Sturmian expansion of Green's function and its application to multiphoton ionization of hydrogen

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We report a study of the Sturmian expansion of Green's function and its convergence properties in the complex energy plane. We take as a model for our study multiphoton ionization of hydrogen. Convergence difficulties arise from the fact that the stationary wave of the outgoing photoelectron contains both outgoing and ingoing parts, whereas the Sturmian functions have outgoing wave character and so do not provide an expansion of the ingoing part of the photoelectron wave. We show how this difficulty can be overcome. We have tested the method for N-photon ionization of hydrogen when $(N-1)$-photon ionization is possible, with $N=2$–5, and for three-photon ionization when ordinary photoionization is possible.

I. INTRODUCTION

The radial Coulomb Green's function can be simply represented by a sum of bilinear products of Sturmian functions, that is, scaled hydrogenic functions.[1,2] This expansion has been widely used in the calculation of cross sections for multiphoton ionization of hydrogen in the case where no more than the minimum number of photons required to ionize the atom are absorbed.[2,3] In the case where additional photons are absorbed, that is, where photons are absorbed above the ionization threshold, the expansion, as it stands, diverges. Nevertheless, for two- and three-photon absorption it has proved possible, using a variety of techniques,[4–8] to analytically continue the Sturmian expansion from an intermediate energy below threshold to above threshold. Thereby, cross sections for two- and three-photon absorption, from both ground and excited states of hydrogen, have been calculated at frequencies where ordinary photoionization is possible. However, the extension to absorption of an arbitrary number of photons using these previous techniques, where possible, may involve considerable difficulties. Recently, a simplification was suggested,[9] and it will be elaborated on in this paper. The primary difficulty in using the Sturmian expansion to treat absorption above the ionization threshold is that the outgoing electron is described by a stationary wave, consisting of both ingoing and outgoing waves, whereas the Sturmian functions have outgoing wave character and thus do not provide an expansion of the electron wave function. We will see below how this difficulty can be circumvented. In Sec. II we present a general analysis of the problem, and in Sec. III we specialize to the hydrogenlike ion.

II. GENERAL THEORY

A. Sturmian functions

Rather than limit our discussion to the Coulomb potential we consider the electron to move in a local, real, spherically symmetric potential $V=V(r)$, with $r=|\mathbf{x}|$ and $\mathbf{x}$ the electron coordinate. We assume that $V(r)$ vanishes for $r\sim\infty$ and that $V(r)$ does not change sign over the interval $0\le r\le\infty$. We use atomic units throughout this paper. The radial kinetic energy operator T_l is represented in coordinate space by

$$T_l=-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}\ .$$

The Sturmian functions $S_{nl}^k(r)\equiv\langle r\,|\,S_{nl}^k\rangle$ are the solutions to the Sturm-Liouville eigenvalue problem[10] posed by the equation

$$(T_l+\lambda_{nl}^k V-E)\,|\,S_{nl}^k\rangle=0 \tag{2.1}$$

subject to the boundary conditions that the $S_{nl}^k(r)$ vanish at $r=0$ and $r\sim\infty$. Here $E\equiv-\frac{1}{2}k^2$ is fixed. The boundary conditions cannot be satisfied for E real and positive and for the present we assume that E is real and negative. Drawing a branch cut along the positive real axis in the complex E plane, we take that branch of k which is real and positive when E is real and negative. $S_{nl}^k(r)$ is damped by the exponential factor $\exp(-kr)$. We assume that the potential V is such that the eigenvalues $\{\lambda_{nl}^k\}$ form a countable infinite set $(n=l+1,l+2,\ldots)$ and that the $\{S_{nl}^k(r)\}$ form a complete set in the space L_V^{l+1} of all piecewise continuous functions $f(r)=\langle r\,|\,f\rangle$ for which $\langle f\,|\,V\,|\,f\rangle$ is finite and $f(r)/r^{l+1}$ is bounded for $r\sim0$. We define the scalar product $\langle a\,|\,b\rangle$ as $\int_0^\infty dr\,a(r)^*b(r)$ when a one-dimensional integral over the radial coordinate is implied.

Noting that E is real, the operator (T_l-E) is Hermitian in L_V^{l+1} and we have that

$$\langle S_{ml}^k\,|\,(T_l-E)\,|\,S_{nl}^k\rangle=\langle S_{nl}^k\,|\,(T_l-E)\,|\,S_{ml}^k\rangle^*\ . \tag{2.2}$$

Using Eq. (2.1) it follows that

$$\lambda_{nl}^k\langle S_{ml}^k\,|\,V\,|\,S_{nl}^k\rangle=(\lambda_{ml}^k)^*\langle S_{ml}^k\,|\,V\,|\,S_{nl}^k\rangle\ . \tag{2.3}$$

Since $\langle S_{nl}^k\,|\,V\,|\,S_{nl}^k\rangle$ does not vanish [recall $V(r)$ does not change sign] we see, putting $m=n$, that λ_{nl}^k is real. Since the boundary conditions are real it follows that all $S_{nl}^k(r)$

can be chosen to be real. Provided that the eigenvalues are nondegenerate, i.e., that $\lambda_{ml}^k \neq \lambda_{nl}^k$ for $m \neq n$, we also see that

$$\langle S_{ml}^k \mid V \mid S_{nl}^k \rangle = \beta_{nl}^k \delta_{nm} , \tag{2.4a}$$

$$\beta_{nl}^k = \langle S_{nl}^k \mid V \mid S_{nl}^k \rangle . \tag{2.4b}$$

We may use Eqs. (2.4) to derive a simple expansion of V in terms of separable potentials:

$$\langle \mathbf{x} \mid V \mid \mathbf{x}' \rangle = \sum_l \sum_m Y_{lm}(\hat{\mathbf{x}}) \frac{V_l(r,r')}{rr'} Y_{lm}^*(\hat{\mathbf{x}}') , \tag{2.5}$$

where $Y_{lm}(\hat{\mathbf{x}})$ is the usual spherical harmonic and where $V_l(r,r') = \langle r \mid V_l \mid r' \rangle$, with

$$V_l = \sum_{n=l+1}^{\infty} (1/\beta_{nl}^k) \mid \phi_{nl}^k \rangle \langle \phi_{nl}^k \mid , \tag{2.6a}$$

$$\mid \phi_{nl}^k \rangle = V \mid S_{nl}^k \rangle . \tag{2.6b}$$

Note that closure in L_V^{l+1} is expressed as

$$1 = \sum_n (1/\beta_{nl}^k) \mid S_{nl}^k \rangle \langle \phi_{nl}^k \mid . \tag{2.7a}$$

We assume that $V(r)$ behaves as r^q for $r \sim 0$, where $q+1$ is a non-negative integer. The $\{ \mid \phi_{nl}^k \rangle \}$ form a complete set in $L_{1/V}^{l+1+q}$, and closure in $L_{1/V}^{l+1+q}$ is expressed as

$$1 = \sum_n (1/\beta_{nl}^k) \mid \phi_{nl}^k \rangle \langle S_{nl}^k \mid . \tag{2.7b}$$

B. Green's function

The resolvent operator in three dimensions is $G(\Omega) \equiv 1/(\Omega - T - V)$ where T is the kinetic energy operator in three dimensions. We can make a partial-wave decomposition of $G(\Omega)$ in terms of $g_l(\Omega) \equiv 1/(\Omega - T_l - V)$. In coordinate space we have

$$G(\mathbf{x},\mathbf{x}';\Omega) = \langle \mathbf{x} \mid G(\Omega) \mid \mathbf{x}' \rangle = \sum_l \sum_m Y_{lm}(\hat{\mathbf{x}}) \frac{g_l(r,r';\Omega)}{rr'} Y_{lm}^*(\hat{\mathbf{x}}') ,$$

where $g_l(r,r';\Omega) = \langle r \mid g_l(\Omega) \mid r' \rangle$ is the radial Green's function.

