mu'|+\mu+|\mu|)}2^{-(1/2)(|\mu'|+|\mu|)}\frac{\tau}{4n'n}\frac{1}{[(|m-\mu|)!]^2}$$
$$\times\left[\frac{(n'_\xi+|m'|)!(n'_\eta+|m'|)!(n_\xi+|m|)!(n_\eta+|m|)!}{n'_\xi!n'_\eta!n_\xi!n_\eta!}\right]^{1/2}(\beta_{n',n})^{|m-\mu|+1}\frac{1}{|m-\mu|+1-\tau}$$
$$\times\sum_{\tilde M'=0,M'}\sum_{\tilde M=0,M}\sum_{s'=-1,1}\sum_{s=-1,1}\left[\frac{n'-\tau}{n'+\tau}\right]^{n'-s'}\left[\frac{n-\tau}{n+\tau}\right]^{n-s}(1-\tfrac{1}{2}\delta_{M'-\tilde M'+s',\tilde M'})(1-\tfrac{1}{2}\delta_{M-\tilde M+s,\tilde M})$$
$$\times\{d^{(M',\tilde M',s')}_{n'_\xi,n'_\eta,|m'|}[d^{(M,\tilde M,s)}_{n_\xi,n_\eta,|m|}\;{}_2F_E(|m-\mu|+1-\tau;n'+n-s'-s\;,-n'_\xi+M'-\tilde M'+s',-n'_\eta+\tilde M'\;,$$
$$-n_\xi+M-\tilde M+s,-n_\eta+\tilde M;|m-\mu|+1\;,|m-\mu|+1;$$
$$|m-\mu|+2-\tau;\zeta_{n',n},\zeta_{-n',n},\zeta_{n',-n},\beta_{n',n})$$
$$-(-1)^{\mu}d^{(M,\tilde M,s)}_{n_\eta,n_\xi,|m|}(M-\tilde M+s\leftrightarrow\tilde M)]-(-1)^{\mu'}d^{(M',\tilde M',s')}_{n'_\eta,n'_\xi,|m'|}(M'-\tilde M'+s'\leftrightarrow\tilde M')\}\;. \quad (28)$$

In Eq. (28), we have used the indices $M'=|m'-\mu'|-|m'|$, $M=|m-\mu|-|m|$, defined by Eq. (A14) of I, and the coefficients $d^{(M,\tilde M,s)}_{n_\xi,n_\eta,|m|}$ listed in Table III of I. The symbol $(M-\tilde M+s\leftrightarrow\tilde M)$ stands for the preceding function ${}_2F_E$ with the quoted parameters interchanged, while by $[M'-\tilde M'+s'\leftrightarrow\tilde M']$ we mean the expressions within the preceding square brackets with the specified numbers interchanged. ${}_2F_E$ is a new generalized hypergeometric function with nine parameters and four variables, defined by a contour integral similar to that of Eq. (20),

$${}_2F_E(a;b,a_1,a_2,b_1,b_2,c_1,c_2;c;x,x',x'',z)$$
$$\equiv\frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)}\frac{-ie^{-i\pi a}}{2\sin(\pi a)}\int_1^{(0+)}d\rho\,\rho^{a-1}(1-\rho)^{c-a-1}(1-x\rho)^{-b}(1-x'\rho)^{-(a_1+a_2)}(1-x''\rho)^{-(b_1+b_2)}$$
$$\times{}_2F_1\left[a_1,b_1;c_1;\frac{z\rho}{(1-x'\rho)(1-x''\rho)}\right]$$
$$\times{}_2F_1\left[a_2,b_2;c_2;\frac{z\rho}{(1-x'\rho)(1-x''\rho)}\right], \quad (29)$$

where $a\neq1,2,3,\ldots$, $\mathrm{Re}(c-a)>0$, $c_1,c_2\neq0,-1,-2,\ldots$, and, as required in this paper, a_1, a_2, b_1, and b_2 are *non-positive integers*. Consequently, on account of Eqs. (A3) and (A4), the function (29) is a *finite* sum of Gauss hypergeometric functions,

