First-order perturbed wave functions for the hydrogen atom in a harmonic uniform external electric field

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We investigate the linear response of a nonrelativistic hydrogenlike atom to a harmonic uniform electric field, which is switched on adiabatically. For the electron initially in an arbitrary bound $|nlm\rangle$ state, the first-order correction to the wave function has been written in terms of a vector function \mathbf{w}_{nlm} . We report an exact closed-form expression of the vector \mathbf{w}_{nlm} that we have derived using the Coulomb Green's function. Our general analytic results prove to be useful in a systematic study of two-photon processes involving the hydrogen atom.

I. INTRODUCTION

The problem of determining the linear response of the hydrogen atom to a monochromatic electromagnetic plane wave was investigated by Podolsky¹ soon after the creation of quantum mechanics. Assuming a stationary $|nlm\rangle$ state as the initial atomic state, the specific question was how does one get an analytic expression of the corresponding first-order perturbed wave function. The electric dipole approximation (DA) to Podolsky's problem consists in calculating the linear response of the hydrogen atom to a harmonic uniform electric field. This is the subject considered in the following.

In his paper, Podolsky has treated only the ground-state case in the DA, expressing the first-order correction $\psi_{100}^{(1)}$ to the wave function as an infinite series of orthogonal functions, the Coulomb Sturmian functions. With his noncompact result Podolsky has obtained the dynamic dipole polarizability of the hydrogen atom in the ground state.

Much later, a simple closed-form expression of $\psi_{100}^{(1)}$ has been derived by Luban, Nudler, and Freund.^{2,3} The linear-response function for the ground state has been given as an integral representation, strictly valid for field frequencies below the first excitation frequency. This result has been extended to higher frequencies not, however, exceeding the photoionization threshold.

It is worth mentioning that for the hydrogen atom in the presence of a *static* electric field, Jhanwar and Meath⁴ have derived a compact expression of the first-order correction to *any* energy eigenstate $|nlm\rangle$. Using these corrections they have written general formulas for the atomic static dipole polarizabilities.

All the quoted results¹⁻⁴ have been obtained by solving appropriate inhomogeneous differential equations with adequate boundary conditions.

Recently⁵ we have reconsidered the linear-response problem, using the Green's-function method. In the ground-state case we have taken into account retardation, giving the *exact* solution of Podolsky's problem. In the same work we have derived the DA corrections $\psi_{nlm}^{(1)}$ corresponding to the excited states with n = 2 and 3.

Meanwhile, we have generalized our DA results to any

excited $|nlm\rangle$ state.⁶ The analytic formulas obtained are very convenient for calculating the matrix elements of two-photon transitions.⁵ In analytic work, this method has never been used as yet, although in numerical work the calculation of the first-order perturbed wave functions, as a first step for evaluating two-photon matrix elements, has been applied for a long time.⁷

The purpose of this paper is to present our general nonrelativistic DA formulas for the linear-response functions $\psi_{nlm}^{(1)}$. The method of derivation relies on the consistent use of the Coulomb Green's function. Mathematical details are omitted and will be given in a separate paper. An alternative method of derivation, using Podolsky's differential equations,¹ will be also described elsewhere.

In Sec. II we point out that the correction $\psi_{nlm}^{(1)}$ is entirely determined by a vector function \mathbf{w}_{nlm} which in its turn includes two radial scalar functions $\mathscr{B}_{nll'}$ $(l'=l\pm 1)$. In Sec. III we write the functions $\mathscr{B}_{nll'}$ as closed-form integral representations, while in Sec. IV they are expressed in terms of Humbert functions ϕ_1 . In particular, we examine the result corresponding to the ground state. The detailed expressions of the functions $\mathscr{B}_{nll'}$ for the excited states with n=2 are also given. In Sec. V the static limit of the linear-response problem is briefly discussed. Section VI summarizes the results and stresses their importance for applications.

