Representation of a complex Green function on a real basis: Integral representation

Robin Shakeshaft
Physics Department, University of Southern California, Los Angeles, California 90089-0484
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We describe a decomposition of the resolvent $G(E)=1/(E-H)$ into two parts, $G_{\rm int}(E)$ and $G_{\rm ext}(E)$, each of which can be computed, potentially, with moderate cost. Using an integral representation, $G_{\rm int}(E)$ is built from a Hermitian Hamiltonian matrix constructed on a real discrete basis, and it incorporates the interaction in the interior region where the dynamics take place. The term $G_{\rm ext}(E)$ takes into account the flux passing into the exterior region, and it can be replaced by a Padé approximant by means of a simple connection between $G_{\rm int}(E)$ and $G_{\rm ext}(E)$. We illustrate the method by application to the examples of photoionization of a hydrogen atom and scattering of a particle from a $1/(1+r)^4$ potential.

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I. INTRODUCTION

The approximation of a system's Hamiltonian H by a matrix H is a common simplification in theoretical physics. It leads to the straightforward approximation of the resolvent $G(E)\equiv 1/(E-H)$ by $G(E)=1/(ES-H)$, where S is the overlap matrix of the discrete basis on which H is constructed. However, whereas $G(E)$ has poles *and* branch points, $G(E)$ has only poles, whose positions are the eigenvalues of $S^{-1}H$. Some of the poles of $G(E)$ correspond to bound states, while the others are spurious and simulate the branch cuts of $G(E)$, which extend from the continuum thresholds to infinity. If H is Hermitian, the eigenvalues of $S^{-1}H$ are real, and the spurious poles of $G(E)$ mock a series of overlapping cuts along the real energy axis. Unfortunately, any physical value E that lies in the continuum sits directly on one or more of these makeshift cuts and, consequently, the branch of $G(E)$ is ambiguous. The standard remedy [1] is to rotate the cuts, which can be accomplished by either rotating the particle coordinates through an angle θ, where $0<\theta<\pi/2$ or, equivalently, approximating H by a non-Hermitian matrix constructed on a complex basis that has the character of outgoing waves, i.e., a basis whose members oscillate with distance r as $e^{i\kappa r}$, where $\kappa=i|\kappa|e^{-i\theta}$.

A complex basis that has outgoing-wave character is well suited for calculating the inclusive rate at which a half-collision (e.g., autoionization or photoionization) proceeds since the wave function of a localized system undergoing decay behaves asymptotically as a superposition of outgoing waves. However, a complex basis is not well suited for calculating the rate at which a full collision proceeds since the entrance-channel component of the wave function describing a full collision is a *real standing* wave, comprised of *both* outgoing *and* ingoing waves; a complex basis cannot simulate standing-wave behavior over a distance of the order of the effective range of the interaction—unless the effective range is very short, i.e., it falls off at least exponentially [2]. Moreover, since an outgoing or ingoing wave is a linear combination of standing waves with complex coefficients, it should be possible to calculate either a full- or half-collision rate by representing the resolvent on a real discrete basis, irrespective of the particular asymptotic boundary conditions that pertain to the system. It is our purpose to describe one method for accomplishing this goal.

The work reported on here is an outgrowth of earlier work [3] on the development of a series representation of $G(E)$ which permits H to be approximated by a Hermitian matrix. Our starting point was the observation that all the particles in a system evolve according to a common time. The asymptotic behavior of the system's wave function emerges from the initial boundary conditions, at the inception of the system's evolution, say time $t=0$. The temporal behavior is governed by the time-evolution operator e^{-iHt} (we set $\hbar=1$ throughout), in terms of which $G(E)$ has, for $\mathrm{Im}\,E>0$, the well-known representation

$$G(E)=-it_0\int_0^\infty d\tau\, e^{i(t_0E)\tau}e^{-i(t_0H)\tau}, \tag{1}$$

where t_0 defines the time scale on which the evolution of the system proceeds and where τ is the dimensionless time $\tau\equiv t/t_0$. The unit of time t_0 is the characteristic time it takes for the wave packet on which $G(E)$ acts to change appreciably when it evolves under e^{-iHt}. Roughly speaking, t_0 depends on both the duration of the interaction between the fragments of the system, a time characterized by $1/E$, and the strength of this interaction, characterized by the ground-state binding energy Δ of the system. A suitable definition of t_0 is therefore