$${}_2F_E(a;b,a_1,a_2,b_1,b_2,c_1,c_2;c;x,x',x'',z)$$
$$=\sum_{\nu_1=0}^{\infty}\sum_{\nu_2=0}^{\infty}\sum_{\nu'=0}^{\infty}\sum_{\nu''=0}^{\infty}\frac{(a)_{\nu_1+\nu_2+\nu'+\nu''}}{(c)_{\nu_1+\nu_2+\nu'+\nu''}}\frac{(a_1)_{\nu_1}(b_1)_{\nu_1}(a_2)_{\nu_2}(b_2)_{\nu_2}}{(c_1)_{\nu_1}(c_2)_{\nu_2}}$$
$$\times\frac{(a_1+a_2+\nu_1+\nu_2)_{\nu'}(b_1+b_2+\nu_1+\nu_2)_{\nu''}}{\nu_1!\nu_2!\nu'!\nu''!}z^{\nu_1+\nu_2}(x')^{\nu'}(x'')^{\nu''}$$
$$\times{}_2F_1(a+\nu_1+\nu_2+\nu'+\nu'',b;c+\nu_1+\nu_2+\nu'+\nu'';x)\quad\text{for } x'\neq x'',\ x'\neq1,\ x''\neq1\;, \quad (30)$$

and

$${}_2F_E(a;b,a_1,a_2,b_1,b_2,c_1,c_2;c;x,x',x'',z)$$
$$=\sum_{\nu_1=0}^{\infty}\sum_{\nu_2=0}^{\infty}\frac{(a)_{\nu_1+\nu_2}(c-a)_{-a_1-a_2-b_1-b_2-2(\nu_1+\nu_2)}}{(c)_{-a_1-a_2-b_1-b_2-(\nu_1+\nu_2)}}\frac{(a_1)_{\nu_1}(b_1)_{\nu_1}(a_2)_{\nu_2}(b_2)_{\nu_2}}{(c_1)_{\nu_1}(c_2)_{\nu_2}\nu_1!\nu_2!}z^{\nu_1+\nu_2}$$
$$\times{}_2F_1(a+\nu_1+\nu_2,b;c-a_1-a_2-b_1-b_2-(\nu_1+\nu_2);x)\quad\text{for } x'=x''=1\;. \quad (31)$$

The function (29) is obviously symmetric with respect to the indices 1 and 2 and also invariant under a simultaneous interchange $a_1 \leftrightarrow b_1$, $a_2 \leftrightarrow b_2$, $x' \leftrightarrow x''$. We notice that each function ${}_2F_E$ included in the tensor (29) has only six parameters and three variables that are independent. Similar to the case of angular momentum states, one has to use the expansion (30) for Raman scattering and the simpler one (31) for Rayleigh scattering.

The ϕ-gauge tensor $\Xi^p_{n'_\xi n'_\eta m', m_\xi n_\eta m}(\Omega)$ may be obtained in the same manner, and its final expression is similar to that of the A-gauge tensor $\Pi^p_{n'_\xi n'_\eta m', n_\xi n_\eta m}(\Omega)$, Eq. (28). Instead of writing it explicitly, it is sufficient to indicate the substitution in Eq. (28) which converts *formally* $\Pi^p_{n'_\xi n'_\eta m', n_\xi n_\eta m}(\Omega)$ into $\Xi^p_{n'_\xi n'_\eta m', n_\xi n_\eta m}(\Omega)$,

$$\sum_{s'=-1,1}\sum_{s=-1,1} d^{(M',\tilde{M}',s')}_{n'_\xi,n'_\eta,|m'|} d^{(M,\tilde{M},s)}_{n_\xi,n_\eta,|m|} \rightarrow \sum_{s'=-2}^{2}\sum_{s=-2}^{2} n'^2 n^2 c^{(M',\tilde{M}',s')}_{n'_\xi,n'_\eta,|m'|} c^{(M,\tilde{M},s)}_{n_\xi,n_\eta,|m|} \; . \tag{32}$$