II. THE FIRST-ORDER CORRECTION $\psi_{nlm}^{(1)}$ AND THE VECTOR FUNCTION \mathbf{w}_{nlm}

The unperturbed system is an electron in the Coulomb field of a point nucleus of charge Ze. The external perturbation is a weak electric field

$$\mathscr{E}(t) = \mathscr{E}_0 \cos(\omega t) , \qquad (1)$$

that we describe by the potentials

$$\phi = 0, \quad \mathbf{A}(t) = -\frac{c}{\omega} \mathscr{C}_0 \sin(\omega t) \;.$$
 (2)

The corresponding interaction Hamiltonian (with the A^2 term neglected) is

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$$H^{(1)}(t) = \frac{e}{m_e c} \mathbf{A} \cdot \mathbf{P} , \qquad (3)$$

where m_e is the electron mass, and **P** denotes the momentum operator. We suppose that the electric field is switched on adiabatically, i.e., for t < 0 the operator (3) is multiplied by a factor $\exp[(\epsilon/\hbar)t]$, with $\epsilon \to +0$ eventually. In the remote past $(t \to -\infty)$ the atom is assumed to be in a stationary $|nlm\rangle$ state,

$$\psi_{nlm}^{(0)}(\mathbf{r},t) = \exp\left[-\frac{i}{\hbar}E_n t\right] u_{nlm}(\mathbf{r}) . \qquad (4)$$

Then the first-order correction to the wave function (4), given by time-dependent perturbation theory, has the form

$$\psi_{nlm}^{(1)}(\mathbf{r},t) = \frac{ie}{2m_e\omega} \exp\left[-\frac{i}{\hbar}E_n t\right]$$
$$\times \mathscr{B}_0 \cdot \left[\exp(-i\omega t)\mathbf{w}_{nlm}(\Omega_1;\mathbf{r}) - \exp(i\omega t)\mathbf{w}_{nlm}(\Omega_2;\mathbf{r})\right].$$
(5)

The vector function \mathbf{w}_{nlm} is defined by the equation

$$\mathbf{w}_{nlm}(\Omega;\mathbf{r}) \equiv \sum_{n'} \sum_{l',m'} \frac{\langle u_{n'l'm'} | \mathbf{P} u_{nlm} \rangle}{E_{n'} - \Omega} u_{n'l'm'}(\mathbf{r}) , \qquad (6)$$

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where the summation is extended over all the energy eigenstates (bound and continuum) of the electron in the Coulomb field. The parameters Ω_1 and Ω_2 in Eq. (5) are

$$\Omega_1 = E_n + \hbar\omega + i\epsilon, \quad \Omega_2 = E_n - \hbar\omega . \tag{7}$$

We notice that the linear-response function (5) is completely determined by the vector function \mathbf{w}_{nlm} .

Equation (6) can be written alternatively as

$$\mathbf{w}_{nlm}(\Omega;\mathbf{r}) = -\int d^3x' G(\mathbf{r},\mathbf{r}';\Omega) \mathbf{P}' u_{nlm}(\mathbf{r}') , \qquad (8)$$

where $G(\mathbf{r},\mathbf{r}';\Omega)$ is the Coulomb Green's function.

Using the definition (6) we decompose the vectors \mathbf{w}_{nlm} in terms of vector spherical harmonics,⁸

$$\mathbf{w}_{nlm}(\Omega;\mathbf{r}) = \frac{im_e}{\hbar} \left[-\left[\frac{l+1}{2l+1}\right]^{1/2} \mathscr{B}_{nll+1}(\Omega;\mathbf{r}) \mathbf{V}_{l+1lm} \left[\frac{\mathbf{r}}{\mathbf{r}}\right] + \left[\frac{l}{2l+1}\right]^{1/2} \mathscr{B}_{nll-1}(\Omega;\mathbf{r}) \mathbf{V}_{l-1lm} \left[\frac{\mathbf{r}}{\mathbf{r}}\right] \right], \quad l > 0.$$
(9)

For l=0 only the first term exists, so that

$$\mathbf{w}_{n00}(\Omega;\mathbf{r}) = \frac{im_e}{\hbar} (4\pi)^{-1/2} \mathscr{B}_{n01}(\Omega;\mathbf{r}) \frac{\mathbf{r}}{\mathbf{r}} . \tag{10}$$

