Integral representation of the Coulomb Green function derived from the Sturmian expansion

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We recast the Sturmian expansion of the one-particle Coulomb Green function as an integral which, through an appropriate choice of contour, is applicable anywhere on the Riemann energy surface (excluding the neighborhood of the negative real axis on the physical energy sheet, a region to which the series representation is ideally suited). As a numerical test we have used this integral representation, in conjunction with a two-particle convolution of one-particle Coulomb Green functions, to calculate the cross sections for both partial and complete breakup of the negative hydrogen ion by one-photon absorption.

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I. INTRODUCTION

Consider a smoothly varying potential $V(r)$ which vanishes at asymptotically large distances and does not change sign over the allowed range of the distance r. The "Sturmian" functions are bound-state solutions of the Schrödinger equation for a potential $\lambda_n V(r)$ whose overall strength parameter λ_n is *variable* while the energy $\mathcal{E}$ is *fixed* to be real and negative. This is a Sturm-Louiville eigenvalue problem; the eigenvalue is λ_n. The eigenvalue spectrum is discrete, yet the eigenfunctions span a vector space of square-integrable functions. Furthermore, the Green function for the actual potential $V(r)$, at the energy $\mathcal{E}$, is *diagonal* on the Sturmian basis, and hence can be represented by a series whose discrete index n runs over the eigenvalue spectrum.

The "Coulomb-Sturmian" functions, popularized by Rotenberg [1], have the merit that they can be expressed in closed form. Furthermore, they exhibit the cusp-behavior at the origin which is a characteristic of the singularity of the Coulomb potential. Hence a Coulomb-Sturmian basis is well suited to the description of few-body atomic systems, at least over finite distances [2]. However, despite its simplicity, the Coulomb-Sturmian series representation of the Coulomb Green function is of limited use; it is defined on the negative real energy axis, where it is indeed useful, but it does not converge on the positive real energy axis. Various methods have been employed for analytically continuing the series to positive energies—see, e.g., Refs. [3,4]—but sometimes high-precision arithmetic is needed to avoid a serious loss in accuracy. However, Papp [5] observed that matrix elements of the Coulomb Green function on a Coulomb-Sturmian basis satisfy a very useful three-term recurrence relation which can be analytically continued to all energies without significant roundoff error. Papp and collaborators [6,7] have used this recurrence relation, together with a two-particle convolution of one-particle Coulomb Green functions, to numerically solve to high accuracy the Faddeev-Merkuriev integral equations for several three-body atomic processes.

In the present paper we reexpress the series representation of the Coulomb Green function as an integral, again in diagonal form. After making an appropriate choice of contour this integral representation is applicable over the entire Riemann energy surface (excluding the neighborhood of the negative real axis on the physical energy sheet, a region to which the series representation is ideally suited). The primary distinction of our integral representation is that it pertains to the Green function itself, and therefore it can be used to evaluate matrix elements on any basis, including a Coulomb-Sturmian basis. Its accuracy can be regulated by varying the number of quadrature points. As a numerical test we have used it to perform a desktop calculation of the cross sections for both partial and complete breakup of the negative hydrogen ion by one-photon absorption. In common with Papp *et al.* we employ a two-particle convolution of one-particle Coulomb Green functions.

II. THE ONE-PARTICLE COULOMB GREEN FUNCTION

Let $g(\mathcal{E})$ denote a one-particle resolvent, which has the partial-wave expansion

$$\langle \vec{r}|g(\mathcal{E})|\vec{r}'\rangle = \sum_{lm} Y^*_{lm}(\hat{\mathbf{r}}) \frac{\langle r|g_l(\mathcal{E})|r'\rangle}{rr'} Y_{lm}(\hat{\mathbf{r}}'). \tag{1}$$

The wave number k is a two-valued function of the energy $\mathcal{E}$,

$$k = \sqrt{2\mu\mathcal{E}}/\hbar, \tag{2}$$

and we distinguish its two branches by a cut along the positive energy axis; this is the "unitarity" cut, the line along which the spectral decomposition of $g_l(\mathcal{E})$ is singular. The "physical" branch of $g_l(r,r';\mathcal{E}) \equiv \langle r|g_l(\mathcal{E})|r'\rangle$ has as its domain the "physical" energy sheet $0 < \arg(\mathcal{E}) < 2\pi$, and it is bounded as r and/or r' increase. Consequently, if $\langle r|\Phi\rangle$ and $\langle r|\Psi\rangle$ are two well-behaved functions of r which vanish at least as fast as r^{l+1} at the origin and faster than $1/r$ at infinity, the matrix element $\langle\Phi|g_l(\mathcal{E})|\Psi\rangle$ formally exists for all values of $\mathcal{E}$ on the physical sheet, save for bound-state poles which occur on the negative real axis. The "unphysical" branch of $g_l(r,r';\mathcal{E})$ has as its domain the "unphysical" energy sheet $-2\pi < \arg(\mathcal{E}) < 0$, and it is unbounded as r and/or r' increase. Nevertheless, $\langle\Phi|g_l(\mathcal{E})|\Psi\rangle$ can be defined on the unphysical sheet by analytic continuation from the physical sheet.

A. Series representation

The Coulomb-Sturmian functions $S^k_{nl}(r)$ are

$$S_{nl}^{k}(r) = \sqrt{\frac{e^{-i\pi/2}k(n-l-1)!}{n[(n+l)\,!\,]}}(-2ikr)^{l+1}L_{n-l-1}^{2l+1}(-2ikr)e^{ikr} \tag{3}$$

normalized here as

$$\int_0^\infty dr[S_{nl}^{k}(r)]^2 = 1. \tag{4}$$

The Coulomb-Sturmian eigenvalue is $\lambda_n = -ink/Z$, which multiplies the attractive Coulomb potential $-Ze^2/r$, where $Z>0$. The radial Green function has the series representation [8]

$$g_l(r,r';\mathcal{E}) = \frac{i}{2\mathcal{E}}\sum_{n=l+1}^{\infty}\left(\frac{nka_0}{Z+inka_0}\right)S_{nl}^{k}(r)S_{nl}^{k}(r'). \tag{5}$$

Each term of this series has its own bound-state pole at a pure imaginary value of the wave number, i.e., $ka_0 = iZ/n$, or, equivalently, at a real negative value of the energy, i.e., $\mathcal{E} = -Z^2e^2/(2n^2a_0)$, on the physical sheet. The ordinal number (number of nodes) of the eigenfunction $S_{nl}^{k}(r)$ is $n-l-1$, and this is in one-one correspondence with the eigenvalue λ_n. If $\mathcal{E}$ is real and negative λ_n is real; otherwise λ_n is complex. In order to analytically continue the series representation of $g_l(r,r';\mathcal{E})$ to the entire Riemann energy surface we must allow the ordinal number to become complex, i.e., we must replace the integer n by a complex variable z, and we must transform the sum over n to an integral over z.