Comparison of Eqs. (27) and (32) for angular momentum states and Stark states respectively shows in both cases the same "correspondence" between the explicit forms of the tensors (5) and (8).[14] However, an inspection of Tables II and III of I, allows us to notice that while the ϕ-gauge tensor $\Xi^p_{n'_\xi n'_\eta m', n_\xi n_\eta m}(\Omega)$ is composed at the most of $33^2=1089$ functions ${}_2F_E$, the A-gauge tensor $\Pi^p_{n'_\xi n'_\eta m', n_\xi n_\eta m}(\Omega)$ involves at the most $8^2=64$ such functions. This remark, as well as the similar one that concludes Sec. III, shows that, although the ϕ-and A-gauge tensors $\Xi_{N',N}(\Omega)$ and $\Pi_{N',N}(\Omega)$ have the same explicit structure, the former includes considerably more terms than the latter, both for angular momentum and Stark states.

V. TWO-PHOTON TRANSITIONS INVOLVING THE GROUND STATE

Our DA A-gauge results become remarkably simple when either the initial or the final atomic state in a two-photon transition is the ground state. We shall write compactly the Cartesian components of the tensor (5), by specializing N to label the atomic ground state.

First, from Eqs. (9) and (11) it follows that

$$\Pi^s_{n'l'm',100;ij}(\Omega)=\delta_{l'0}\delta_{m'0}\delta_{ij}\tfrac{1}{3}b^{(1,1)}_{n'0,10}(\tau) + \delta_{l'2}\left[\sum_{m''=-2}^{2}\delta_{m'm''}C^*_{2m'',ij}\right] \times \tfrac{2}{15}b^{(-1,1)}_{n'2,10}(\tau) \; , \tag{33}$$

where the coefficients $C_{2m,ij}$ are specified by Eq. (10). The invariant amplitudes in Eq. (33) corresponding to the allowed $1s \rightarrow n's$ and $1s \rightarrow n'd$ DA transitions are, respectively,

$$b^{(1,1)}_{n'0,10}(\tau)=2^6 n'^{3/2}\frac{\tau^5}{(1+\tau)^4}\frac{(n'-\tau)^{n'-3}}{(n'+\tau)^{n'+3}}\frac{1}{2-\tau} \times[(n'+1)(n'+2)(n'-\tau)^2F_1(2-\tau;n'+3,-n'+1;3-\tau;\zeta_{n',1},\zeta_{-n',1}) -(n'-1)(n'-2)(n'+\tau)^2F_1(2-\tau;n'+1,-n'+3;3-\tau;\zeta_{n',1},\zeta_{-n',1})] \tag{34}$$

and

$$b^{(-1,1)}_{n'2,10}(\tau)=2^6 n'^{3/2}[(n'^2-1)(n'^2-4)]^{1/2}\frac{\tau^5}{(1+\tau)^4}\frac{(n'-\tau)^{n'-3}}{(n'+\tau)^{n'+3}} \times\frac{1}{2-\tau}[(n'-\tau)^2F_1(2-\tau;n'+3,-n'+1;3-\tau;\zeta_{n',1},\zeta_{-n',1}) -(n'+\tau)^2F_1(2-\tau;n'+1,-n'+3;3-\tau;\zeta_{n',1},\zeta_{-n',1})] \; . \tag{35}$$

The amplitudes (34) and (35) are expressed in terms of two Appell functions F_1,[15] which are *finite* sums of Gauss functions ${}_2F_1$ of the variable $\zeta_{n',1}$.

Secondly, from Eqs. (9) and (28) we get

$$\Pi^p_{n'_\xi n'_\eta m',000;ij}(\Omega)=2^6 n'\frac{\tau^5}{(1+\tau)^4}\frac{(n'-\tau)^{n'-3}}{(n'+\tau)^{n'+3}}\frac{1}{2-\tau} \times[B^{(-1)}_{n'k'm';ij}(n'-\tau)^2F_1(2-\tau;n'+3,-n'+1;3-\tau;\zeta_{n',1},\zeta_{-n',1}) -B^{(1)}_{n'k'm';ij}(n'+\tau)^2F_1(2-\tau;n'+1,-n'+3;3-\tau;\zeta_{n',1},\zeta_{-n',1})] \; , \tag{36}$$