The radial functions $\mathscr{B}_{nll'}(\Omega;r)$ in Eqs. (9) and (10), $(l'=l\pm 1, \text{ if } l>0, \text{ and } l'=1, \text{ if } l=0)$, have the following expansion in terms of Coulomb radial eigenfunctions:

$$\mathscr{B}_{nll'}(\Omega;r) = \sum_{n'} \frac{Q_{nl}^{n'l'}}{E_{n'} - \Omega} R_{n'l'}(r) , \qquad (11)$$

with

$$Q_{nl}^{n'l'} \equiv \int_0^\infty dr \, r^2 R_{n'l'}(r) \left(\frac{d}{dr} + \frac{1 + \lambda_{l',l}}{r} \right) R_{nl}(r) , \qquad (12)$$

and

$$\lambda_{l+1,l} = -(l+1), \ l \ge 0,$$

$$\lambda_{l-1,l} = l, \ l > 0.$$
 (13)

The sum in Eq. (11) is extended over energy eigenvalues: negative values $E_{n'}$, with n' > l', and the positive values. For E > 0 the energy eigenfunctions are normalized in the energy scale. An alternative form of the expansion (11) is

$$\mathscr{B}_{nll'}(\Omega;r) = rR_{nl}(r) - (E_n - \Omega) \sum_{n'} \frac{R_{nl}^{n'l'}}{E_{n'} - \Omega} R_{n'l'}(r) , \quad (14)$$

where we have used the standard notation⁹

$$R_{nl}^{n'l'} \equiv \int_0^\infty dr \, r^3 R_{n'l'}(r) R_{nl}(r) \; . \tag{15}$$

Equation (14) displays some analytic properties of the radial functions $\mathscr{B}_{nll'}$ in the complex Ω plane, namely, their behavior in the vicinity of the poles $\Omega = E_{n'} < 0$ $(n' \neq n)$, and the compact expressions of $\operatorname{Im} \mathscr{B}_{nll'}$ along the cut $\Omega = E > 0$.

III. THE RADIAL FUNCTIONS *B*_{nll}. AS INTEGRAL REPRESENTATIONS

We have found a closed form of the functions $\mathscr{B}_{nll'}(\Omega; r)$ using Schwinger's integral representation of the Coulomb Green's function in momentum space.¹⁰ This starting point was adopted for the first time by Gavrilă¹¹ and proved to be very efficient in the study of two-photon processes.

We have first calculated the function

$$\mathscr{F}(\mathbf{q},\lambda,\Omega;\mathbf{r}) \equiv -\int d^{3}x' G(\mathbf{r},\mathbf{r}';\Omega) \frac{1}{r'} \exp\left[\frac{i}{\hbar}\mathbf{q}\cdot\mathbf{r}' - \frac{1}{\hbar}\lambda r'\right],$$
(16)

depending on the real parameters q and $\lambda > 0$. Then, by suitable operations, we have derived the functions (11) from their "generating function" (16). The explicit relationship between $\mathcal{B}_{nll'}$ and \mathcal{F} , as well as the details of the calculation, will not be presented here. We have eventually found the following integral representation of $\mathcal{B}_{nll'}$:

where
$$\kappa_n = 27 m_0$$
, u_0 is the boin radius, and

where $\kappa = 7/nq$, q is the Bohr radius and

$$X \equiv (-2m_e\Omega)^{1/2} \ (\text{Re}X > 0), \ \tau \equiv \frac{n\kappa_1}{X},$$
 (18)

$$\mathcal{N}_{n,\tau} \equiv n + \tau + (n - \tau)\rho , \qquad (19)$$

$$b_{nll'}(\rho,\tau;r) = \frac{1}{(2l'+1)!} \left[\frac{(n+l)!}{(n-l-1)!2n} \right]^{1/2} 4n\tau \frac{\mathcal{N}_{n,-\tau}^{n-2}}{\mathcal{N}_{n,\tau}^{n+2}} (2\kappa_n r_{n,\tau})^{l'} \\ \times \left[d_{n,l}^{l',1} \mathcal{N}_{n,-\tau}^2 \phi(l'-n,2l'+2;2\kappa_n r_{n,\tau}) + d_{n,l}^{l',-1} \mathcal{N}_{n,\tau}^2 \phi(l'+2-n,2l'+2;2\kappa_n r_{n,\tau}) \right],$$
(20)