Since the eigenvectors $\mid S_{nl}^k \rangle$ form a complete set in L_V^{l+1} we can expand $g_l(\Omega)$ in terms of these eigenvectors. We can write

$$g_l(\Omega) = \sum_m \sum_p a_{pm} \mid S_{ml}^k \rangle \langle S_{pl}^k \mid . \tag{2.8}$$

Premultiplying both sides of this equation by $(\Omega - T_l - V)$ and using Eq. (2.1) we obtain

$$1 = \sum_m \sum_p a_{pm} [\Omega - E + (\lambda_{ml}^k - 1)V] \mid S_{ml}^k \rangle \langle S_{pl}^k \mid . \tag{2.9}$$

Now premultiplying both sides of this last equation by $\langle S_{nl}^k \mid$ and using Eqs. (2.4) yields

$$\langle S_{nl}^k \mid = \sum_m \sum_p a_{pm} M_{mn} \langle S_{pl}^k \mid , \tag{2.10}$$

where

$$M_{mn} = (\Omega - E) \langle S_{nl}^k \mid S_{ml}^k \rangle + \delta_{nm} (\lambda_{nl}^k - 1) \beta_{nl}^k . \tag{2.11}$$

Equating coefficients of $\langle S_{pl}^k \mid$ yields an infinite set of linear equations for the coefficients a_{pm}:

$$\delta_{pn} = \sum_m a_{pm} M_{mn} . \tag{2.12}$$

Defining matrices $\underline{A}$ and $\underline{M}$ whose elements are a_{pm} and M_{mn}, respectively, we can write Eq. (2.12) in matrix form as $\underline{A}\,\underline{M} = \underline{1}$ where $\underline{1}$ is the identity matrix. Hence the determination of $g_l(\Omega)$, according to Eq. (2.8), amounts to the inversion of the matrix $\underline{M}$. If V is either a Coulomb potential or a harmonic-oscillator potential we have $\langle S_{nl}^k \mid S_{ml}^k \rangle = 0$ for $\mid m - n \mid > 1$, and then $\underline{M}$ is a tridiagonal matrix which can be easily inverted; this is the approach exploited by Heller[11] and collaborators, and also Fainshtein *et al.*[8] If, however, we have $\Omega = E$, the matrix $\underline{M}$ becomes diagonal for all allowed V and we obtain

$$a_{pn} = \delta_{pn} / [\beta_{nl}^k (\lambda_{nl}^k - 1)] ; \tag{2.13}$$

the double sum of Eq. (2.8) collapses to a single sum which is the familiar Sturmian expansion of the radial Green's function:

$$g_l(r,r';E) = \sum_{n=l+1}^{\infty} \frac{S_{nl}^k(r) S_{nl}^k(r')}{\beta_{nl}^k (\lambda_{nl}^k - 1)} . \tag{2.14}$$

If one of the λ_{nl}^k equals unity, the Green's function has a pole, corresponding to the presence of a bound state at energy E. Note that we have just written $\langle S_{nl}^k \mid r' \rangle$ as $S_{nl}^k(r')$, and not its complex conjugate. There is no discrepancy since we have assumed E to be real and negative, and have chosen $S_{nl}^k(r')$ to be real. We intend, however, to analytically continue the Sturmian expansion into the complex E plane, and it is important to remember that it is $S_{nl}^k(r')$, and not its complex conjugate, which is an analytic function of E in the cut E plane.

Before proceeding further we give a somewhat different derivation of the Sturmian expansion, one which illuminates the connection with the expansion of V in separable potentials—recall Eqs. (2.5) and (2.6). Note first that Eq. (2.9), and therefore $g_l(\Omega)$, are unaffected if we replace V by V_l. This is simply a consequence of the fact that $g_l(\Omega)$ is a partial-wave component of $G(\Omega)$. We now consider

$$\mid \psi_{nl}^k \rangle \equiv g_l(E) \mid \phi_{nl}^k \rangle .$$

We have

$$(T_l + V - E) \mid \psi_{nl}^k \rangle = -V \mid S_{nl}^k \rangle . \tag{2.15}$$

A particular solution of this equation is, recalling Eq. (2.1),

$$\mid \psi_{nl}^k \rangle = \frac{1}{(\lambda_{nl}^k - 1)} \mid S_{nl}^k \rangle . \tag{2.16}$$

This is, in fact, the unique solution satisfying the boundary conditions that $\langle r \mid \psi_{nl}^k \rangle$ vanish at $r = 0$ and $r \sim \infty$. We next introduce the free-particle resolvent $g_{0l}(\Omega) \equiv 1/(\Omega - T_l)$. Following the derivation of Eq. (2.16), it is straightforward to show that

$$g_{0l}(E)\,|\,\phi^k_{nl}\rangle=(1/\lambda^k_{nl})\,|\,S^k_{nl}\rangle\ . \tag{2.17}$$

We now make use of the relationship

$$g_l(\Omega)=g_{0l}(\Omega)+g_{0l}(\Omega)Vg_l(\Omega)\ . \tag{2.18}$$

We can replace V by V_l without affecting Eq. (2.18), in accordance with our previous observation. If, further, we approximate V_l by a finite sum of separable potentials, namely,

$$V_l\approx\sum_{n=l+1}^{N}(1/\beta^k_{nl})\,|\,\phi^k_{nl}\rangle\langle\phi^k_{nl}\,|\ , \tag{2.19}$$

and use Eqs. (2.16) and (2.17), setting $\Omega=E$ in Eq. (2.18) and noting that $g_l(E)$ is Hermitian for E real and negative, we obtain

$$g_l(E)\approx g_{0l}(E)+\sum_{n=l+1}^{N}\frac{|\,S^k_{nl}\rangle\langle S^k_{nl}\,|}{\beta^k_{nl}\lambda^k_{nl}(\lambda^k_{nl}-1)}\ . \tag{2.20}$$

Equation (2.20), which is exact for $N\sim\infty$, expresses in a simple form the deviation of $g_l(E)$ from $g_{0l}(E)$. Writing $g_{0l}(E)=g_{0l}(E)1$, and using the closure relation (2.7b) with Eq. (2.17), we obtain

$$g_{0l}(E)=\sum_{n=l+1}^{\infty}\frac{|\,S^k_{nl}\rangle\langle S^k_{nl}\,|}{\beta^k_{nl}\lambda^k_{nl}}\ . \tag{2.21}$$

Letting $N\sim\infty$, and combining Eqs. (2.20) and (2.21), we obtain once again the Sturmian expansion of $g_l(E)$, namely Eq. (2.14).