with

$$k' \equiv n'_\xi - n'_\eta \tag{37}$$

and

$$\begin{aligned}B^{(\mp 1)}_{n'k'm';ij} = {} & \delta_{m',0}\{\tfrac{1}{2}(\delta_{i1}\delta_{j1}+\delta_{i2}\delta_{j2})[(n'\pm 1)^2-k'^2]+\delta_{i3}\delta_{j3}[k'^2 \pm (n'\pm 1)]\}\\ & -[\delta_{m',-1}(D_{1,i}\delta_{j3}+\delta_{i3}D_{1,j})+\delta_{m',1}(D_{-1,i}\delta_{j3}+\delta_{i3}D_{-1,j})]\tfrac{1}{2}k'(n'^2-k'^2)^{1/2}\\ & +(\delta_{m',-2}D_{2,ij}+\delta_{m',2}D_{-2,ij})\tfrac{1}{8}\{[(n'-1)^2-k'^2][(n'+1)^2-k'^2]\}^{1/2} .\end{aligned} \tag{38}$$

The coefficients $D_{\pm 1,i}$ and $D_{\pm 2,ij}$ in Eq. (38) occur in the polynomials of degree 1 and 2 belonging to the class of the homogeneous harmonic polynomials in the coordinates x_1 and x_2,

$$\rho^{|m|}e^{im\varphi} = \sum_{(j=1,2)} D_{m,j_1 \cdots j_{|m|}} x_{j_1} \cdots x_{j_{|m|}}$$

$$[\rho = (x_1^2+x_2^2)^{1/2}, \quad m = \pm 1, \pm 2, \pm 3, \ldots] . \tag{39}$$

It is worth mentioning that the tensors (33) and (36) include the *same* Appell functions F_1. In particular, for $n'=1$, they clearly reduce to Gavrilă's formula[16]

$$\begin{aligned}\Pi^s_{100,100;ij}(\Omega) &= \Pi^p_{000,000,ij}(\Omega)\\ &= \delta_{ij}\frac{2^7\tau^5}{(1+\tau)^8}\frac{1}{2-\tau}\\ &\quad \times {}_2F_1(2-\tau,4;3-\tau;\zeta_{1,1}) .\end{aligned} \tag{40}$$

VI. DISCUSSION

We do not intend to explain here in a comprehensive way the connection between our results in Sec. III and the earlier ones by Karule[4] and Gazeau.[6] Nevertheless, prior to any comment, it is convenient to present briefly a simplified version of Karule's method.

First, we introduce Eq. (48) of I into Eq. (24):

$$\begin{aligned}a^{(q',q)}_{n'l',nl}(\tau) = {} & \frac{4|E_1|^2}{e^2 a_0}\sum_{\nu=0}^{\infty}\frac{\tau}{\nu+l+q+1-\tau}\\ & \times \int_0^\infty dr\, r^3 R_{n'l'}(r) S_{\nu l+q}(\Omega;r)\\ & \times \int_0^\infty dr' r'^3 S_{\nu l+q}(\Omega;r') R_{nl}(r')\\ & (l'=l+q-q') .\end{aligned} \tag{41}$$

Note that, in contrast with the eigenvalue expansion (25), the Sturmian expansion (41) of the ϕ-gauge scalar amplitudes (24) involves merely a discrete sum. The next steps to be made are the same as in our method described in Sec. III: we use Eq. (A6) of I and then perform the radial integrations by means of Eq. (A2). Our final result,