(17)

with ϕ denoting the confluent hypergeometric function, and

$$2\kappa_n r_{n,\tau} \equiv \frac{4n^2 \rho}{\mathcal{N}_{n,-\tau} \mathcal{N}_{n,\tau}} 2\kappa_n r , \qquad (21)$$

 $\times \int_{1}^{(0+)} d\rho \rho^{-\tau} b_{nll'}(\rho,\tau;r) \\ \times \exp\left[-\frac{n+\tau-(n-\tau)\rho}{\mathcal{N}_{n,\tau}}\frac{Xr}{\hbar}\right],$

$$d_{n,l}^{l+1,1} = (n+l+1)(n+l+2),$$

$$d_{n,l}^{l-1,1} = 1,$$

$$d_{n,l}^{l',-1} = -d_{-n,l}^{l',1}.$$
(22)

One notices that the two confluent hypergeometric functions in Eq. (20) are in fact proportional to Laguerre polynomials of the variable (21). It is remarkable that the general formulas (17) and (20) are valid for any value of the parameter τ , i.e., for *any* field frequency.

We shall now discuss in some detail the ground-state case. By taking n = 1 in Eqs. (20)-(22) one finds

$$b_{101} = 2^{7/2} \tau \frac{\rho}{\mathcal{N}_{1,\tau}^4} 2\kappa_1 r .$$
 (23)

Equations (10), (17), and (23) then give our previous result⁵

$$\mathbf{w}_{100}(\Omega;\mathbf{r}) = \frac{im_e}{\hbar} \frac{2^{7/2} (2\kappa_1)^{3/2}}{(4\pi)^{1/2}} \tau \, \mathbf{r} e^{-Xr/\hbar} \frac{ie^{i\pi\tau}}{2\sin(\pi\tau)} \\ \times \int_1^{(0+)} d\rho \frac{\rho^{1-\tau}}{\mathcal{N}_{1,\tau}^4} \exp\left[\frac{2(1-\tau)\rho}{\mathcal{N}_{1,\tau}} \frac{Xr}{\hbar}\right].$$
(24)

To Ω_1 and Ω_2 having the expressions (7) correspond τ_1 and τ_2 defined by Eq. (18). At frequencies below the ionization threshold, $\omega_{\infty 1} = |E_1| / \hbar$, one has $1 < \tau_1 < \infty$ and

$$1 > \tau_2 > 1/\sqrt{2}$$
, while above the threshold τ_1 becomes purely imaginary and τ_2 decreases monotonically from $1/\sqrt{2}$ to zero. Equation (24) is valid both below and above the threshold.

For real values $0 < \tau < 2$, the integration path in Eq. (24) may be reduced to the interval [0,1] on the real ρ axis. Then, with the change of variable $\rho = [(1+\tau)/(|1-\tau|)][s/(s+1)]$ ($\tau \neq 1$), we get the integral representations given by Luban *et al.* [Eqs. (20) and (23) of Ref. 3]. The quoted formulas, unlike our result (24), hold only below the first excitation frequency, $\omega_{21} = (E_2 - E_1)/\hbar$, where $1 < \tau_1 < 2$ and $1 > \tau_2 > 2/\sqrt{7}$.