$$t_0\equiv 1/(E+\Delta), \tag{2}$$

which is roughly the shorter of the ''collision'' time $1/E$ and the ground-state orbital period $1/\Delta$. The preceding representation of $G(E)$ can be analytically continued to all sectors of the E plane, excluding the discrete set of points at which $G(E)$ has poles, by rotating the contour of integration into the complex τ plane. Thus a particular branch of $G(E)$ on the positive energy axis can be specified by the integration contour. By performing the integration over τ in such a way that a vestige of this contour—namely, its angle of rotation ϕ—is preserved, we arrived in Ref. [3] at a series representation of $G(E)$ whose branch is specified by a complex unit of time $t_\phi\equiv t_0e^{i\phi}$:

$$G(E)=e^{-t_\phi H}\left(\frac{1}{E}+it_\phi(2t_\phi H)\sum_{n=1}^{\infty}\frac{1}{n}\mathcal{I}_n(Et_\phi)L_{n-1}^{(1)}(2t_\phi H)\right), \tag{3}$$

where $L_{n-1}^{(1)}(2t_\phi H)$ is an associated Laguerre polynomial of degree $n-1$ in the operator $2t_\phi H$, and where the coefficient $\mathcal{I}_n(Et_\phi)$ is a number defined by the integral

$$\mathcal{I}_n(a)\equiv\int_0^\infty d\tau\, e^{ia\tau}\left(\frac{\tau+i}{\tau-i}\right)^n. \tag{4}$$

We show in the Appendix that this series can be resummed to yield the integral representation

$$G(E)=-\left(\frac{e^{i\phi}}{E+\Delta}\right)\int_0^\infty dy\, yK_0(ye^{i(\phi-\pi)/2})J_0 \times\left(y\sqrt{\frac{e^{i\phi}(H+\Delta)}{(E+\Delta)}}\right), \tag{5}$$

where $J_n(z)$ and $K_n(z)$ are the regular and modified irregular (cylindrical) Bessel functions. There is no difficulty in dealing with the square root of $H+\Delta$, which appears in the argument of the regular Bessel function, since $H+\Delta$ is positive definite.

The integral representation of Eq. (5) can be used to calculate matrix elements of the form

$$M(E)=\langle\psi'|P_{\text{open}}G(E)|\psi\rangle,$$

where $|\psi\rangle$ and $|\psi'\rangle$ are normalizable kets and where P_{open} projects onto open channels. The branch of $M(E)$ is specified by the phase ϕ; the branch cuts lie along the lines $\arg(E-E_\nu)=-\phi$, where E_ν is the position of any continuum threshold. However, once H is approximated by a Hermitian matrix the integral over y does not formally converge. Consequently, the upper (infinite) limit of the integral must be replaced by a finite value Y, and the limit $Y\to\infty$ taken after the integration over y has been performed. To this end, and in the spirit of the R-matrix method [4], we break the resolvent into two parts:

$$G(E)=G_{\text{int}}(E)+G_{\text{ext}}(E), \tag{6}$$

where $G_{\text{int}}(E)$ is the integral on the right side of Eq. (5) but with the upper limit replaced by a fixed value

$$G_{\text{int}}(E)=-t_\phi\int_0^Y dy\, yK_0(ye^{i(\phi-\pi)/2})J_0[y\sqrt{t_\phi(H+\Delta)}]. \tag{7}$$

Our intention is to approximate H, in the integrand of $G_{\text{int}}(E)$, by a Hermitian matrix H constructed on a real discrete basis which is sufficiently large that its characteristic spatial range R extends over the interior region where the dynamics take place. The boundary value Y is related to R (see below). The remaining integral over the region $y>Y$ is $G_{\text{ext}}(E)$, and this term accounts for the flux in open channels which passes from the interior region to the exterior region. We show below that it is unnecessary to explicitly perform the integration over $y>Y$; by means of a simple connection between $G_{\text{ext}}(E)$ and $G_{\text{int}}(E)$ we can replace $P_{\text{open}}G_{\text{ext}}(E)$ by a Padé approximant [5]. Potentially, both $G_{\text{int}}(E)$ and the open-channel components of $G_{\text{ext}}(E)$ can be computed with moderate cost—most of the computation involves matrix-vector multiplications, which are ideally suited to parallel processing.