As a first step towards this goal we express the Laguerre polynomial as a confluent hypergeometric function, i.e.,

$$(2l+1)\,!\,L_{z-l-1}^{2l+1}(-2ikr) = (z-l)_{2l+1}\,{}_1F_1(l+1-z,2l+2;-2ikr). \tag{6}$$

Writing $(n+m)!$ as $\Gamma(z+m+1)$ we obtain a generalization of the Coulomb-Sturmian function which is analytic in z,

$$S_{zl}^{k}(r) = \sqrt{\frac{e^{-i\pi/2}k}{z(z-l)_{2l+1}}}(-2ikr)^{l+1}L_{z-l-1}^{2l+1}(-2ikr)e^{ikr}, \tag{7}$$

where we used $\Gamma(z+l+1)/\Gamma(z-l) = (z-l)_{2l+1}$, with $(z-l)_{2l+1}$ a Pochhammer symbol, a polynomial of degree $2l+1$ in z.

Since we are interested in matrix elements of $g_l(\mathcal{E})$ on a space of square-integrable functions it is expedient to choose a basis composed of real Sturmian functions $S_{nl}^{i\kappa}(r)$ where κ is a real positive number. Using the Sturmian expansion of $g_l(r,r';\mathcal{E})$, i.e., Eq. (5), together with Eqs. (3) and (7), we obtain the following series representation of the matrix element $\langle S_{ml}^{i\kappa}|g_l(\mathcal{E})|S_{m'l}^{i\kappa}\rangle$, where $m, m' \geqslant l+1$:

$$\langle S_{ml}^{i\kappa}|g_l(\mathcal{E})|S_{m'l}^{i\kappa}\rangle = -iC_{mm'}^{(l)}\frac{\tan\theta}{8\mathcal{E}}(-4\sin^2 2\theta)^{l+1} \times \sum_{n=l+1}^{\infty}(n-l)_{2l+1}e^{4in\theta}\left(\frac{I_m^{(l)}(n,\theta)I_{m'}^{(l)}(n,\theta)}{n-i(Z/ka_0)}\right), \tag{8}$$

where

$$C_{mm'}^{(l)} = \sqrt{\frac{(m-l-1)\,!\,(m'-l-1)!}{mm'(m+l)\,!\,(m'+l)!}} \tag{9}$$

and

$$\left(\frac{(z-l)_{2l+1}e^{2i\theta z}}{(k^2+\kappa^2)^{l+1}}\right)I_m^{(l)}(z,\theta) \equiv 2\kappa\int_0^\infty dr\, r^{2l+2}e^{(-\kappa+ik)r}L_{z-l-1}^{2l+1}(-2ikr)L_{m-l-1}^{2l+1}(2\kappa r), \tag{10}$$

with the angle θ defined by

$$e^{2i\theta} = \frac{\kappa+ik}{\kappa-ik} \tag{11}$$

or, equivalently,

$$\tan\theta = k/\kappa. \tag{12}$$

The integrals $I_m^{(l)}(z,\theta)$ can be evaluated in closed form; for example,

$$I_{l+1}^{(l)}(z,\theta) = 4(l+1+iz\tan\theta)\cos^2\theta. \tag{13}$$

However, the direct evaluation of $I_m^{(l)}(z,\theta)$ is tedious and prone to numerical roundoff error when $m \gg l$. It is preferable to evaluate $I_m^{(l)}(z,\theta)$ by recurrence.

B. Recurrence relation

We digress briefly to derive a suitable recurrence relation for the $I_m^{(l)}(z,\theta)$. We start with a standard recurrence relation for the Laguerre polynomials,

$$xL_{m-l-1}^{2l+1}(x) = 2mL_{m-l-1}^{2l+1}(x) - (m+l)L_{m-l-2}^{2l+1}(x) - (m-l)L_{m-l}^{2l+1}(x). \tag{14}$$

We use this for $(2\kappa r)L_{m-l-1}^{2l+1}(2\kappa r)$ in Eq. (10), which for $m \geqslant l+2$ allows us to express $I_m^{(l)}(z,\theta)$ as a linear combination of integrals $J_m^{(l)}(z,\theta)$ and $J_{m\pm1}^{(l)}(z,\theta)$ whose integrands have one less power of r,

$$I_m^{(l)}(z,\theta) = 2mJ_m^{(l)}(z,\theta) - (m+l)J_{m-1}^{(l)}(z,\theta) - (m-l)J_{m+1}^{(l)}(z,\theta), \tag{15}$$

where

$$\left(\frac{(z-l)_{2l+1}e^{2i\theta z}}{(k^2+\kappa^2)^{l+1}}\right)J_m^{(l)}(z,\theta) \equiv \int_0^\infty dr\, r^{2l+1}e^{(-\kappa+ik)r}L_{z-l-1}^{2l+1}(-2ikr)L_{m-l-1}^{2l+1}(2\kappa r). \tag{16}$$

The integral $J_m^{(l)}(z,\theta)$ has the merit that it can be expressed directly in terms of a single Gauss-hypergeometric function [9],

$$J_m^{(l)}(z,\theta) = (-1)^{m-l-1}\left(\frac{e^{2i(m-l-1)\theta}(z-l)_{m+l}}{(m-l-1)\,!\,(z-l)_{2l+1}}\right) \times F(l+1-z, l+1-m; 1-z-m, e^{-4i\theta}). \quad (17)$$

For the purpose of deriving a recurrence relation for the $J_m^{(l)}(z,\theta)$ we employ the property [10]

$$F(l+1-z, l+1-m; 1-z-m, u) = \frac{(l+m)\,!\,(z-l)_{2l+1}}{(2l+1)\,!\,(z-l)_{m+l}} F(l+1-z, l+1-m; 2l+2, 1-u) \quad (18)$$

which allows us to re-express $J_m^{(l)}(z,\theta)$ in terms of another Gauss-hypergeometric function, only one of whose arguments depends on the variable integer m,

$$J_m^{(l)}(z,\theta) = (-1)^{m-l-1}\left(\frac{e^{2i(m-l-1)\theta}(l+m)!}{(m-l-1)\,!\,(2l+1)!}\right) \times K_m^{(l)}(z, 1-e^{-4i\theta}), \quad (19)$$

where

$$K_m^{(l)}(z,u) \equiv F(l+1-z, l+1-m; 2l+2, u). \quad (20)$$

Now we use one of the standard recurrence relations [9] for a Gauss-hypergeometric function, i.e., for $m \geqslant l+2$,

$$(l+m+1)K_{m+1}^{(l)}(z,u) = [2m+(z-m)u]K_m^{(l)}(z,u) + (l+1-m) \times (1-u)K_{m-1}^{(l)}(z,u) \quad (21)$$

with $K_{l+1}^{(l)}(z,u)=1$ and $K_{l+2}^{(l)}(z,u)=1-(l+1-z)u/(2l+2)$. Thereby we arrive at the recurrence relation

$$(m-l)J_{m+1}^{(l)}(z,\theta) = -2(m\cos 2\theta + iz\sin 2\theta)J_m^{(l)}(z,\theta) - (m+l)J_{m-1}^{(l)}(z,\theta), \quad (22)$$

which can be started using

$$J_{l+1}^{(l)}(z,\theta) = 1, \quad (23)$$

$$J_{l+2}^{(l)}(z,\theta) = -2(l+1)\cos 2\theta - 2iz\sin 2\theta. \quad (24)$$

We infer from Eqs. (19) and (20) that $J_m^{(l)}(z,\theta)$ is a polynomial in z of degree $(m-l-1)$, and hence, using Eq. (15), $I_m^{(l)}(z,\theta)$ is a polynomial in z of degree $(m-l)$.