As a further example, we list the functions (20) for the first excited states, with n = 2,

$$b_{201} = 2^{15/2} \tau \rho 2 \kappa_2 r \left[\frac{2 - \tau + (2 + \tau)\rho}{\mathcal{N}_{2,\tau}^5} - \frac{4\rho}{\mathcal{N}_{2,\tau}^6} 2 \kappa_2 r \right], \quad (25)$$

$$b_{212} = \frac{2^{19/2}}{3^{1/2}} \tau \frac{\rho^2}{\mathcal{N}_{2,\tau}^6} (2\kappa_2 r)^2 , \qquad (26)$$

$$b_{210} = \frac{2^{11/2}}{3^{1/2}} \tau \left[-\frac{3\tau(1-\rho^2)}{\mathcal{N}_{2,\tau}^4} - \frac{6\rho[2-\tau+(2+\tau)\rho]}{\mathcal{N}_{2,\tau}^5} 2\kappa_2 r + \frac{16\rho^2}{\mathcal{N}_{2,\tau}^6} (2\kappa_2 r)^2 \right].$$
(27)

IV. THE EXPLICIT FORM OF THE RADIAL FUNCTIONS $\mathscr{B}_{nll'}$

Equations (17)-(22) lead to the following compact expression of the function $\mathcal{B}_{nll'}$:

$$\mathscr{B}_{nll'}(\Omega;r) = (2\kappa_n)^{1/2} \frac{(2n)^{l'+\tau}}{(2l'+1)!} \left[\frac{(n+l)!}{(n-l-1)!2n} \right]^{1/2} \frac{2\tau}{l'+1-\tau} \frac{(n-\tau)^{n-l'-2}}{(n+\tau)^{n+\tau+1}} (2\kappa_n r)^{l'} e^{-Xr/\hbar} \\ \times \sum_{k=-1,1} d_{n,l}^{l',-k} (n-\tau)^{1-k} (n+\tau)^{1+k} \\ \times \phi_H \left[l'+1-\tau; -n-\tau+1+k, l'+1+k-n, 2l'+2; l'+2-\tau; \frac{n-\tau}{2n}, -\frac{(n+\tau)^2}{2n(n-\tau)}, \frac{n-\tau}{2\tau} 2\kappa_n r, \frac{2n}{n-\tau} 2\kappa_n r \right].$$
(28)

 $\mathscr{B}_{nll'}(\Omega;r) = (2\kappa_n)^{1/2} \frac{ie^{i\pi\tau}}{2\sin(\pi\tau)}$

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In Eq. (28) ϕ_H is a generalized hypergeometric function with five parameters and four variables, defined by its expansion into a double series of Humbert functions ϕ_1 ,

$$\phi_{H}(a;b_{1},b_{2},b';c;x_{1},x_{2},x,y)$$

$$\equiv \sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\infty} \frac{(a)_{\mu+\nu}(b_{2})_{\mu+\nu}}{(c)_{\mu+\nu}(b')_{\nu}} \frac{x_{\mu}^{\mu}y^{\nu}}{\mu!\nu!}$$

$$\times \phi_{1}(a+\mu+\nu,b_{1}+\mu,c+\mu+\nu;x_{1},x)$$

 $(|x_2| < 1)$. (29)

 $(a)_n$ is Pochhammer's symbol and the function ϕ_1 is the sum of the double power series

$$\phi_1(a,b,c\,;x,y) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(a)_{m+n}(b)_m}{(c)_{m+n}} \frac{x^m}{m!} \frac{y^n}{n!} , \quad (30)$$

which converges when $|x| < 1.^{12}$

We note that the third parameter in the functions ϕ_H occurring in Eq. (28) is a negative integer or zero. It follows, according to Eq. (29), that the function $\mathcal{B}_{nll'}$ can be expressed in terms of a *finite* number of Humbert functions ϕ_1 depending on the variables

$$\xi_n \equiv \frac{n-\tau}{2n}, \quad \eta_n \equiv \frac{n-\tau}{2\tau} 2\kappa_n r \quad . \tag{31}$$