C. Analytic continuation

Consider the matrix element

$$M_l(E)=(a\,|\,g_l(E)\,|\,b)\ , \tag{2.22}$$

where the scalar product $(a\,|\,c)$ is defined as $\int_0^\infty dr\,a(r)c(r)$; we do not complex-conjugate $a(r)$. The Sturmian expansion of $M_l(E)$, obtained from Eq. (2.14), is

$$M_l(E)=\sum_{n=l+1}^{\infty}\frac{(a\,|\,S^k_{nl})(S^k_{nl}\,|\,b)}{\beta^k_{nl}(\lambda^k_{nl}-1)}\ . \tag{2.23}$$

We can attempt to analytically continue this expansion from the negative real axis into the complex E plane, cut along the positive real axis, by analytically continuing each term in the sum. We now explore, in a heuristic fashion, the conditions under which the expansion converges.

The $\{\,|\,\phi^k_{nl}\rangle\}$ form a complete set in $L^{l+1+q}_{1/V}$, for E real and negative. Therefore, provided that $|\,a\rangle$ and $|\,b\rangle$ belong to $L^{l+1+q}_{1/V}$ we can expand these vectors in terms of the $|\,\phi^k_{nl}\rangle$:

$$|\,a\rangle=\sum_{n=l+1}^{\infty}(\beta^k_{nl})^{-1}(S^k_{nl}\,|\,a)\,|\,\phi^k_{nl}\rangle\ , \tag{2.24a}$$

$$|\,b\rangle=\sum_{n=l+1}^{\infty}(\beta^k_{nl})^{-1}(S^k_{nl}\,|\,b)\,|\,\phi^k_{nl}\rangle\ . \tag{2.24b}$$

Substituting for $|\,a\rangle$ and $|\,b\rangle$ in Eq. (2.22), and making use of Eqs. (2.4a) and (2.16), we obtain Eq. (2.23). The condition for the convergence of the Sturmian expansion of $M_l(E)$, when $E<0$, is therefore that $|\,a\rangle$ and $|\,b\rangle$ belong to $L^{l+1+q}_{1/V}$.

If $|\,a\rangle$ and $|\,b\rangle$ belong to $L^{l+1+q}_{1/V}$ it is reasonable to expect that Eqs. (2.24), and hence (2.23), can be continued off the negative real axis. We write $E=|\,E\,|\exp(i\theta)$, with $0\le\theta<2\pi$, so that $k=|\,2E\,|^{1/2}\exp(-i\phi)$ where $\phi=(\pi-\theta)/2$ and $-\pi/2<\phi\le\pi/2$. Note that the orthogonality property, Eq. (2.4a), may be analytically continued in the form $(\phi^k_{ml}\,|\,S^k_{nl})=\beta^k_{nl}\delta_{nm}$. A case of special interest is that where $a(r)=(r\,|\,a)$ and/or $b(r)=(r\,|\,b)$ are exponentially damped. Thus suppose that $a(r)=g(r)\exp(-\alpha r)$ where $r^{-(l+1+q)}g(r)$ is bounded for $r\sim0$ and where $\alpha=|\,\alpha\,|\exp(-i\chi)$ with $0\le\chi<\pi/2$. The function $a(r)$ is a damped outgoing wave. If we let r take the complex value $|\,r\,|\exp(i\chi-i\pi/2)$, $a(r)$ becomes a pure (undamped) outgoing wave whose real and imaginary parts oscillate infinitely many times, with undiminished amplitude, as $|\,r\,|$ varies from 0 to ∞. [We assume that $g(r)$ does not dampen the oscillations.] Now suppose that we expand $a(r)$ in terms of the $\phi^k_{nl}(r)$ and allow k to be complex, $k=|\,k\,|\exp(-i\phi)$. As we let r approach $|\,r\,|\exp(i\chi-i\pi/2)$ we obtain an expansion of a pure outgoing wave in terms of (generally damped) waves that are outgoing if $|\,\chi-\phi\,|<\pi/2$ but ingoing if $\pi>|\,\chi-\phi\,|>\pi/2$. Since it is unphysical to express a pure outgoing wave in terms of (albeit damped) ingoing waves, we intuit that the expansion of $a(r)$ in terms of the $\phi^k_{nl}(r)$ will converge (in some sense) only for complex k such that $|\,\chi-\phi\,|<\pi/2$. We arrive at the same conclusion if $-\pi/2<\chi\le0$, that is, if $a(r)$ is a damped ingoing wave. Note, however, that a *damped* outgoing wave can always be expressed as a linear combination of damped ingoing waves, and vice versa. In other words, if $|\,\chi-\phi\,|\ge\pi/2$ we can approximate $a(r)$, to arbitrary accuracy, by a linear combination of waves that have the character of $\exp(-\kappa r)$, where $\kappa=|\,\kappa\,|\exp(-i\zeta)$, with $-\pi/2<\zeta<\pi/2$, $|\,\chi-\zeta\,|<\pi/2$, and $|\,\zeta-\phi\,|<\pi/2$. A suitable approximation to $a(r)$ is obtained by putting $k=\kappa$ in Eq. (2.24a) and truncating the expansion after a sufficient number of terms. This approximation to $a(r)$ can then be expanded in terms of the $\phi^k_{nl}(r)$, with k having the value of interest. Note that while $\mathrm{Re}\alpha$ must be positive we can let it be infinitesimally small since in any scalar product involving $|\,a\rangle$ and $|\,S^k_{nl}\rangle$ we can rotate the path of integration from the positive real axis into the complex r plane, thereby ensuring the convergence of the integral as we let $\mathrm{Re}\alpha\to0$.

A similar analysis applies to $b(r)$. In conclusion: If $a(r)$ and $b(r)$ belong to $L^{l+1+q}_{1/V}$ and are damped by factors $\exp(-\alpha r)$ and $\exp(-\beta r)$, respectively, with $\mathrm{Re}(\alpha,\beta)\ge0$ and $\mathrm{Im}(\alpha,\beta)\le0$, we conjecture that the Sturmian expansion of $M_l(E)$ converges as E approaches the positive real axis from above. [If $\mathrm{Im}\alpha=0$ ($\mathrm{Im}\beta=0$) we must approximate $|\,a\rangle$ ($|\,b\rangle$) by a damped outgoing wave; this is possible provided $\mathrm{Re}\alpha>0$ ($\mathrm{Re}\beta>0$).]

In the radial matrix element for two-photon ionization of hydrogen, $a(r)$ and $b(r)$ are, respectively, the initial and final radial wave functions of the electron multiplied by the dipole interaction. Here we restrict E to real (positive or negative) values, these being the values of interest, but we add an infinitesimal positive imaginary part $i\eta$ to

ensure that positive values of E lie on the upper side of the cut. We may assume that both $a(r)$ and $b(r)$ are real functions; $b(r)$ is a stationary wave, consisting of both ingoing and outgoing waves. We decompose $|b\rangle$ as

$$|b\rangle=|b^+\rangle+|b^-\rangle\ , \tag{2.25}$$

where $|b^+\rangle$ and $|b^-\rangle$ are, respectively, the outgoing and ingoing parts of $|b\rangle$. We decompose $M_l(E+i\eta)$ as

$$M_l(E+i\eta)=M_l^+(E+i\eta)+M_l^-(E+i\eta)\ , \tag{2.26a}$$

$$M_l^{\pm}(E+i\eta)=(a\,|\,g_l(E+i\eta)\,|\,b^{\pm})\ ; \tag{2.26b}$$

the matrix element $M_l^-(E+i\eta)$ does not have a convergent Sturmian expansion and we seek to express it in terms of $M_l^+(E+i\eta)$. To do this we use the relationship