To gain some insight into the behavior of $J_m^{(l)}(z,\theta)$ when m is large we expand $L_{z-l-1}^{2l+1}(-2ikr)$ in a series of Bessel functions [11]; this allows us to perform the integration over r on the right hand side of Eq. (16), to yield the series

$$J_m^{(l)}(z,\theta) = \sec^{2l+2}\theta e^{2iz(\tan\theta-\theta)}\sum_{n=0}^{\infty} A_n(z)(-\tan^2\theta)^{n/2} Y_{nm}^{nl}(z,\theta), \quad (25)$$

where

$$Y_{0m}^{nl}(z,\theta) = (-1)^{m-l-1} L_{m-l-1}^{2l+1+n}(-4iz\tan\theta), \quad (26)$$

$$Y_{j+1,m}^{nl}(z,\theta) = Y_{j,m}^{nl}(z,\theta) - Y_{j,m-1}^{nl}(z,\theta), \quad (27)$$

$$Y_{j0}^{nl}(z,\theta) = Y_{00}^{nl}(z,\theta), \quad (28)$$

and

$$A_0(z) = 1, \quad (29)$$

$$A_1(z) = 0, \quad (30)$$

$$A_2(z) = l+1, \quad (31)$$

$$(n+1)A_{n+1}(z) = (n+2l+1)A_{n-1}(z) - 2zA_{n-2}(z). \quad (32)$$

If $m-l-1$ is much larger than both unity and $|4z\tan\theta|$ the first term of the series on the right-hand side of Eq. (25) gives an order-of-magnitude estimate of $J_m^{(l)}(z,\theta)$, and using the asymptotic form of $L_n^{\alpha}(u)$ for $n \gg |u|$ and $\sqrt{n|u|} \gg 1$ we find that

$$J_m^{(l)}(z,\theta) \sim (-1)^m \frac{\sec^{2l+2}\theta}{\sqrt{-4i\pi z\tan\theta}}\left(\frac{m-l-1}{-4iz\tan\theta}\right)^{l+1/4} \times e^{-2iz\theta}\cos\left(2\sqrt{-4i(m-l-1)z\tan\theta}+\frac{\pi}{4}\right). \quad (33)$$

Consequently, if $m \gg l+1$, the polynomials $J_m^{(l)}(z,\theta)$, and therefore $I_m^{(l)}(z,\theta)$, oscillate rapidly as z is varied over the region $m|\cot\theta| \gtrsim |z|$. If, in addition, $iz\tan\theta$ is complex, the amplitude of oscillation grows exponentially as $\sqrt{m}$ increases.

C. Integral representation

To analytically continue matrix elements of $g_l(\mathcal{E})$ onto the unphysical sheet we use a variant of the Sommerfeld-Watson transform to rewrite the series representation of $g_l(\mathcal{E})$ as an integral. We start by introducing the weight function

$$w(z) = \left(\frac{1}{2\pi i}\right)\left(\frac{\pi e^{\mp i\pi z}}{\sin\pi z}\right), \quad (34)$$

where the sign of the exponent of $e^{\mp i\pi z}$ is minus if $|\arg(\mathcal{E})| < \pi$ and plus if $\pi < |\arg(\mathcal{E})| \leqslant 2\pi$; the negative real energy axis of the physical sheet, along which $\arg(\mathcal{E})=\pi$, is excluded, but this exclusion is of no practical concern since the series representation is ideally suited to energies on this line. The weight function $w(z)$ has poles at integer values of z, each with residue $(1/2\pi i)$. Therefore if $\mathcal{E}$ is any point on the physical sheet, excluding the real axis, we can use the Cauchy theorem to replace the sum by an integral over a closed contour $\mathcal{C}_1$ which (see Fig. 1) wraps around the segment $\mathrm{Re}(z) > l$ of the real z-axis and which excludes the pole at $i(Z/ka_0)$; we have

$$g_l(r,r';\mathcal{E}) = \frac{i}{2\mathcal{E}}\left(\frac{1}{2\pi i}\right)\int_{C_1} dz\left(\frac{\pi e^{\mp i\pi z}}{\sin\pi z}\right)\left(\frac{zka_0}{Z+izka_0}\right) \times S_{zl}^k(r)S_{zl}^k(r'). \quad (35)$$

This integral representation can be analytically continued

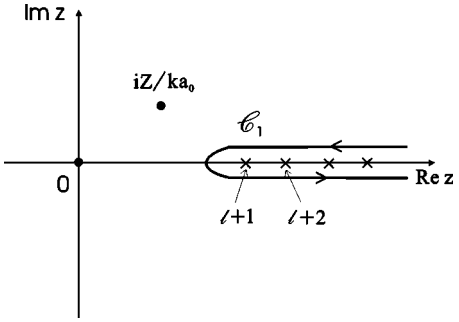

FIG. 1. The Sturmian expansion of the Coulomb Green can be transformed from a sum to an integral over a complex variable z. The path of integration, $\mathcal{C}_1$, wraps around the segment $\mathrm{Re}(z)>l$ of the real axis; it encloses simple poles at integer values $l+1$, $l+2,\cdots$ of z but excludes the pole at $i(Z/ka_0)$.

onto the unphysical sheet by an appropriate distortion of the contour of integration, as described below.

Combining Eqs. (35), (7), and (10) yields an integral representation of the matrix elements $\langle S^{i\kappa}_{ml}|g_l(\varepsilon)|S^{i\kappa}_{m'l}\rangle$; if $m,m' \geqslant l+1$ we have

$$\langle S^{i\kappa}_{ml}|g_l(\mathcal{E})|S^{i\kappa}_{m'l}\rangle = -iC^{(l)}_{mm'}\left(\frac{\mu a_0}{8\kappa\hbar^2}\right)(-4\sin^2 2\theta)^{l+1} \times \int_{C_1} dz\left(\frac{e^{\mp i\pi z}}{\sin \pi z}\right)(z-l)_{2l+1} \times e^{4i\theta z}\left(\frac{I^{(l)}_m(z,\theta)I^{(l)}_{m'}(z,\theta)}{Z+zika_0}\right). \quad (36)$$