We write now the detailed expressions of the functions $\mathscr{B}_{nll'}$ for the ground state (n = 1),

$$\mathscr{B}_{101}(\Omega;r) = \kappa_1^{1/2} \frac{\tau}{2-\tau} \left[\frac{2}{1+\tau} \right]^{2+\tau} \exp\left[-\frac{Xr}{\hbar} \right] \\ \times 2\kappa_1 r \phi_1(2-\tau, -1-\tau, 3-\tau; \xi_1, \eta_1) , \qquad (32)$$

and for the excited states with n = 2,

$$\mathscr{B}_{201}(\Omega; r) = \kappa_{2}^{1/2} \frac{\tau}{4^{2}} \left[\frac{4}{2+\tau} \right]^{3+\tau} \exp\left[-\frac{Xr}{\hbar} \right] 2\kappa_{2}r$$

$$\times \left[4\phi_{1}(2-\tau, -2-\tau, 3-\tau; \xi_{2}, \eta_{2}) + \frac{(2+\tau)^{2}}{3-\tau} \phi_{1}(3-\tau, -1-\tau, 4-\tau; \xi_{2}, \eta_{2}) - \frac{4}{3-\tau} 2\kappa_{2}r\phi_{1}(3-\tau, -2-\tau, 4-\tau; \xi_{2}, \eta_{2}) \right], \qquad (33)$$

$$\mathscr{B}_{212}(\Omega; r) = \kappa_2^{1/2} \frac{1}{3^{1/2} 4} \frac{\tau}{3 - \tau} \left[\frac{4}{2 + \tau} \right]^{3 + \tau} \exp\left[-\frac{Xr}{\hbar} \right] (2\kappa_2 r)^2 \phi_1(3 - \tau, -2 - \tau, 4 - \tau; \xi_2, \eta_2) , \qquad (34)$$
$$\mathscr{B}_{212}(\Omega; r) = \kappa_2^{1/2} \frac{\tau}{3 - \tau} \left[\frac{4}{2 + \tau} \right]^{3 + \tau} \exp\left[-\frac{Xr}{\hbar} \right] (2\kappa_2 r)^2 \phi_1(3 - \tau, -2 - \tau, 4 - \tau; \xi_2, \eta_2) ,$$

$$\times \left[-\frac{48\tau}{1-\tau} \phi_1(1-\tau, -2-\tau, 2-\tau; \xi_2, \eta_2) + \frac{3\tau(2+\tau)^2}{3-\tau} \phi_1(3-\tau, -\tau, 4-\tau; \xi_2, \eta_2) - \frac{6(2\kappa_2 r)}{4\phi_1(2-\tau, -2-\tau, 3-\tau; \xi_2, \eta_2) + \frac{(2+\tau)^2}{3-\tau} \phi_1(3-\tau, -1-\tau, 4-\tau; \xi_2, \eta_2)} \right] + \frac{16}{3-\tau} (2\kappa_2 r)^2 \phi_1(3-\tau, -2-\tau, 4-\tau; \xi_2, \eta_2) \left].$$

$$(35)$$

Equations (32)-(35) result from Eqs. (28) and (29); however, some transformations are needed in order to get Eq. (35).

Making use of Eqs. (29) and (30), the function (28) can be written as a double power series. The resulting expansion is particularly useful in deriving approximate formulas valid at low field frequencies. One can also take advantage of it in a numerical evaluation of the functions $\mathscr{B}_{nll'}$.

V. THE STATIC LIMIT

The analysis of the linear response at low frequencies requires special caution. Without going into details, we only mention here the two steps to be made in order to get correct wave functions in the low-frequency range.

First, Eqs. (3) and (5) show that perturbation theory using the gauge (2) fails as $\omega \rightarrow 0$. It is easy to overcome this difficulty, replacing the gauge (2) by the following one,

$$\phi'(\mathbf{r},t) = -\mathscr{C}_0 \cdot \mathbf{r}\cos(\omega t), \quad \mathbf{A}' = \mathbf{0} , \qquad (36)$$

and carrying out the corresponding gauge transformation of the wave function.⁵ Nevertheless, in our general calculation we have preferred the gauge (2), because it originates in the one with retardation included⁵ and introduces the basic functions \mathbf{w}_{nlm} .