$$g_l(E+i\eta)=g_l(E-i\eta)-2\pi i\delta(E-T_l-V) \tag{2.27}$$

to obtain

$$M_l^-(E+i\eta)=(a\,|\,g_l(E-i\eta)\,|\,b^-)-2\pi i J_l(E)\ , \tag{2.28a}$$

where

$$\begin{aligned}J_l(E)&=(a\,|\,\delta(E-T_l-V)\,|\,b^-)\\&=\langle a\,|\,R_{kl}\rangle\langle R_{kl}\,|\,b^-\rangle\Theta(E)\ ,\end{aligned} \tag{2.28b}$$

where $|R_{kl}\rangle$ is the (stationary wave) eigenvector of T_l+V with eigenvalue E and where $\Theta(E)$ is the Heaviside step function: $\theta(E)$ is zero for $E<0$ and unity for $E>0$. Noting that $(r\,|\,b^-)=(r\,|\,b^+)^*$, that $g_l(E-i\eta)$ is the complex conjugate of $g_l(E+i\eta)$, and that $a(r)$ is real, we have

$$(a\,|\,g_l(E-i\eta)\,|\,b^-)=(a\,|\,g_l(E+i\eta)\,|\,b^+)^* \tag{2.29}$$

and hence that

$$M_l(E+i\eta)=2\,\mathrm{Re}[M_l^+(E+i\eta)]-2\pi i J_l(E)\ . \tag{2.30}$$

We need therefore consider only $M_l^+(E+i\eta)$. Now $a(r)$ is real and exponentially damped ($\chi=0$). Therefore if $E>0$ we must first approximate $a(r)$ by a linear combination of (damped) outgoing waves before attempting a Sturmian expansion of $M_l^+(E+i\eta)$. Moreover, while $b^+(r)$ does have the character of an outgoing wave, in general its behavior is irregular for $r\sim 0$ and therefore $b^+(r)$ does not belong to $L^{l+1+q}_{1/r}$. Nevertheless, in the case where $V(r)$ is a Coulomb potential, and probably more generally, $(S_{nl}^k\,|\,a)$ diminishes sufficiently rapidly as n increases [provided $a(r)$ is replaced by an outgoing wave] that the Sturmian expansion of $M_l^+(E+i\eta)$ converges in spite of the behavior of $(b^+\,|\,S_{nl}^k)$. We can, in any case, always regularize $b^+(r)$ using the following method. We introduce a function $f_m(r)$, whose form for $r\sim 0$ is $1+O(r^{m+1})$, where m is a non-negative integer. A function with this property is

$$f_m(r)=\exp(-\xi r)\sum_{p=0}^{m}\frac{(\xi r)^p}{p!}\ , \tag{2.31}$$

where we take ξ to be real and positive. We now write

$$\begin{aligned}M_l(E+i\eta)&=(a\,|\,g_l(E+i\eta)\,|\,c_m)\\&\quad+(a\,|\,g_l(E+i\eta)\,|\,d_m)\ ,\end{aligned} \tag{2.32}$$

where the *real* functions $c_m(r)=(r\,|\,c_m)$ and $d_m(r)=(r\,|\,d_m)$ are defined as

$$c_m(r)=[1-f_m(r)]b(r)\ , \tag{2.33a}$$

$$d_m(r)=f_m(r)b(r)\ . \tag{2.33b}$$

We decompose $|c_m\rangle$ into outgoing and ingoing parts, $|c_m^+\rangle$ and $|c_m^-\rangle$, and apply the same analysis as above to the first matrix element on the right-hand side of Eq. (2.32). Since $b^+(r)$ is multiplied by $[1-f_m(r)]$ in $c_m^+(r)$ we can, by choosing m sufficiently large, ensure that $c_m^+(r)/r^{l+1+q}$ is bounded for $r\sim 0$. Hence the Sturmian expansion of $(a\,|\,g_l(E+i\eta)\,|\,c_m^+)$ converges. If $|K|$ is the wave number of the outgoing electron, the function $d_m(r)$ oscillates for large r as a damped wave $\exp(-\xi r)\sin(|K|r)$. The ingoing part of this wave, and hence the complete wave, can be expanded in terms of outgoing waves $\phi_{nl}^{\kappa}(r)$ if, according to our previous discussion,

$$|\arg(\xi+i\,|\,K\,|\,)-\arg(\kappa)|<\pi/2\ . \tag{2.34}$$

This condition can be reexpressed as

$$\xi\,\mathrm{Re}(\kappa)+|K|\,\mathrm{Im}(\kappa)>0\ . \tag{2.35}$$

[Note that we require $\mathrm{Im}\kappa<0$ for $\phi_{nl}^{\kappa}(r)$ to be an outgoing wave.] With $d_m(r)$ approximated by a finite sum of outgoing waves $\phi_{nl}^{\kappa}(r)$, the second matrix element on the right-hand side of Eq. (2.32) has a convergent Sturmian expansion.

The preceding analysis of the two-photon matrix element applies also to an N-photon matrix element, if $N-1$ photons are required to ionize the atom. Thus $a(r)$ becomes the product of $N-2$ Green's functions with intermediate energies that are negative, $N-1$ dipole interactions, and the initial bound state; this $a(r)$ has the properties assumed above. It is straightforward to extend the analysis when more than one photon is absorbed above the ionization threshold. Thus, we again decompose $|b\rangle$ into $|b^+\rangle$ and $|b^-\rangle$, and in the matrix element involving $|b^-\rangle$ we replace all those $g_l(E+i\eta)$ with positive E by $g_l(E-i\eta)$, using Eq. (2.27); the analysis continues as before.

III. COULOMB POTENTIAL

A. General properties

In this section we consider the Coulomb potential $V(r)=-Z/r$. By simply scaling the coordinate as $r\to r/\lambda_{nl}^k$ in Eq. (2.1) we see by comparison with the Schrödinger equation for the hydrogen atom that the eigenvalues are $\lambda_{nl}^k=nk/Z$; these eigenvalues are independent of l. The eigenfunctions, normalized so that $\beta_{nl}^k=-Z$, are given by

$$S_{nl}^k(r)=A_{nl}(kr)^{l+1}\exp(-kr)\,{}_1F_1(l+1-n;2l+2;2kr)\ , \tag{3.1a}$$

$$A_{nl}=\frac{2^{l+1}}{(2l+1)!}\left[\frac{(n+l)!}{(n-l-1)!}\right]^{1/2}. \tag{3.1b}$$