Since the poles of $1/\sin z$ at $z=-l,\cdots,l$ are eliminated by the factor $(z-l)_{2l+1}$ in the integrand on the right-hand side of Eq. (36) we can extend the contour $\mathcal{C}_1$ so that it wraps around the entire positive real axis, not just the segment $\mathrm{Re}(z)>l$. Furthermore, since $w(z)e^{4i\theta z}$ decays exponentially at asymptotically large z we can open up the contour, provided it crosses neither the real axis [on which the poles of $w(z)$ lie] nor the pole at $i(Z/ka_0)$. Suppose that ε is real and positive and lies on the upper edge of the unitarity cut on the physical sheet; thus k is real and positive and the "unitarity" pole at $i(Z/ka_0)$ lies on the positive imaginary z axis. We can open up $\mathcal{C}_1$ into an infinite semicircle whose base $\mathcal{C}_2$ runs along the imaginary z axis, except for an infintesimal indentation to the right of the unitarity pole; see Fig. 2. The integral over the semicircular arc at infinity, in the right half of the z plane, vanishes [recall that $w(z)e^{4i\theta z}$ decays exponentially at z]. The integral along the imaginary z axis is the principal-value contribution. From Eqs. (12),(15), and (22)–(24) we see that when z is pure imaginary $J^{(l)}_{l+1}(z,\theta)$, and therefore $I^{(l)}_{l+1}(z,\theta)$, are real (κ and k are both real). Thus, setting $z=ix$ where x is real, and noting that $(ix-l)_{2l+1}=(-1)^l ix|(ix+l)_l|^2$, which is purely imaginary, the principal-value integral is real. On the other hand, the contribution to $\langle S^{i\kappa}_{ml}|g_l(\mathcal{E})|S^{i\kappa}_{m'l}\rangle$ from the unitarity pole is pure imaginary. If we move $\mathcal{E}$ to the lower edge of the unitarity cut on the physical energy sheet k becomes real and negative. The principal-value integral does not change; it is a single-valued function of $\mathcal{E}$. However, the contribution from the unitarity pole changes sign. To verify that $\langle S^{i\kappa}_{ml}|g_l(\mathcal{E})|S^{i\kappa}_{m'l}\rangle$ does behave as stated when $\mathcal{E}$ is moved from the upper to the lower edge of the unitarity cut, note that we must change the sign in the exponent of $w(z)$; note further that Eqs. (12),(15), and (22)–(24) imply θ changes sign while $I^{(l)}_{l+1}(z,\theta)$ is invariant under a simultaneous change in the signs of z and k. Introducing $\xi\equiv(Z/ka_0)$, with $\mathcal{E}$ real and positive, we have (where P denotes principal value)

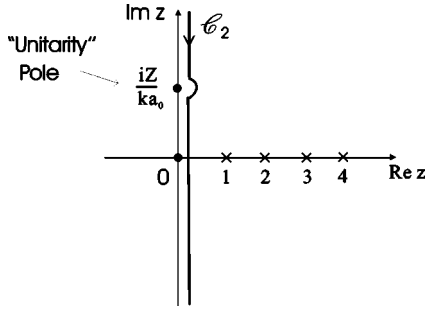

FIG. 2. If ε lies on either edge of the unitarity cut the path of integration $\mathcal{C}_1$ can be distorted into a line $\mathcal{C}_2$ which runs down the imaginary z axis, with an infinitesimal indentation to the right of the "unitarity" pole.

$$\langle S^{i\kappa}_{ml}|g_l(\mathcal{E}\pm i0)|S^{i\kappa}_{m'l}\rangle = \mathrm{P}\langle S^{i\kappa}_{ml}|g_l(\mathcal{E})|S^{i\kappa}_{m'l}\rangle \mp i\pi 2^{4l+1}C^{(l)}_{mm'} \times\left(\frac{Z}{\mathcal{E}\kappa a_0}\right)\left(\frac{\kappa k}{\kappa^2+k^2}\right)^{2l+2}|(i\xi+l)_l|^2 \times\frac{e^{-4\theta\xi}}{1-e^{\mp 2\pi\xi}}I^{(l)}_m(i\xi,\theta)I^{(l)}_{m'}(i\xi,\theta). \quad (37)$$

It is straightforward to deduce from the imaginary part of this expression the familiar rate for photoionization of atomic hydrogen from its ground state. The discontinuity in $g_l(\mathcal{E})$ at two points on opposite sides of the cut, but on the same sheet, arises from the unitarity pole of the integral representation. This discontinuity accounts for the loss of flux in a scattering process, and leads to the optical theorem, an expression of the unitarity of the scattering operator.

Now we allow $\mathcal{E}$ to lie anywhere on the Riemann energy surface, on either sheet, excluding the negative real axis. We choose the contour $\mathcal{C}_1$ so that the integral on the right-hand side of Eq. (36) is suited to numerical integration. Thus we deform the contour into two straight lines, $z=x_0+ipx$ and $z=x_0+iqx$, where x_0 is a real constant in the interval $0\leqslant x_0<l+1$, e.g., $x_0=l+\frac{1}{2}$, where x is real and runs from 0 to ∞, and where

$$p = 1/(4\theta), \quad (38)$$

$$q = \mp 1/(2\pi \mp 4\theta). \quad (39)$$

Note that $p\to\infty$ as $k\to 0$ and $q\to\infty$ as $k\to\infty$. The q-dependent sign is determined as follows: It is minus if

$$|\arg(\mathcal{E})| < \pi, \tag{40}$$

in which case $\mathrm{Re}(k)>0$, $\mathrm{Re}(p)>0$, but $\mathrm{Re}(q)<0$; it is plus if

$$|\arg(\mathcal{E})| > \pi, \tag{41}$$

in which case $\mathrm{Re}(k)<0$, $\mathrm{Re}(p)<0$, but $\mathrm{Re}(q)>0$. As $\mathcal{E}$ moves onto the second sheet the contour crosses the unitarity pole, and the contribution of this pole must be included.

Selecting the contour just described, we arrive at

$$\langle S^{i\kappa}_{ml}|g_l(\mathcal{E})|S^{i\kappa}_{m'l}\rangle = -iC^{(l)}_{mm'}\frac{\tan\theta}{8\mathcal{E}}(-4\sin^2 2\theta)^{l+1}\int_0^\infty dx\, e^{-x}\left[\frac{(x_0+ipx-l)_{2l+1}}{1-e^{\mp 2\pi(px-ix_0)}}\left(\frac{I^{(l)}_m(x_0+ipx,\theta)I^{(l)}_{m'}(x_0+ipx,\theta)}{x-(ix_0+Z/ka_0)/p}\right)e^{ix_0/p}\right.$$
$$\left.+\frac{(x_0+iqx-l)_{2l+1}}{1-e^{\pm 2\pi(qx-ix_0)}}\left(\frac{I^{(l)}_m(x_0+iqx,\theta)I^{(l)}_{m'}(x_0+iqx,\theta)}{x-(ix_0+Z/ka_0)/q}\right)e^{ix_0/q}\right], \tag{42}$$