$$\begin{aligned}a^{(q',q)}_{n'l',nl}(\tau) = {} & \frac{n'n\tau}{4}\frac{1}{\{[2(l+q)+1]!\}^2}\left[\frac{(n'+l')!(n+l)!}{(n'-l'-1)!(n-l-1)!}\right]^{1/2}(\beta_{n',n})^{l+q+1}\\ & \times \sum_{s'=-2}^{2}\sum_{s=-2}^{2} c^{(q',s')}_{n',l'} c^{(q,s)}_{n,l}\left[\frac{n'-\tau}{n'+\tau}\right]^{n'-s'}\left[\frac{n-\tau}{n+\tau}\right]^{n-s}\\ & \times \sum_{\nu=0}^{\infty}\frac{1}{\nu+l+q+1-\tau}\frac{[\nu+2(l+q)+1]!}{\nu!}(\zeta_{n',n})^\nu\\ & \times {}_2F_1\left[-\nu,l+q+1+s'-n';2(l+q)+2;-\frac{4n'\tau}{(n'-\tau)^2}\right]\\ & \times {}_2F_1\left[-\nu,l+q+1+s-n;2(l+q)+2;-\frac{4n\tau}{(n-\tau)^2}\right] \quad (l'=l+q-q') ,\end{aligned} \tag{42}$$

is equivalent to Karule's original ϕ-gauge formula for bound-bound two-photon transitions.[17]

In the same manner one can get the Sturmian expansion of the **A**-gauge invariant amplitudes (12). However, it is much easier to infer the result from Eq. (42) simply by inverting the correspondence rule (27),

$$b_{n'l',nl}^{(q',q)}(\tau)=\frac{\tau}{4n'n}\frac{1}{\{[2(l+q)+1]!\}^2}\left[\frac{(n'+l')!(n+l)!}{(n'-l'-1)!(n-l-1)!}\right]^{1/2}(\beta_{n',n})^{l+q+1}$$
$$\times\sum_{s'=-1,1}\sum_{s=-1,1}d_{n',l'}^{(q',s')}d_{n,l}^{(q,s)}\left[\frac{n'-\tau}{n'+\tau}\right]^{n'-s'}\left[\frac{n-\tau}{n+\tau}\right]^{n-s}$$
$$\times\sum_{\nu=0}^{\infty}\frac{1}{\nu+l+q+1-\tau}\frac{[\nu+2(l+q)+1]!}{\nu!}(\zeta_{n',n})^{\nu}$$
$$\times{}_2F_1\left[-\nu,l+q+1+s'-n';2(l+q)+2;-\frac{4n'\tau}{(n'-\tau)^2}\right]$$
$$\times{}_2F_1\left[-\nu,l+q+1+s-n;2(l+q)+2;-\frac{4n\tau}{(n-\tau)^2}\right]\quad(l'=l+q-q')\ . \tag{43}$$

Now we are in a position to mention two important points. On one hand, starting from the definition (20) of the function ${}_1F_E$, we have managed, after performing a rather intricate Gauss-hypergeometric-function algebra, to establish the expansion formula

$$\frac{1}{l+q+1-\tau}{}_1F_E(l+q+1-\tau;n'+n-s'-s,l+q+1+s'-n',l+q+1+s-n,2(l+q)+2\ ;$$
$$l+q+2-\tau;\zeta_{n',n},\zeta_{n',n},\zeta_{-n',-n},\beta_{n',n})$$
$$=\frac{1}{[2(l+q)+1]!}\sum_{\nu=0}^{\infty}\frac{1}{\nu+l+q+1-\tau}\frac{[\nu+2(l+q)+1]!}{\nu!}(\zeta_{n',n})^{\nu}$$
$$\times{}_2F_1\left[-\nu,l+q+1+s'-n';2(l+q)+2;-\frac{4n'\tau}{(n'-\tau)^2}\right]$$
$$\times{}_2F_1\left[-\nu,l+q+1+s-n;2(l+q)+2;-\frac{4n\tau}{(n-\tau)^2}\right]\ . \tag{44}$$

By substituting Eq. (44) into our closed-form results (26) and (17), we recover the noncompact expressions (42) and (43), respectively, derived by Karule's method.

On the other hand, we have examined Gazeau's **A**-gauge formulas also. Taking into account his different phase convention for the eigenfunctions, and apart from some misprints and minor inconsistencies, we have succeeded in casting Gazeau's results[18] into our more compact and flexible form, Eqs. (11) and (17), both for the $N'\neq N$ and $N'=N$ cases. However, this conversion involves a suitable rearrangement in the finite sum of Gauss functions ${}_2F_1$.