(In Ref. 9 the normalization was chosen to be $\beta_{nl}^{k}=-Zk/n$.) Note that r appears in the combination kr in the eigenfunctions. This is a consequence of the fact that, for the Coulomb potential, Eq. (2.1) is invariant under the simultaneous transformations $r\to r\exp(i\phi)$ and $k\to k\exp(-i\phi)$. We now use this property to investigate the expansion coefficients of $a(r)$, assuming $a(r)$ belongs to $L^{l}_{1/V}$. For r and k real ($r\geq 0$, $k>0$) we know from general considerations[10] that since $\lambda_{nl}^{k}\to\infty$ as $n\to\infty$ the $\{\phi_{nl}^{k}(r)\}$ span $L^{l}_{1/V}$, and therefore $a(r)$ can be expanded, according to Eq. (2.24a), as

$$a(r)=-(1/Z)\sum_{n=l+1}^{\infty}(S_{nl}^{k}\,|\,a)\phi_{nl}^{k}(r)\,, \tag{3.2}$$

where $\phi_{nl}^{k}(r)=-(Z/r)S_{nl}^{k}(r)$. The coefficients $(S_{nl}^{k}\,|\,a)$ tend to zero rapidly as $n\to\infty$ since the integrand of

$$(S_{nl}^{k}\,|\,a)=\int_{0}^{\infty}dr\,S_{nl}^{k}(r)a(r) \tag{3.3}$$

oscillates many times—$S_{nl}^{k}(r)$ has $n-l-1$ nodes on the positive real axis for k real. Suppose that we now choose $k=|k|\exp(-i\phi)$ where $\phi=(\pi-\theta)/2$. Provided that $a(r)$ has no singularities in the sector $0\leq(1/\phi)\arg(r)\leq 1$, and provided that $rS_{nl}^{k}(r)a(r)$ vanishes for $r\sim\infty$ in this sector, we can rotate the path of integration in the above integral from the positive real axis to the line $r=|r|\exp(i\phi)$. Since $S_{nl}^{k}(r)=S_{nl}^{|k|}(|r|)$ we see that $(S_{nl}^{k}\,|\,a)=\exp(i\phi)(S_{nl}^{|k|}\,|\,a')$, where $a'(r)=a(r\exp(i\phi))$. It follows that $(S_{nl}^{k}\,|\,a)$ tends rapidly to zero as $n\to\infty$ if (reverting to r real) $a'(r)$ belongs to $L^{l}_{1/V}$. This condition, and a similar condition with $|a\rangle$ replaced by $|b\rangle$, guarantee the convergence of the Sturmian expansion of $M_l(E)$. Note that if $a(r)=\exp(-\alpha r)$, with $\mathrm{Re}\alpha>0$, we require that $\mathrm{Re}[\alpha\exp(i\phi)]>0$, that is, $|\arg(\alpha)+\phi|<\pi/2$, in accord with the heuristic analysis of Sec. II C.

The Coulomb wave, $u_{KL}(r)$, describing an electron moving with positive energy $-\frac{1}{2}K^{2}$ (note $K=-i|K|$) and angular momentum $L(L+1)$ is

$$u_{KL}(r)=c_{KL}(Kr)^{L+1}\exp(-Kr)\times{}_1F_1(L+1-Z/K;2L+2;2Kr)\,, \tag{3.4a}$$

$$c_{KL}=(2\pi|K|)^{-1/2}(2i)^{L+1}|\Gamma(L+1-Z/K)|\times\exp(\pi Z/2|K|)/(2L+1)!\,. \tag{3.4b}$$

[Note that in Ref. 9, K appears as $|K|$ and $u_{KL}(r)$ differs from $R_{KL}(r)$ by a factor r.] We have normalized $u_{KL}(r)$ on the energy scale. We can expand $\exp(-\xi r)u_{KL}(r)$ in terms of damped outgoing waves $S_{nl}^{\kappa}(r)$, where $\mathrm{Re}\kappa\geq 0$, $\mathrm{Im}\kappa\leq 0$. Thus, we have

$$u_{KL}(r)=\exp(\xi r)\sum_{n=L+1}^{\infty}a_nS_{nL}^{\kappa}(r)\,, \tag{3.5a}$$

where the coefficients a_n are given by the orthogonality condition:

$$a_n=-(1/Z)\int_{0}^{\infty}dr\exp(-\xi r)u_{KL}(r)\phi_{nL}^{\kappa}(r)\,. \tag{3.5b}$$

This last integral is a standard one (see, e.g., Ref. 12) and we obtain

$$a_n=-(K\kappa)^{L+1}c_{KL}A_{nL}(2L+1)!\lambda^{-(n+Z/K)}\times(\lambda-2\kappa)^{(n-L-1)}(\lambda-2K)^{(Z/K-L-1)}\times{}_2F_1(L+1-n,L+1-Z/K;2L+2;\zeta)\,, \tag{3.5c}$$

$$\lambda=\xi+K+\kappa\,, \tag{3.5d}$$

$$\zeta=4K\kappa/[(\lambda-2K)(\lambda-2\kappa)]\,. \tag{3.5e}$$

Putting $\xi=0$ we recover the expansion of $u_{KL}(r)$ derived by Yamani and Reinhardt.[13] The condition for the coefficients a_n to vanish as $n\to\infty$ is

$$\mathrm{Re}(\xi)\,\mathrm{Re}(\kappa)+\mathrm{Im}(\xi)\mathrm{Im}(\kappa)+|K|\,\mathrm{Im}(\kappa)>0\,; \tag{3.6}$$

this condition is the generalization of Eq. (2.35) to ξ complex.

We can decompose $u_{KL}(r)$ into outgoing and ingoing parts as follows:

$$u_{KL}(r)=u_{KL}^{+}(r)+u_{KL}^{-}(r)\,, \tag{3.7a}$$

$$u_{KL}^{\pm}(r)=d_{KL}^{\pm}(Kr)^{L+1}\exp(\mp Kr)\times\Psi(L+1\mp Z/K;2L+2;\pm 2Kr)\,, \tag{3.7b}$$

$$d_{KL}^{\pm}=(-2i)^{L+1}(2\pi|K|)^{-1/2}\times\exp[\pm i\eta_L-(\pi Z/2|K|)]\,, \tag{3.7c}$$

$$\eta_L=\arg\Gamma(L+1-Z/K)\,; \tag{3.7d}$$

here $\Psi(a;b;z)$ is the irregular Kummer function.[12] These expressions are useful in the calculation of cross sections for multiphoton ionization of a hydrogenlike ion. Note that $u_{KL}^{\pm}(r)$ diverges as r^{-L} for $r\sim 0$.

In some applications a generalized resolvent $G(\varepsilon_n)Q_n$ is useful, where $\varepsilon_n=-(Z^2/2n^2)$ is a bound-state energy of the hydrogenlike ion and Q_n projects out all bound-state eigenvectors with eigenvalue ε_n. [Thus Q_n removes the poles of $G(E)$ at $E=\varepsilon_n$.] By carefully letting $E\to\varepsilon_n$ in Eq. (2.14) we can obtain a Sturmian expansion of $G(\varepsilon_n)Q_n$. Here we record the result for $n=1$. The partial-wave decomposition of $G(\varepsilon_1)Q_1$ differs from that of $G(\varepsilon_1)$ only in that $g_0(r,r';\varepsilon_1)$ is replaced by

$$-2Zrr'(3-Zr)(3-Zr')\exp[-Z(r+r')]-\sum_{n=3}^{\infty}\frac{1}{Z(n-1)}S_{n0}^{k}(r)S_{n0}^{k}(r')\,.$$

This result was recently used[14] in an application of the Schwinger variational principle to the treatment of two-photon ionization of ground-state hydrogen; the presence of the generalized Green's function partially takes account of virtual absorption or emission.