where the upper sign of the exponents of $e^{\mp 2\pi(px-ix_0)}$ and $e^{\pm 2\pi(qx-ix_0)}$ applies if $|\arg(\mathcal{E})|<\pi$, and the lower sign applies if $|\arg(\mathcal{E})|>\pi$ (so the exponentials decrease in magnitude with increasing x). In general, the unitarity pole lies off the real x axis, at $x=ix_0+(Z/ska_0)$ where $s=p$ if $\mathrm{Re}(p)>0$ or $s=q$ if $\mathrm{Re}(q)>0$. In any case it is expedient to subtract this pole using

$$\int_0^\infty dx\frac{e^{-x}f(x)}{x-w} = \int_0^\infty dx\frac{e^{-x}[f(x)-f(w)]}{x-w} + f(w)e^{-w}E_1(-w), \tag{43}$$

where $E_1(z)$ is the exponential integral. Since $(x_0+isx-l)_{2l+1}I^{(l)}_m(x_0+isx,\theta)I^{(l)}_{m'}(x_0+isx,\theta)$ is a polynomial in x of degree $m+m'+1$, the integrand which results upon removal of the unitarity pole is, aside from the term $1/[1-e^{\pm 2\pi(sx-ix_0)}]$, a polynomial in x of degree $m+m'$ weighted by e^{-x}, and the resulting integral can be conveniently evaluated using Gauss-Laguerre quadrature. However, recall that if $m\gg l+1$ the function $I^{(l)}_m(x_0+isx,\theta)$ oscillates rapidly as x varies, possibly (if θ is complex) with very large amplitude, so the presence of the nonpolynomial factor $1/[1-e^{\pm 2\pi(sx-ix_0)}]$ might undermine the accuracy of Gauss-Laguerre quadrature.

III. THE CONVOLUTION OF TWO ONE-PARTICLE GREEN FUNCTIONS

Consider a system of two particles, 1 and 2 say, moving under the influence of both their mutual interaction W_{12} and a fixed center of force. Let E be the total energy of the two particles; E is real, but may be positive or negative. If $G_0(E)$ is the resolvent for the motion in the absence of W_{12}, the full two-particle resolvent is

$$G(E) = G_0(E) + G_0(E)W_{12}G(E) \tag{44}$$

$$= [1 - W_{12}G_0(E)]^{-1}G_0(E) \tag{45}$$

$$= [W_{12} - W_{12}G_0(E)W_{12}]^{-1}W_{12}G_0(E). \tag{46}$$

The merit of Eq. (46) is that $[W_{12}-W_{12}G_0(E)W_{12}]$ is a symmetric operator, a property that is useful in reducing the effort of taking the inverse. If W_{12} is positive or negative definite (as is the Coulomb potential) $[W_{12}-W_{12}G_0(E)W_{12}]$ is positive or negative definite on the negative real energy axis below the bound-state poles of $G_0(E)$. Along this segment $[W_{12}-W_{12}G_0(E)W_{12}]$ has a Cholesky decomposition [13], i.e., it can be expressed as the product of a lower triangular matrix and its transpose. The Cholesky decomposition can be analytically continued to other regions of the complex E plane, in particular to either edge of the unitarity cut. This yields a further reduction in the effort of taking the inverse.

Let $g(1;\mathcal{E})$ and $g(2;\mathcal{E})$ be the one-particle resolvents for particles 1 and 2 when these particles move on their own in the presence of the center of force (the nucleus). Introducing

$$\mathcal{E}_0 \equiv \tfrac{1}{2}E, \tag{47}$$

the physical branch of $G_0(E)$ can be expressed as the standard convolution integral [12], as yet unsymmetrized with respect to particle exchange,

$$G^{(\mathrm{I})}_0(E+i0) = \frac{1}{2\pi i}\int_{\mathcal{C}_3} d\mathcal{E} \times g^{(\mathrm{I})}(1;\mathcal{E}_0+i0-\mathcal{E})g^{(\mathrm{I})}(2;\mathcal{E}_0+i0+\mathcal{E}), \tag{48}$$

where $\mathcal{C}_3$ runs along real axis from ∞ to $-\infty$ and where the superscript I indicates that the branch is the physical one. The contour $\mathcal{C}_3$ runs just beneath the cut and the bound-state poles of $g^{(\mathrm{I})}(1;\mathcal{E}_0+i0-\mathcal{E})$, and just above the cut and the bound-state poles of $g^{(\mathrm{I})}(2;\mathcal{E}_0+i0+\mathcal{E})$; see Fig. 3. The integrand of the convolution integral has branch points at $\mathcal{E}_0$ and $-\mathcal{E}_0$. If the center of force is attractive and Coulombic the integrand also has bound-state poles which accumulate at $\mathcal{E}_0$ and $-\mathcal{E}_0$, in which case the branch points are essential singu-

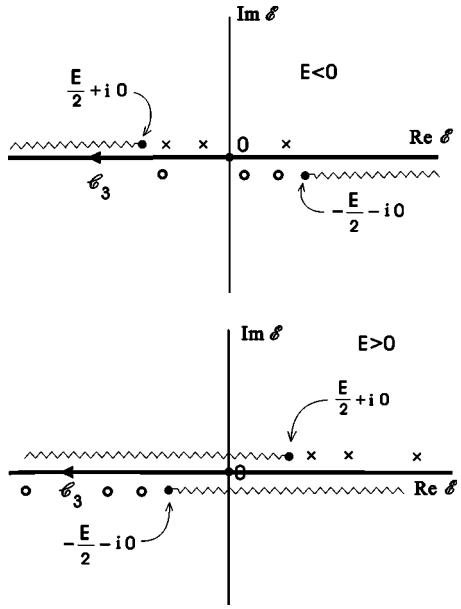

FIG. 3. The path of integration of the convolution integral is the whole real $\mathcal{E}$ axis, from ∞ to $-\infty$. The bound-state poles which are associated to the thresholds at $\frac{1}{2}E$ and $-\frac{1}{2}E$ are shown schematically as crosses and open circles, respectively. The zigzag lines are the unitarity branch cuts.

larities. However, by rotating the contour about the origin through an angle ϕ in the range $[-\pi/2,\pi/2]$ we can avoid these singularities. Thus we set $\mathcal{E}=\mathcal{E}_0te^{i\phi}$ where t runs from ∞ to $-\infty$. If E is negative ϕ is positive, and the contour remains on the physical sheet but sweeps past those poles further than $|\mathcal{E}_0|$ from threshold; while if E is positive ϕ is negative, and the contour sweeps over the unitarity cuts and moves onto the unphysical sheet. See Fig. 4.

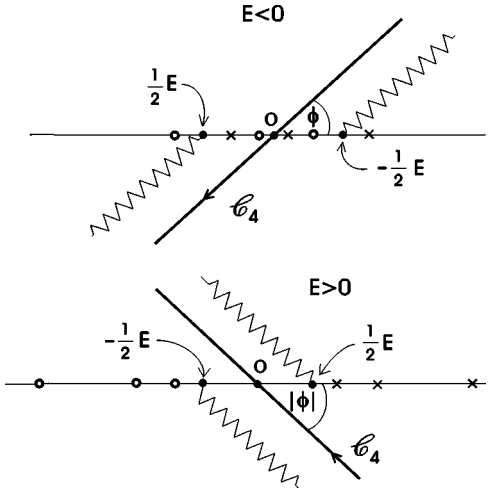

FIG. 4. The path of integration of the convolution integral is rotated about the origin. For clarity we have also rotated the branch cuts along with the contour; the rotated cuts differ from the "unitarity" cuts. The rotation is counterclockwise ($\phi>0$) if $E<0$ and clockwise ($\phi<0$) if $E>0$. The counterclockwise rotation sweeps over those bound-state poles which are further than $\frac{1}{2}|E|$ from the pertinent threshold. The clockwise rotation sweeps over the unitarity cuts.