To recapitulate, our main results are the explicit forms of the **A**-gauge KH tensors for angular momentum states, $\Pi^{s}_{n'l'm',nlm}(\Omega)$, Eqs. (11) and (17), and for Stark states, $\Pi^{p}_{n'_\xi n'_\eta m',n_\xi n_\eta m}(\Omega)$, Eq. (28). We have pointed out the rules (27) and (32) by means of which they may be converted formally into the corresponding ϕ-gauge KH tensors $\Xi^{s}_{n'l'm',nlm}(\Omega)$ and $\Xi^{p}_{n'_\xi n'_\eta m',n_\xi n_\eta m}(\Omega)$. Our general formulas are *compact* and have been derived in a *unitary* way by a *simple* algebraic method. They are also versatile enough to get easy, by specializing the quantum numbers, all the earlier DA results concerning particular bound-bound two-photon transitions of hydrogenic atoms.

APPENDIX: TWO USEFUL INTEGRALS

In Secs. III, IV, and VI we have to evaluate integrals of the form

$$J_{c-1}^{(0,0)}(\lambda;a',a;K',K)\equiv\int_0^\infty dr\,e^{-\lambda r}r^{c-1}{}_1F_1(a',c;K'r)\times{}_1F_1(a,c;Kr)\ , \tag{A1}$$

with a' and a nonpositive integers, $\mathrm{Re}c>0$, $\mathrm{Re}\lambda>0$. In the special case $\lambda=\frac{1}{2}(K'+K)$, the integral (A1) belongs to a class of integrals calculated by Gordon.[19] One obtains[20]

$$J_{c-1}^{(0,0)}(\lambda;a',a;K',K)=\Gamma(c)\lambda^{a'+a-c}(\lambda-K')^{-a'}\times(\lambda-K)^{-a}\times{}_2F_1\left[a',a;c;\frac{K'K}{(\lambda-K')(\lambda-K)}\right]\ . \tag{A2}$$

In establishing the explicit form of the functions ${}_1F_E$ and ${}_2F_E$, we have made use of Lauricella's hypergeometric functions F_D.[21] A function F_D is defined by the contour integral

$$F_D(a;b_1,\ldots,b_n;c;x_1,\ldots,x_n)\equiv\frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)}\frac{-ie^{-i\pi a}}{2\sin(\pi a)}\int_1^{(0+)}d\rho\,\rho^{a-1}(1-\rho)^{c-a-1}\times(1-x_1\rho)^{-b_1}\cdots(1-x_n\rho)^{-b_n}\,,\quad \mathrm{Re}(c-a)>0 \tag{A3}$$

and has the expansion

$$F_D(a;b_1,\ldots,b_n;c;x_1,\ldots,x_n)=\sum_{\nu_1=0}^{\infty}\cdots\sum_{\nu_{n-1}=0}^{\infty}\frac{(a)_{\nu_1+\cdots+\nu_{n-1}}}{(c)_{\nu_1+\cdots+\nu_{n-1}}}\frac{(b_1)_{\nu_1}\cdots(b_{n-1})_{\nu_{n-1}}}{\nu_1!\cdots\nu_{n-1}!}x_1^{\nu_1}\cdots x_{n-1}^{\nu_{n-1}}\times{}_2F_1(a+\nu_1+\cdots+\nu_{n-1}),b_n;c+\nu_1+\cdots+\nu_{n-1};x_n)\,, \tag{A4}$$

provided $|x_p|<1$ and/or b_p is a negative integer, for $p=1,\ldots,n-1$. In the special cases $n=1$ and $n=2$, Lauricella's hypergeometric function F_D reduces, respectively, to the Gauss function ${}_2F_1$ and the Appell function F_1.

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[14]It is precisely the idea to assure a unique form of the "rules" (27) and (32) that persuaded us to define the coefficients $c_{n,l}^{(q,s)}$ listed in Table I of I, in such a way that two of them may take on half-odd-integer values.

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[16]Reference 1, Eq. (53).

[17]Reference 4, Eqs. (4)–(6) written for $N=2$.

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