B. Multiphoton ionization of H-like ion

The generalized differential cross section $d\hat{\sigma}_N/d\Omega$ for N-photon ionization of a one-electron system by a monochromatic, spatially independent, classically describable radiation field of frequency ω, polarization $\hat{\epsilon}$, intensity I,

and photon flux $F=I/\omega$ is (recall we use atomic units)

$$d\hat{\sigma}_N/d\Omega=(2\pi\rho/F^N)\,|R_{fi}|^2\,; \tag{3.8}$$

ρ is a phase-space factor ($\rho\,d\Omega$ is the density of final states per unit energy) and R_{fi} is the transition matrix element which, to Nth order in the dipole interaction

$$W=(2\pi I/c)^{1/2}(\hat{\epsilon}\cdot\mathbf{x})\,, \tag{3.9}$$

can be written as

$$R_{fi}=\langle f\,|\,WG(E_{N-1})WG(E_{N-2})\cdots G(E_1)W\,|\,i\rangle\,, \tag{3.10}$$

where $|\,i\rangle$ and $|\,f\rangle$ represent the initial and final states and $E_1,E_2,\ldots,E_{N-1}$ are the intermediate energies of the electron. We write

$$\langle\,\mathbf{x}\,|\,i\,\rangle=Y_{lm}(\hat{\mathbf{x}})u_{n_0l}(r)/r\,, \tag{3.11a}$$

$$\langle\,\mathbf{x}\,|\,f\,\rangle=4\pi\sum_{L,M}i^LY^*_{LM}(\hat{\mathbf{K}})Y_{LM}(\hat{\mathbf{x}})u_{KL}(r)/r\,; \tag{3.11b}$$

n_0, l, and m are the quantum numbers of the initial state, L and M are the angular-momentum quantum numbers of the final state, $|\,K\,|$ is the wave number of the outgoing electron, and $\hat{\mathbf{K}}$ its direction of motion ($d\Omega=d\hat{\mathbf{K}}$). Since $u_{KL}(r)$ is normalized on the energy scale, $\rho=(1/16\pi^2)$. We obtain

$$\frac{d\hat{\sigma}_N}{d\Omega}=2\pi\left[\frac{2\pi\omega}{c}\right]^N\left|\sum_{L,M}i^LY_{LM}(\hat{\mathbf{K}})\sum_{l_{N-1},m_{N-1}}\cdots\sum_{l_1,m_1}A(l_{N-1},\ldots,l_1;m_{N-1},\ldots,m_1)M^{(N)}\right|^2, \tag{3.12}$$

where $l_1,l_2,\ldots,l_{N-1}$ and $m_1,m_2,\ldots,m_{N-1}$ are the allowed intermediate angular momentum quantum numbers, and $A(l_{N-1},\ldots)$ is a geometrical factor, given as the following product:

$$A(l_{N-1},\ldots)=\prod_{n=1}^{N}\int d\hat{\mathbf{x}}\,Y^*_{l_n,m_n}(\hat{\mathbf{x}})(\hat{\epsilon}\cdot\hat{\mathbf{x}})Y_{l_{n-1},m_{n-1}}(\hat{\mathbf{x}})\,, \tag{3.13}$$

with $l_0=l$, $m_0=m$, $l_N=L$, and $m_N=M$. The matrix element $M^{(N)}$ is defined as

$$M^{(N)}=\int dr_N\int dr_{N-1}\cdots\int dr_1u_{KL}(r_N)\times r_Ng_{l_{N-1}}(r_N,r_{N-1};E_{N-1})r_{N-1}g_{l_{N-2}}(r_{N-1},r_{N-2};E_{N-2})\cdots r_2g_{l_1}(r_2,r_1;E_1)r_1u_{n_0l}(r_1)\,. \tag{3.14}$$

We have calculated cross sections for N-photon ionization of ground-state hydrogen, applying the above formalism to the matrix element $M^{(N)}$. The evaluation of $M^{(N)}$ reduces to the evaluation of two types of matrix elements, $(S^k_{nl}\,|\,r\,|\,S^{k'}_{n'l'})$ and $(u^+_{KL}\,|\,r\,|\,S^k_{nl})$; the first of these is a standard integral[12] and the second is evaluated in the Appendix. We did not regularize $u^+_{KL}(r)$ since the convergence of the Sturmian expansion of $M^{(N)}$ is assured simply if

$$|\,a\,\rangle=g_{l_{P-1}}(E_{P-1})rg_{l_{P-2}}(E_{P-2})\cdots r\,|\,u_{n_0l}\,\rangle \tag{3.15}$$

is expanded in (damped) outgoing waves; here P is the minimum number of photons required to ionize the atom. Following the discussion of Sec. II C we have, in general, that

$$M^{(N)}=2\,\mathrm{Re}(M^{+(N)})-2\pi i\sum_{n=1}^{N-P}J^{(N)}_nM^{(N-n)}\,, \tag{3.16a}$$

where [with $|\,a\,\rangle$ as in Eq. (3.15)]

$$M^{+(N)}=(u^+_{KL}\,|\,rg_{l_{N-1}}(E_{N-1})r\cdots g_l(E_P)r\,|\,a)\,, \tag{3.16b}$$

$$J^{(N)}_n=(u^+_{KL}\,|\,rg_{l_{N-1}}(E_{N-1})\cdots g_{l_{N-n+1}}(E_{N-n+1})r\,|\,u_{k_{N-n},l_{N-n}})^*\,, \tag{3.16c}$$

$$J^{(N)}_1=(u^+_{KL}\,|\,r\,|\,u_{k_{N-1},l_{N-1}})^*\,, \tag{3.16d}$$

where $k_n=\sqrt{-2E_n}$ and E_n has an infinitesimal positive imaginary part. The evaluation of $J^{(N)}_n$ amounts to evaluating matrix elements of the form

$$(b\,|\,g_{l_{j+1}}(E_{j+1})r\,|\,u_{k_jl_j})\,.$$

This latter matrix element can be evaluated by expanding $|\,u_{k_jl_j}\rangle$ according to Eq. (3.5a) and by replacing $g_{l_{j+1}}(E_{j+1})$ by its Sturmian expansion; the resulting expansion of the matrix element converges if the following three conditions are satisfied:

$$\mathrm{Re}(\xi)\mathrm{Re}(\kappa)+\mathrm{Im}(\xi)\mathrm{Im}(\kappa)+|\,k_j\,|\,\mathrm{Im}(\kappa)>0\,, \tag{3.17a}$$

$$\mathrm{Im}(\kappa-\xi)<0\ , \tag{3.17b}$$

$$\mathrm{Re}(\xi)\mathrm{Re}(\kappa)+\mathrm{Im}(\xi)\mathrm{Im}(\kappa)+|k_{j+1}|\,\mathrm{Im}(\kappa)<0\ . \tag{3.17c}$$

The first condition ensures that the expansion of $|u_{k_jl_j}\rangle$ is convergent. The second condition ensures that this expansion consists of *out*going waves. The third condition implies that the truncated expansion of $r^{\Delta l}\exp(-\xi r)u_{k_jl_j}(r)$ (where $\Delta l=l_{j+1}-l_j$) can, in principle, be reexpanded in a series of terms $\exp(-\xi r)S^{k_{j+1}}_{nl_{j+1}}(r)$, thereby ensuring that the replacement of $g_{l_{j+1}}(E_{j+1})$ by its Sturmian expansion is legitimate. All three conditions can be met if ξ and κ are chosen as follows:

$$\mathrm{Re}\xi=\tfrac{1}{4}(|k_{j+1}|+|k_j|)\ ,$$

$$\mathrm{Im}\xi=-\mathrm{Re}\xi\ ,$$

$$\kappa=2\xi\ .$$

In verifying Eqs. (3.17) note that $|k_{j+1}|>|k_j|$.