Suppose hereafter that particles 1 and 2 are identical, and let us (anti)symmetrize $G_0(E)$ with respect to particle exchange. The symmetrized integrand is even in t, and so we can reduce the range of integration to $[0,\infty]$. If E is positive we have (taking into account that the contour sweeps over the unitarity cuts)

$$G_0^{(\mathrm{I})}(E>0+i0)$$
$$=-\frac{\mathcal{E}_0e^{i\phi}}{2\pi i}\int_0^\infty dt[g^{(\mathrm{I})}(1;\mathcal{E}_0-\mathcal{E}_0te^{i\phi})g^{(\mathrm{II})}(2;\mathcal{E}_0+\mathcal{E}_0te^{i\phi})$$
$$\pm g^{(\mathrm{II})}(1;\mathcal{E}_0+\mathcal{E}_0te^{i\phi})g^{(\mathrm{I})}(2;\mathcal{E}_0-\mathcal{E}_0te^{i\phi})], \tag{49}$$
$$\phi<0,$$

where the superscript II indicates that the branch is the unphysical one. If E is negative we have (taking into account that the contour sweeps over the poles)

$$G_0^{(\mathrm{I})}(E<0)$$
$$=\frac{\mathcal{E}_0e^{i\phi}}{2\pi i}\int_0^\infty dt[g^{(\mathrm{I})}(1;\mathcal{E}_0-\mathcal{E}_0te^{i\phi})g^{(\mathrm{I})}(2;\mathcal{E}_0+\mathcal{E}_0te^{i\phi})$$
$$\pm g^{(\mathrm{I})}(1;\mathcal{E}_0+\mathcal{E}_0te^{i\phi})g^{(\mathrm{I})}(2;\mathcal{E}_0-\mathcal{E}_0te^{i\phi})]+R(E), \tag{50}$$
$$\phi>0,$$

where $R(E)$ is the sum of the residues of those bound-state poles crossed by the contour, i.e.,

$$R(E)=\frac{1}{2}\sum_{\mathcal{E}_{\mathrm{bd}}<\mathcal{E}_0}g^{(\mathrm{I})}(1;E+i0-\mathcal{E}_{\mathrm{bd}})|2;\mathcal{E}_{\mathrm{bd}}\rangle\langle 2;\mathcal{E}_{\mathrm{bd}}|$$
$$\pm|1;\mathcal{E}_{\mathrm{bd}}\rangle\langle 1;\mathcal{E}_{\mathrm{bd}}|g^{(\mathrm{I})}(2;E+i0-\mathcal{E}_{\mathrm{bd}}), \tag{51}$$

where $|j;\mathcal{E}_{\mathrm{bd}}\rangle$ is an eigenket of the one-particle Hamiltonian h_j for particle j (1 or 2) with bound-state energy $\mathcal{E}_{\mathrm{bd}}$.

We can express $G_0^{(\mathrm{I})}(E+i0)$ in a common form, which is applicable to both positive and negative E and involves only the physical branches of the one-particle resolvents. To this end we observe that the discontinuity in $g^{(\mathrm{I})}(j;\mathcal{E})$ between two points on opposite edges of the unitarity cut is

$$D(j;\mathcal{E})=-2i\pi\delta(\mathcal{E}-h_j) \tag{52}$$
$$=-2i\pi\rho(j;\mathcal{E})|j;\mathcal{E}\rangle\langle j;\mathcal{E}|, \tag{53}$$

where $|j;\mathcal{E}\rangle$ is an eigenket of h_j with continuum-state energy $\mathcal{E}$ and where $\rho(j;\mathcal{E})$ is the density-of-states factor; if $\mathcal{E}$ is degenerate, summation over eigenstates with the same energy eigenvalue is to be understood. Therefore the analytic continuation of $g(j;\mathcal{E})$ from the physical to the unphysical sheet can be carried out by means of the relation

$$g^{(\mathrm{II})}(j;\mathcal{E})=g^{(\mathrm{I})}(j;\mathcal{E})+D(j;\mathcal{E}), \tag{54}$$

where $D(j;\mathcal{E})$ is the analytic continuation of the discontinuity onto the unphysical sheet. Incidentally, from this relation and the asymptotic expansion [with $\arg(\mathcal{E})\neq 0$]

$$g^{(\mathrm{I})}(j;\mathcal{E}) = \frac{1}{\mathcal{E}}\sum_{n=0}^{\infty}\left(\frac{h_j}{\mathcal{E}}\right)^n \tag{55}$$

we can evaluate rather easily $g^{(\mathrm{II})}(\mathcal{E})$ for large values of $\mathcal{E}$. Combining Eqs. (49), (50), and (54) we have, for E positive or negative,

$$\begin{aligned} G_0^{(\mathrm{I})}(E+i0) &= -\frac{|E|e^{i\phi}}{4\pi i}\int_0^{\infty} dt[g^{(\mathrm{I})}(1;\mathcal{E}_0-\mathcal{E}_0te^{i\phi})g^{(\mathrm{I})}(2;\mathcal{E}_0+\mathcal{E}_0te^{i\phi}) \\ &\pm g^{(\mathrm{I})}(1;\mathcal{E}_0+\mathcal{E}_0te^{i\phi})g^{(\mathrm{I})}(2;\mathcal{E}_0-\mathcal{E}_0te^{i\phi})] \\ &+\Theta(-E)R(E)+\Theta(E)\Delta(E),\quad E\phi<0, \end{aligned} \tag{56}$$

where $\Theta(x)$ is the Heaviside step function and where

$$\begin{aligned} \Delta(E) = -\frac{Ee^{i\phi}}{4\pi i}\int_0^{\infty} dt[g^{(\mathrm{I})}(1;\mathcal{E}_0-\mathcal{E}_0te^{i\phi})D(2;\mathcal{E}_0+\mathcal{E}_0te^{i\phi}) \\ \pm D(1;\mathcal{E}_0+\mathcal{E}_0te^{i\phi})g^{(\mathrm{I})}(2;\mathcal{E}_0-\mathcal{E}_0te^{i\phi})]. \end{aligned} \tag{57}$$

If $E>0(\phi<0)$ the argument $\mathcal{E}_0+\mathcal{E}_0te^{i\phi}(t>0)$ of $D(1;\mathcal{E}_0+\mathcal{E}_0te^{i\phi})$ lies on the unphysical sheet.