We can estimate a suitable value of Y as follows: The variable of integration y is the square root of a dimensionless time, i.e., $y=\sqrt{t/t_0}$. Let μ be the mass of a fragment which is released in the channel whose threshold energy is E_ν. The asymptotic momentum of this fragment is k where $E=E_\nu+k^2/(2\mu)$. If δE is the spacing of the energy eigenvalues of H in the neighborhood of E [6], we have $\delta E=k\,\delta k/\mu$, and the spatial range of the basis is, effectively, $R=1/\delta k$. The time that it takes for the fragment to travel a distance R is roughly $R\mu/k$, which is just $1/\delta E$. Since this time must be larger than t_0, we require that the parameter

$$Y_0\equiv\sqrt{(E+\Delta)/\delta E} \tag{8}$$

be greater than unity. Furthermore, since a fragment must reach the exterior region before it travels the full distance R we require Y to be somewhat less than Y_0. Therefore, we want the inequality

$$1<Y<Y_0 \tag{9}$$

to be satisfied.

In the next section we describe some of the technical details of the method. In Sec. III we present some test results based on two applications (i) photoionization of a hydrogen atom and (ii) s-wave scattering of a particle from a $1/(1+r)^4$ potential. Section IV contains some final remarks. In the Appendix we establish the connection between the series and integral representations of $G(E)$, i.e., Eqs. (3) and (5), which partially justifies the nonrigorous analysis of the next section.

II. TECHNICAL DETAILS

To formulate Eq. (6) we begin with

$$(\alpha^2+\beta^2)\int_0^Y dy\, yK_0(\alpha y)J_0(\beta y) =1+Y[\beta K_0(\alpha Y)J_1(\beta Y)-\alpha K_1(\alpha Y)J_0(\beta Y)]. \tag{10}$$

This formula can be derived from the differential equations that are satisfied by the Bessel functions, i.e.,

$$\left(\frac{d^2}{dy^2}+\frac{1}{y}\frac{d}{dy}+\beta^2\right)J_0(\beta y)=0, \tag{11}$$

$$\left(\frac{d^2}{dy^2}+\frac{1}{y}\frac{d}{dy}-\alpha^2\right)K_0(\alpha y)=0. \tag{12}$$

Premultiplying the left sides of Eqs. (11) and (12) by $K_0(\alpha y)$ and $J_0(\beta y)$, respectively, subtracting the resulting equations, and integrating over y from 0 to Y gives Eq. (10). Putting aside any notion of rigor, we now set $\alpha=-ie^{i\phi}$ and $\beta=\sqrt{t_\phi(H+\Delta)}$ in Eq. (10). This yields

$$-(E-H)t_\phi\int_0^Y dy\, yK_0(ye^{i(\phi-\pi)/2})J_0[y\sqrt{t_\phi(H+\Delta)}] = 1+X, \tag{13}$$

where X is the operator

$$X=Y[\sqrt{t_\phi(H+\Delta)}J_1[Y\sqrt{t_\phi(H+\Delta)}]K_0(Ye^{i(\phi-\pi)/2}) - e^{i(\phi-\pi)/2}K_1(Ye^{i(\phi-\pi)/2})J_0[Y\sqrt{t_\phi(H+\Delta)}]]. \tag{14}$$

It follows from Eqs. (6), (7), and (13) that

$$G_{\rm ext}(E)=-\left(\frac{X}{1+X}\right)G_{\rm int}(E). \tag{15}$$

It suffices to restrict ϕ to the range $0\leqslant\phi<2\pi$.

We now discuss the evaluation of $G_{\rm int}(E)$. Substituting the expansion

$$J_0(z)=\sum_{m=0}^{\infty}(-1)^m\frac{\left(\frac{1}{2}z\right)^{2m}}{(m!)^2} \tag{16}$$

into Eq. (7), and introducing the finite integrals

$$a_m(Y)=\int_0^Y dy\, y^{2m+1}K_0(ye^{i(\phi-\pi)/2}), \tag{17}$$

we obtain

$$G_{\rm int}(E)=-t_\phi\sum_{m=0}^{\infty}(-1)^m\frac{a_m(Y)}{(m!)^2}\left(\frac{t_\phi(H+\Delta)}{4}\right)^m. \tag{18}$$

Provided that Y is not too large the series on the right side of Eq. (18) should converge rapidly. The coefficients $a_m(Y)$ may be readily evaluated [7] and are universal, i.e., they are independent of both E and H. The main part of the computational labor is the evaluation of powers of $(H+\Delta)$, and this is also independent of E. Furthermore, since it is the action of $G(E)$ on a ket, rather than $G(E)$ itself, that is required, and since H is to be replaced by a matrix, most of the labor involves matrix-vector multiplications. Those eigenvectors of $\underline{S}^{-1}\underline{H}$ with the largest few eigenvalues normally play only a minor role, and their omission leads to a substantial enhancement in the rapidity of convergence of the sum on the right side of Eq. (18). Fortunately, the eigenvectors with the largest eigenvalues can be determined easily, using for example, the ''power'' method [8].