We have performed calculations for N equal to $P+1$. Numerous calculations have now been reported for above-threshold ionization of hydrogen (i.e., $N>P$), and so we do not present extensive results here; we refer the reader to calculations involving the Sturmian approach[4–8] and other methods.[15–18] However, to our knowledge, most results presented so far (not those of Refs. 6, 15, and 16) are for $N=2$, $P=1$. In Table I we give results for $P=1$–4.

The expansion of $|a\rangle$ in outgoing waves can be truncated after a few terms; the number of terms required depends on the (complex) wave vector chosen for the outgoing waves, and increases as P increases. In our calculations we retained at most 11 terms in the expansion of $|a\rangle$. The Sturmian expansion of $M^{+(N)}$, with $N=P+1$, converges rapidly for $P=1$—only about 50 terms were required in the final sum to achieve convergence in the second place—but the rate of convergence diminishes as P increases, and for $P=4$ about 450 terms were required in the final sum to achieve convergence in the second place. Furthermore, for $P>2$ the individual terms can become very large and cancel in the sum. For $P=4$ the individual terms in $M^{+(N)}$ reached an order of magnitude of 10^{17}, while the sum is on the order of only 10^6. For this reason we needed to use extended precision in our computations. We hope that further exploration will reveal a path to alleviating this drawback. We note that large terms which cancel in the sum appear in other Sturmian-type methods; the problem can be alleviated to some extent, as demonstrated by Fainshtein *et al.*,[8] by optimally choosing the open wave vectors (which are not uniquely defined).

TABLE I. Generalized cross sections for N-photon ionization of ground-state hydrogen when $(N-1)$-photon ionization is possible. The light polarization is circular, $\hat{\sigma}_N$ has units $\mathrm{cm}^{2N}\mathrm{sec}^{N-1}$, and the wavelength λ is in Å. The number in square brackets is the power of 10 by which the preceding number should be multiplied.

N	2	3	4	5
λ	500	1200	2300	3200
$\hat{\sigma}_{N-1}$	1.2[−18]	1.3[−49]	2.9[−83]	4.0[−116]
$\hat{\sigma}_N$	3.4[−53]	1.4[−83]	2.6[−116]	8.8[−149]

TABLE II. Generalized cross sections for one-, two-, and three-photon ionization of ground-state hydrogen when one-photon ionization is possible. Units of $\hat{\sigma}_N$ are $\mathrm{cm}^{2N}\mathrm{sec}^{N-1}$. Light polarization is circular.

λ (Å)	400	500	600	700
$\hat{\sigma}_1$	6.4[−19]	1.2[−18]	2.0[−18]	3.1[−18]
$\hat{\sigma}_2$	1.0[−53]	3.4[−53]	9.2[−53]	2.2[−52]
$\hat{\sigma}_3$	1.3[−88]	6.3[−88]	2.4[−87]	8.8[−87]

We have also performed calculations of three-photon ionization when ordinary photoionization is possible ($P=1$, $N=P+2$). Some results are given in Table II. The number of terms retained in the expansion of $|u_{kl}\rangle$ was of the order of 20. The number of terms retained in the Sturmian expansion of $g_l(E)$ in $J^{(N)}_n$ was of the order of 100. Where comparison is possible, our results agree to within a few percent with those of Klarsfeld and Maquet[6] and Aymar and Crance.[16]

Progress has been made on extending the ideas of this paper to atoms more complicated than hydrogen.[18] We note that the remarks of this paper have implications for all approaches employing discrete basis functions.

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APPENDIX

We describe here the evaluation of

$$(u^+_{KL}\,|\,r^p\exp(-\zeta r)\,|\,S^k_{nl})=\int_0^\infty dr\,r^p\exp(-\zeta r)u^+_{KL}(r)S^k_{nl}(r)\ , \tag{A1}$$

where $p+l-L+1$ and $p-l+L+1$ are non-negative integers (and V is pure Coulombic). We reduce this integral to a closed-form expression which, though rather complicated, is manageable even when $n\gg l$.

Using the integral representation

$$F(a;b;z)=\frac{\Gamma(1-a)\Gamma(b)}{2\pi i\Gamma(b-a)}\int_C dt\exp(-zt)\frac{(1+t)^{b-a-1}}{t^{1-a}}\ , \tag{A2}$$

to represent $S^k_{nl}(r)$—here C is any contour enclosing the point $t=0$ in the counterclockwise sense, if a and b are integers with $(b-a)>0$—we have, from Eqs. (3.1) and (3.7), that

$$(u^+_{KL}\,|\,r^p\exp(-\zeta r)\,|\,S^k_{nl})=\beta I\ , \tag{A3a}$$

$$I=\frac{1}{2\pi i}\int_C dt\frac{(1+t)^{n+l}}{t^{n-l}}\int_0^\infty dr\,r^{m-1}\exp(-\mu r)\times\Psi(L+1-i\gamma;2L+2;2Kr), \tag{A3b}$$

where $\gamma=Z/|K|$, $m=p+L+l+3$, and

$$\mu=K+k+\zeta+2kt\ , \tag{A3c}$$

$$\beta=(2k)^{l+1}K^{L+1}[(n-l-1)!/(n+l)!]^{1/2}d_{KL}^{+}\ . \tag{A3d}$$

Note that $m-2L-2$ and $m-2l-2$ are non-negative integers, as required in the following analysis. In going from (A1) to (A3) we have interchanged the order of integration, which is legitimate if $\mathrm{Re}\mu>0$ inside and on C. The integral over r is a standard one[12] and we obtain

$$I=\frac{(m-1)!(m-2L-2)!}{\Gamma(m-L-i\gamma)2\pi i}\times\int_C dt\frac{t^{2l}}{\mu^m}\left[1+\frac{1}{t}\right]^{n+l}\times{}_2F_1(L+1-i\gamma,m;m-L-i\gamma;\xi)\ , \tag{A4a}$$

$$\xi=(k+\zeta+2kt-K)/\mu\ . \tag{A4b}$$

In the region outside C the integrand of Eq. (A4a) has branch point singularities at $t=-(K+k+\zeta)/2k$, where $\xi=\infty$, and at $t=\infty$, where $\xi=1$. We draw a branch cut between these two singularities, with the direction of the cut chosen so that ξ is real along the cut. We deform C into a contour C_1 that wraps around this cut and then joins a circle C_2 of infinitely large radius. See Fig. 1. We write $I=I_1+I_2$, where I_1 and I_2 are the contributions from the contours C_1 and C_2, respectively.