The rotated straight-line integration contour $\mathcal{C}_4$ penetrates deep into the region of (complex) unphysical energies. This has the disadvantage that the angle θ acquires a relatively large imaginary part along some segment of the contour (where $|k|\sim\kappa$) so the polynomial $I_m^{(l)}(x_0+isx,\theta)$, with $s=p$ or q, oscillates with a very large amplitude, resulting in significant roundoff error when $m\gg l+1$. Rather than use a straight-line contour it is more helpful to use a contour which remains close to the real energy axis except near the singularities. This can be most conveniently accomplished by invoking the conformal transformation

$$u = \frac{1-te^{i\phi}}{1+te^{i\phi}}, \tag{58}$$

which maps half of the energy plane onto the disk $|u|\leqslant 1$. Since

$$t = \left(\frac{1-u}{1+u}\right)e^{-i\phi}, \tag{59}$$

we have

$$\mathcal{E}_0-\mathcal{E}_0te^{i\phi} = \frac{Eu}{1+u}, \tag{60}$$

$$\mathcal{E}_0+\mathcal{E}_0te^{i\phi} = \frac{E}{1+u}, \tag{61}$$

and

$$-\frac{Ee^{i\phi}}{4\pi i}\int_0^{\infty} dt\cdots = \frac{E}{2\pi i}\int_1^{-1}\frac{du}{(1+u)^2}\cdots. \tag{62}$$

Noting that $g(\mathcal{E}_0+\mathcal{E}_0te^{i\phi})$ has branch points at $u=\infty$ $(t=-e^{-i\phi})$ and $u=-1$ $(t=\infty)$, while $g(\mathcal{E}_0-\mathcal{E}_0te^{i\phi})$ has branch points at $u=0$ $(t=e^{-i\phi})$ and $u=-1$ $(t=\infty)$, the integrand of the convolution integral has a cusp at $u=-1$ and branch points at $u=0$ and $u=\infty$. The contour $\mathcal{C}_5$ (see Fig. 5) in the u plane commences at $u=1$ and terminates at $u=-1$; it remains close to the real u axis except in the region of the origin where it circumvents the branch point at $u=0$ and also the high-lying bound-state poles which accumulate to the left of this branch point. The lower-lying bound-state poles are isolated near singularities of the form

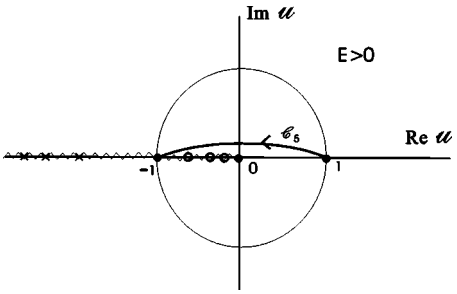

FIG. 5. Half of the energy plane is mapped onto the disk $|u|\leqslant 1$. The integration contour $\mathcal{C}_5$ runs from $u=1$ to $u=-1$, and avoids the high-lying bound-state poles which accumulate below $u=0$. This illustration is for $E>0$; if $E<0$ the integration contour is in the lower half of the disk.

$$\frac{1}{\mathcal{E}_0-\mathcal{E}_0te^{i\phi}-\mathcal{E}_{\mathrm{bd}}} = \frac{1+u}{(E-\mathcal{E}_{\mathrm{bd}})u-\mathcal{E}_{\mathrm{bd}}} \tag{63}$$

which can be subtracted using

$$\int_{u_1}^{-1+i0} du\frac{1}{(E-\mathcal{E}_{\mathrm{bd}})u-\mathcal{E}_{\mathrm{bd}}} = \frac{1}{E-\mathcal{E}_{\mathrm{bd}}} \times\left(i\pi+\ln\frac{E}{(E-\mathcal{E}_{\mathrm{bd}})u_1-\mathcal{E}_{\mathrm{bd}}}\right). \tag{64}$$

IV. NUMERICAL APPLICATION

We have tested the method outlined above by applying it to the problem of one-photon absorption by H^-. We treated the nucleus as an infinitely massive and stationary center of force. Our basis was composed of symmetrized products of real one-particle Sturmian functions.

The interparticle interaction is the pure repulsive Coulomb potential $W_{12}=e^2/r_{12}$ where r_{12} is the interparticle separation. Care must be taken to avoid accumulating roundoff error when evaluating matrix elements of $1/r_{12}$. We eliminated significant roundoff error by constructing the matrix elements of $1/r_{12}$ from those of the inverse square of the Coulomb repulsion, i.e., $r_{12}^2=r_1^2+r_2^2-2r_1r_2\cos\theta_{12}$ where θ_{12} is the angle between the electron coordinates $\vec{r}_1$ and $\vec{r}_2$. The evaluation of the matrix $\underline{M}$ which represents r_{12}^2 is a relatively simple task. Since r_{12} is real, symmetric, positive definite, invariant under the parity operation, and scale invariant, so is both $\underline{M}$ and its square root. Furthermore, the rows and columns of $\underline{M}$ can be labelled so that $\underline{M}$ is tightly banded (e.g., block diagonal or block tridiagonal) with respect to the

TABLE I. Nonvariational estimates of the ground-state energy of H^- in atomic units (1 a.u.=2 Ry) for different basis sizes. The rows and columns are labelled by the maximum values of the ordinal and angular momentum quantum numbers, $n-l-1$ and l, of the real Sturmian functions $S_{nl}^{i\kappa}(r)$ employed in the basis. In composing this table we took $\kappa=1.1$ a.u. A more accurate value [14] for the ground-state energy of H^- is −0.527 751 02 a.u.

	3	5	7	9	11
5	−0.53012	−0.52974	−0.52971	−0.52971	−0.52970
10	−0.52972	−0.52912	−0.52903	−0.52902	−0.52902
15	−0.52951	−0.52877	−0.52863	−0.52860	−0.52860
20	−0.52943	−0.52862	−0.52844	−0.52839	−0.52838
25	−0.52940	−0.52855	−0.52833	−0.52827	−0.52826
30	−0.52939	−0.52851	−0.52827	−0.52820	−0.52817

orbital angular momentum quantum numbers of the particles; this yields a substantial reduction in the effort required to diagonalize $\underline{M}$. Once $\underline{M}$ has been reduced to diagonal form it is trivial to find its square root and inverse. However, since $\underline{M}$ is real, symmetric, and positive definite, its square root and inverse can be found without resorting to diagonalization [13]. Instead we can express $\underline{M}$ as the Cholesky decomposition $\underline{L}\underline{L}^t$ where $\underline{L}$ is a lower triangular matrix which can be expressed without great effort as the singular-value decomposition $\underline{L}=\underline{X}\underline{D}\underline{Y}^t$ where $\underline{X}$ and $\underline{Y}$ are orthogonal matrices and $\underline{D}$ is diagonal; it follows [13] that $\underline{M}^{-1/2}=\underline{X}\underline{D}^{-1}\underline{X}^t$.