Secondly, as pointed out by Chung,¹³ conventional per-

turbation theory does not exhibit the right static limit in the excited-states case. Accordingly, it is necessary to "renormalize" the wave function (see also Ref. 14), and to use, as proper initial states, the energy eigenstates in parabolic coordinates.

When taking into account the above-mentioned points, we have to replace, in characterizing the linear-response functions, the vectors (6) by the similar ones

$$\mathbf{v}_{nlm}'(\Omega;\mathbf{r}) \equiv \sum_{n'}' \sum_{l',m'} \frac{\langle u_{n'l'm'} | \mathbf{r} u_{nlm} \rangle}{E_{n'} - \Omega} u_{n'l'm'}(\mathbf{r}) . \quad (37)$$

The significance of the prime on the sum over the energy eigenvalues is to exclude the contribution of the level E_n . The angular dependence of the vectors (37) is similar to that described by Eqs. (9) and (10),

$$\mathbf{v}_{nlm}'(\Omega;\mathbf{r}) = -\left[\frac{l+1}{2l+1}\right]^{1/2} \mathscr{A}_{nll+1}'(\Omega;r) \mathbf{V}_{l+1lm}\left[\frac{\mathbf{r}}{r}\right] \\ + \left[\frac{l}{2l+1}\right]^{1/2} \mathscr{A}_{nll-1}'(\Omega;r) \mathbf{V}_{l-1lm}\left[\frac{\mathbf{r}}{r}\right] \\ (l>0), \quad (38)$$

$$\mathbf{v}_{n00}'(\Omega;\mathbf{r}) = (4\pi)^{-1/2} \mathscr{A}_{n01}'(\Omega;\mathbf{r}) \frac{\mathbf{r}}{\mathbf{r}}$$
 (39)

The radial functions $\mathscr{A}'_{nll'}(\Omega;r)$ in Eqs. (38) and (39) $(l'=l\pm 1 \text{ if } l>0$, and l'=1 if l=0) have the eigenfunction expansion

$$\mathscr{A}'_{nll'}(\Omega;r) = \sum_{n'}' \frac{R_{nl}^{n'l'}}{E_{n'} - \Omega} R_{n'l'}(r) .$$
(40)

From Eqs. (14) and (40) we get

$$\frac{\partial \mathscr{B}_{nll'}}{\partial \Omega} \bigg|_{\Omega = E_n} = \mathscr{A}'_{nll'}(E_n; r) = \sum_{n'}' \frac{R_{nl}^{n'l'}}{E_{n'} - E_n} R_{n'l'}(r) .$$
(41)

Therefore, when Ω is close to the energy E_n , the function $\mathscr{B}_{nll'}(\Omega;r)$ has the behavior

$$\mathscr{B}_{nll'}(E_n + \delta\Omega; r) = \mathscr{B}_{nll'}(E_n; r) + \mathscr{A}'_{nll'}(E_n; r) \delta\Omega + O((\delta\Omega)^2) .$$
(42)

Making use of Eq. (28), written as a series, we have derived the following compact expression of the radial function (41):

$$\int_{n'}^{r'} \frac{R_{nl}^{n'l'}}{E_{n'} - E_n} R_{n'l}(r) = \frac{(2\kappa_n)^{1/2}}{4|E_n|} \frac{1}{(2l'+1)!} \left[\frac{(n+l)!}{(n-l-1)!2n} \right]^{1/2} e^{-\kappa_n r} (2\kappa_n r)^{l'} \sum_{k=-2}^{2} C_{n,l}^{l',-k} \phi(l'+1+k-n,2l'+2;2\kappa_n r) \\ (l'=l\pm 1 \text{ if } l > 0, \text{ and } l'=1 \text{ if } l=0),$$

$$(43)$$

with

$$C_{n,l}^{l+1,2} = -\frac{1}{2}(n+l+1)(n+l+2)(n+l+3), \quad C_{n,l}^{l-1,2} = -\frac{1}{2}(n+l+1),$$

$$C_{n,l}^{l+1,1} = (n+l+1)(n+l+2)(n+l+3), \quad C_{n,l}^{l-1,1} = n-l+2,$$

$$C_{n,l}^{l+1,0} = (n+l+1)(n-l-1)(2l+5), \quad C_{n,l}^{l-1,0} = -(2l-3),$$

$$C_{n,l}^{l',-k} = C_{-n,l}^{l',k} \quad (k = 1,2).$$
(44)