To evaluate I_1 we change variables from t to $s=1/\xi$. We have

$$t=\left[\frac{k+\zeta+K}{2k}\right]\left[\frac{1-sz}{s-1}\right]\ , \tag{A5a}$$

$$z=(k+\zeta-K)/(k+\zeta+K)\ , \tag{A5b}$$

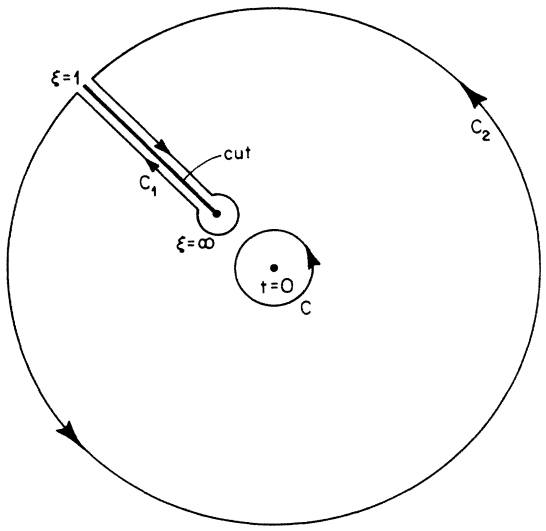

FIG. 1. Contour C in complex t plane is deformed into contour C_1 encircling cut and contour C_2 which is circle of infinite radius.

$$\frac{dt}{ds}=-\frac{K}{k}\frac{1}{(1-s)^2}\ , \tag{A5c}$$

$$1+\frac{1}{t}=\left[\frac{k-\zeta+K}{k+\zeta+K}\right]\left[\frac{s-w}{1-sz}\right]\ , \tag{A5d}$$

$$w=(k-\zeta-K)/(k-\zeta+K)\ , \tag{A5e}$$

$$\mu=2Ks/(s-1)\ . \tag{A5f}$$

Noting that the singular part of

$${}_2F_1(L+1-i\gamma,m;m-L-i\gamma;\xi)\mu^{-m}$$

along C_1 is[12]

$$\frac{\Gamma(m-L-i\gamma)\Gamma(1-\delta)}{(m-1)!(m-2L-2)!}(-s)^{L+1-i\gamma}\times{}_2F_1(L+1-i\gamma,2L+2-m;\delta;s)\mu^{-m}\ ,$$

where $\delta=L+2-m-i\gamma$, we obtain

$$I_1=-\left[\frac{K}{k}\right]\left[\frac{k+\zeta+K}{2k}\right]^{2l}\left[\frac{k-\zeta+K}{k+\zeta+K}\right]^{n+l}\frac{\Gamma(1-\delta)}{(2K)^m2\pi i}\times\int_{C_3}ds(-s)^{\delta-1}(1-s)^{m-2l-2}(1-sz)^{2l}\times\left[\frac{s-w}{1-sz}\right]^{n+l}\times{}_2F_1(L+1-i\gamma,2L+2-m;\delta;s)\ . \tag{A6}$$

Here C_3 is the transform of C_1 under the change of variables $t\to s$; thus, in the complex s plane, C_3 starts at the point $s=1$ and returns to this point after encircling (in the clockwise sense) the cut along the interval $0\le s\le 1$. Note that the hypergeometric function in the integrand of Eq. (A6) is a polynomial in s of degree $m-2L-2$. Note also that if $\zeta=0$ (i.e., $w=z$) and if k and K are both pure imaginary (a case of interest) we have $|z|<1$, and $|(s-z)/(1-sz)|\le 1$ along C_3, where the equality obtains only when s equals 1. Hence if $n\gg 1$ the integrand of (A6) is negligibly small except in the region $|1-s|\sim 1/n$; it follows that $I_1=O(\gamma/n^{m-2l-1})$ if $n\gg 1$, assuming that $\zeta=0$ and that k and K are pure imaginary. To evaluate the integral of (A6) we write

$$(s-w)^{n+l}=\sum_{q=0}^{n+l}C_q^{n+l}s^{n+l-q}(-w)^q\ , \tag{A7a}$$

$${}_2F_1(L+1-i\gamma,2L+2-m;\delta;s)=\sum_{r=0}^{m-2L-2}\frac{(L+1-i\gamma)_r(2L+2-m)_rs^r}{(\delta)_r(r!)}\ , \tag{A7b}$$

where $C_q^n=n!/[q!(n-q)!]$, and we use the integral representation

$${}_2F_1(a,b;c;z)=\frac{1}{2\pi i}\frac{\Gamma(1-a)\Gamma(c)}{\Gamma(c-a)}\times\int_{C_3}ds(-s)^{a-1}(1-s)^{c-a-1}(1-sz)^{-b}\ , \tag{A7c}$$

where $\mathrm{Re}(c-a)>0$. The result is a sum of hypergeometric functions:

$$I_1=B\sum_{q=0}^{n+l}C_q^{n+l}(-w)^q\sum_{r=0}^{m-2L-2}B_{qr}\,{}_2F_1(a,b;c;z)\ , \tag{A8a}$$

$$B=-\left[\frac{K}{k}\right]\left[\frac{k+\zeta+K}{2k}\right]^{2l}\left[\frac{k-\zeta+K}{k+\zeta+K}\right]^{n+l}\times\frac{(m-2l-2)!}{(2K)^m}\frac{1}{\Gamma(\delta)}\ , \tag{A8b}$$

$$B_{qr}=\frac{(L+1-i\gamma)_r(2L+2-m)_r}{(\delta)_r(r!)(a)_{m-2l-1}}\ , \tag{A8c}$$

$$a=\delta+n+l-q+r\ , \tag{A8d}$$

$$b=n-l\ , \tag{A8e}$$

$$c=a+m-2l-1\ . \tag{A8f}$$

Along C_2 the singular part of ${}_2F_1(L+1-i\gamma,m;m-L-i\gamma;\xi)$ is[12]

$$\frac{(2L)!\Gamma(m-L-i\gamma)}{\Gamma(L+1-i\gamma)(m-1)!}\times\sum_{q=0}^{2L}\frac{(-L-i\gamma)_q}{q!}\frac{(m-2L-1)_q}{(-2L)_q}(1-\xi)^{q-2L-1}$$

We therefore have

$$I_2=(2L)!\frac{(m-2L-2)!}{\Gamma(L+1-i\gamma)}\times\sum_{q=0}^{2L}\frac{(-L-i\gamma)_q}{q!}\frac{(m-2L-1)_q}{(-2L)_q}(2K)^{q-2L-1}I_{2q}\ , \tag{A9a}$$

$$I_{2q}=\frac{1}{2\pi i}\int_{C_2}dt\frac{t^{2l}}{\mu^{q'}}\left[1+\frac{1}{t}\right]^{n+l}\ , \tag{A9b}$$

where $q'=m+q-2L-1$. If we expand $\mu^{-q'}(1+1/t)^{n+l}$ in powers of $1/t$, only the term in $1/t^{2l+1}$ contributes to the integral I_{2q}; in fact, the integral is just the coefficient of this term. We therefore have

$$I_{2q}=(2k)^{-q'}\sum_{r=0}^{R}(-1)^jC_r^{n+l}\frac{(q')_j}{j!}\left[\frac{K+k+\zeta}{2k}\right]^j\ , \tag{A10}$$

where $j=2l+1-r-q'$ and where R is the smaller of $2l+1-q'$ and $n+l$; with the restriction imposed on p, we have, in fact, $R=2l+1-q'$, and hence that $j=R-r$. Note that I_{2q} increases with n as n^R and therefore, since R has maximum value $l+L-p-1$, I_2 increases as $n^{l+L-p-1}$.

The values $p=1$ and $L=l\pm1$ are of particular interest. We have $m=2l+4\pm1$; for $n\gg1$ we have I_2 increases as $n^{2l-2\pm1}$ whereas if $\zeta=0$ and k and K are pure imaginary we have $I_1=O(\gamma/n^{3\pm1})$. In this case we can neglect I_1 for $n\gg1$ and we have only to deal with the relatively simple computation of I_2.

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