While our values of the matrix elements of $1/r_{12}$ are not plagued by roundoff error they do suffer from truncation error due to the truncation of the basis. As a consequence our estimate of the ground-state energy of H^- is not variational, i.e., its error is of first rather than second order in the error of the ground-state wave function. (Nor does the minimum principle apply, i.e., our estimate is not bounded from below.) Hence the convergence towards the exact ground-state energy, with increasing basis size, is rather slow, as indicated in Table I. We see from this table that the convergence with increasing angular momentum quantum number is moderately rapid, as is the convergence with increasing ordinal number for smaller angular momentum quantum numbers; but the convergence with increasing ordinal number is very slow for larger angular momentum quantum numbers. The "exact" value [14] of the ground-state energy is −0.527 751 0.2 a.u.. The error in our estimate of the ground-state energy diminishes only slowly, from 0.4% in the upper left corner of the table to 0.08% in the lower right corner of the table. Nevertheless, in our calculations of the photoabsorption cross section, reported on below, our estimate of the ground-state energy was sufficiently accurate that it was not the principal source of error; and, besides, our expression for the photoabsorption cross section is not variational either.

If $|\Phi\rangle$ represents the initial ground state of the H^- system the response to one-photon absorption, mediated by an external perturbation V in the entrance channel, is represented by

$$|\Psi\rangle = G(E)V|\Phi\rangle, \tag{65}$$

where E is the total energy (ground-state plus photon energy). The inclusive rate for photoabsorption is

$$\Gamma = -2\,\mathrm{Im}\langle\Phi|V^\dagger|\Psi\rangle. \tag{66}$$

Let Γ_α be the rate for the system to undergo a transition to the open (sub)channel α. We express Γ_α in a form which requires only the response ket $|\Psi\rangle$ as input. To this end we introduce the operator $P_{i\alpha}$ which, for $i=1,2$, projects onto the subspace in which a particular electron, the ith, has the energy range and other single-particle quantum numbers specified by the index α. As shown elsewhere [15], by first expressing the rate in terms of the flux through the surface of a hypersphere of asymptotically large radius we deduce that

$$\Gamma_\alpha = -2\,\mathrm{Im}\sum_{i=1}^{2}\{\langle\Phi|V^\dagger P_{i\alpha}|\Psi\rangle + \langle\Psi|W_{12}P_{i\alpha}|\Psi\rangle\}. \tag{67}$$

In the first of the two terms on the right-hand side of Eq. (67) the perturbation V acts in a spatial region whose linear dimensions are of the order of the initial bound-state radius. This term describes the direct excitation by V of the system to (sub)channel α; it does not take into account the possibility that the system is directly excited by V to (sub)channels other than α, after which—and perhaps over distances far larger than the initial bound-state radius—the system migrates to (sub)channel α under the influence of the correlation interaction $\Sigma_{i=1}^2(1-P_{i\alpha})W_{12}P_{i\alpha}$. It is the second of the two terms on the right-hand side of Eq. (67) which takes into account this indirect excitation of the system to (sub)channel α.

The rate for single-electron escape is $\Gamma_{\mathrm{single}}=\Sigma_{\alpha=\mathrm{bd}}\Gamma_\alpha$ where the sum is over one-electron bound states. The rate for double-electron escape is $\Gamma_{\mathrm{double}}=\Sigma_{\alpha=\mathrm{ct}}\Gamma_\alpha$ where the sum is over one-electron continuum states in the energy region $0 \leqslant \mathcal{E} < E/2$. Alternatively, we can express the rate for double-electron escape as $\Gamma_{\mathrm{double}}=\Gamma-\Gamma_{\mathrm{single}}$; the degree to which these two different expressions for Γ_{double} have the same value is an indication of the accuracy of the calculations. Our calculations were done in the velocity gauge. We took the maximum ordinal number of the Sturmian functions to be 25, and the maximum angular momentum quantum number to be 7, at all photon energies. We choose κ, the wave number of the basis, to be 0.5 a.u. at photon energies below 25 eV, 0.7 a.u. in the range 23–29 eV, and 0.9 a.u. above 29 eV. In Fig. 6 we show results for the ratio of the cross sections for double- and single-electron escape over a range

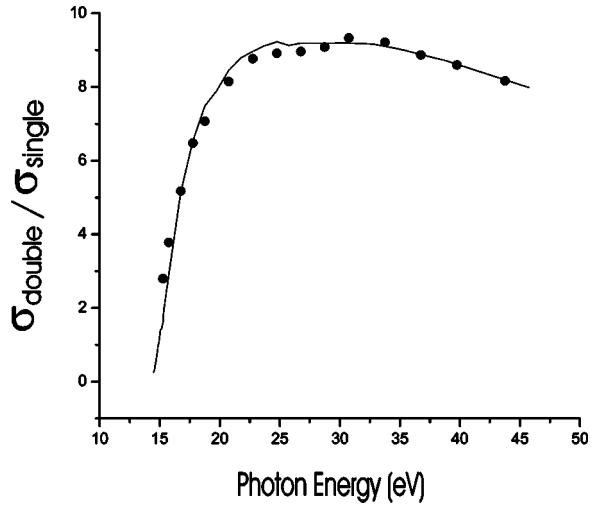

FIG. 6. The ratio of cross sections for double- and single-electron escape from H^- by one-photon absorption. The solid curve corresponds to the results of Kheifets and Bray [16]. The solid circles are the present results.

of photon energies above the threshold for double escape. We show both our results and those of Kheifets and Bray [16]. The results of Kheifets and Bray agree well with the earlier results (not shown) of Meyer, Greene, and Esry [17] and Edah, Foumouo, and Piraux [18]. The agreement with our results is also reasonable, especially in view of the simplicity of our expressions for the single- and double-escape rates, which require no direct input on the asymptotic boundary conditions.

V. SUMMARY

Starting from an expansion in Sturmian functions we derived an integral representation of the Coulomb Green function which, through an appropriate choice of the path of integration, can be used at any point on the Riemann energy surface (excluding the negative axis on the physical sheet). We applied it, in conjunction with a two-particle convolution of one-particle Green functions, to the problem of partial and complete breakup of H^- by one-photon absorption. Our method does not demand enormous computer resources; our application was accomodated on a single-processor (Pentium 4, 1.7 GHz) desktop machine with 1.25 Gb of internal memory. We choose H^- as the system to study since the correlation between the two electrons is strongest in this system, and poses more of a challenge than does helium or other helium-like ions. While we presented results only at positive energies (i.e., above the threshold for complete breakup) we checked that the method is also useful at negative energies, where there are resonances. The partial resolvent $G_0(E)$ has no resonance poles; the resonance poles of the full resolvent $G(E)$ arise from the Coulomb repulsion W_{12}, as zeroes of $W_{12}-W_{12}G_0(E)W_{12}$—recall Eq. (46). However, $G_0(E)$ does have poles at negative energies; they arise from one-particle bound states, and some of them are "picked out" by the counterclockwise rotation of the contour of the convolution integral—recall Fig. 4 and Eqs. (50) and (51).

ACKNOWLEDGMENT

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