In their work⁴ Jhanwar and Meath have calculated the z-axis component of the vector $v'_{nlm}(E_n;\mathbf{r})$, which determines the linear response of the atom to a static uniform electric field. Our sum rules, Eqs. (43) and (44), are equivalent to their results, contained in Eqs. (19), (20), (23)-(28), (31), and (32) of Ref. 4.

VI. SUMMARY AND CONCLUSIONS

We have presented in this paper the solution of Podolsky's problem in the dipole approximation, for an arbitrary $|nlm\rangle$ state. The linear-response correction $\psi_{nlm}^{(1)}$, Eq. (5), is completely determined by a mathematical object that we have studied, namely the vector function \mathbf{w}_{nlm} , defined by Eq. (6). Its expansion in terms of vector spherical harmonics [Eqs. (9) and (10)] has coefficients proportional to the radial functions $\mathcal{B}_{nll'}$, Eq. (11). Our main results are the integral representation of the functions $\mathscr{B}_{nll'}$ [Eqs. (17) and (20)] and their explicit expression (28).

Finally, we emphasize the importance of the vectors \mathbf{w}_{nlm} , beyond characterizing the linear-response wave functions. Our Eqs. (9), (10), (17), and (20) allow a *straightforward* calculation of the Kramers-Heisenberg matrix element for hydrogenic atoms.⁵ We think that with our results, two-photon bound-bound, bound-free, and free-free transitions in the DA can be treated in a general and unitary manner. Work on these lines is in progress.

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- ¹B. Podolsky, Proc. Natl. Acad. Sci. USA 14, 253 (1928).
- ²M. Luban, B. Nudler, and I. Freund, Phys. Lett. **47A**, 447 (1974).
- ³M. Luban and B. Nudler-Blum, J. Math. Phys. 18, 1871 (1977).
- ⁴B. L. Jhanwar and W. J. Meath, Mol. Phys. 40, 713 (1980).
- ⁵V. Florescu and T. Marian, Report No. FT-245-1984, Central Institute of Physics, Bucharest (unpublished).
- ⁶V. Florescu and T. Marian, in Proceedings of the Joint Romanian-USA Seminar in Mathematical Physics, Bucharest, June 14-20, 1985 (unpublished).
- ⁷G. E. Brown, R. E. Peierls, and J. B. Woodward, Proc. R. Soc. London A 227, 51 (1954); Sheila Brenner, G. E. Brown, and J. B. Woodward, *ibid.* 227, 59 (1954).
- ⁸A. R. Edmonds, Angular Momentum in Quantum Mechanics (Princeton University Press, Princeton, 1957), p. 84, Eq.

(5.9.16). Edmonds denotes the vector spherical harmonics by \mathbf{Y}_{jlm} , while our notation is \mathbf{V}_{ljm} .

- ⁹H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One*and Two-Electron Atoms (Springer, Berlin, 1957), p. 253, Eq. (60.8).
- ¹⁰J. Schwinger, J. Math. Phys. 5, 1606 (1964).
- ¹¹M. Gavrilă, Phys. Rev. 163, 147 (1967).
- ¹²The hypergeometric function ϕ_H has been defined in the present work in order to write our result (28) in the most compact form. For the function ϕ_1 , see P. Appell and J. Kampé de Fériet, Fonctions Hypergéométriques and Hypersphériques (Gauthier-Villars, Paris, 1926), p. 126.
- ¹³K. T. Chung, Phys. Rev. 163, 1343 (1967).
- ¹⁴P. W. Langhoff, S. T. Epstein, and M. Karplus, Rev. Mod. Phys. 44, 602 (1972).