Turning to the evaluation of $P_{\rm open}G_{\rm ext}(E)$, note that the operator X, defined by Eq. (14), contains the numerical factors $K_n(Ye^{i(\phi-\pi)/2})$, $n=0,1$, and that since $K_n(z)$ behaves for large z as $\sqrt{(\pi/2z)}e^{-z}$ these factors decrease exponentially, as $e^{-Y\sin(\phi/2)}$ as Y increases. In contrast, since $J_n(z)$ behaves for large z as $\sqrt{(2/\pi z)}\cos(z-\frac{1}{2}n\pi-\frac{1}{4}\pi)$, the operators

$$J_n[Y\sqrt{t_\phi(H+\Delta)}]$$

would be unbounded as Y increases if H were approximated by a Hermitian matrix. However, since the resolvent satisfies complex outgoing-wave boundary conditions in the exterior region, it is appropriate to approximate H in the integrand of $G_{\rm ext}(E)$ by a non-Hermitian matrix H_θ that is constructed from complex basis functions that oscillate with distance r as $e^{i\kappa r}$ where κ, the basis wave number, is $|\kappa|e^{i(\pi/2)-i\theta}$ with $0<\theta<\pi/2$. Therefore we temporarily replace H by $\underline{H}_\theta$; ultimately we let θ vanish, so that in the final step we approximate H by the Hermitian matrix H. As is well known [9], the bound-state eigenvalues of H_θ are, very nearly, real and the continuum eigenvalues lie, approximately, along the lines $\arg(H-E_\nu)=-2\theta$. Writing $t_0(H+\Delta)=A+B$ where

$$A=\frac{H-E_\nu}{E+\Delta}, \tag{19}$$

$$B=\frac{E_\nu+\Delta}{E+\Delta}, \tag{20}$$

we have, approximately, that $A=|A|e^{-i2\theta}$ and that B is real and positive. Let us temporarily put $\theta=\phi/2$. It follows that

$$\arg[e^{i\phi}(A+B)]\leqslant\phi, \tag{21}$$

where the equality obtains only if $A=0$. Noting that $B<1$ if $E>E_\nu$, we conclude that $J_n[Y\sqrt{e^{i\phi}(A+B)}]$ increases less rapidly than $e^{Y\sin(\phi/2)}$ if $E>E_\nu$, i.e., if channel ν is open. Consequently, $P_{\rm open}X$ is exponentially small for large Y and, provided that neither Y nor ϕ are too small, the series

$$P_{\rm open}\left(\frac{X}{1+X}\right)=-P_{\rm open}\sum_{m=1}^{\infty}(-X)^m \tag{22}$$

should converge rapidly. Hence $P_{\rm open}G_{\rm ext}(E)$ can be computed by repeated multiplication of $G_{\rm int}(E)$ by X followed by multiplication by $P_{\rm open}$. We now remove the constraint $\theta=\phi/2$, and we analytically continue $P_{\rm open}G_{\rm ext}(E)$ in θ to $\theta=0$. In order to do this we replace the (truncated) power series in X, i.e., the right side of Eq. (22), by a Padé approximant, which yields a convergent expression even when $\theta=0$.

To evaluate X it is necessary to evaluate $J_n[Y\sqrt{e^{i\phi}(A+B)}]$, and to this end the Bessel function expansion, Eq. (16), can be used again after eliminating the closed channels. The operator $P_{\rm open}$ is understood to project onto *asymptotic* channels, wherein the different fragments of the system are well separated. A one- or two-particle system has only one channel, and assuming it is open $P_{\rm open}$ is the identity operator. We briefly consider the construction of $P_{\rm open}$ for a three-particle system in Sec. IV.

We conclude this section by considering the analogous expressions for $G_{\rm int}(E)$ and $G_{\rm ext}(E)$ that we would have obtained were we to have used the integral representation of

Eq. (1) rather than Eq. (5). Let us rotate the contour of integration through the angle ϕ on the right side of Eq. (1), replace the upper limit of the integral over τ by $Y^2e^{i\phi}$, add Δ to both E and H in the exponent, expand $e^{-it_0(H+\Delta)\tau}$ as a power series in τ, and integrate term by term. In place of Eq. (18) we obtain

$$G_{\rm int}(E)=-t_\phi\sum_{m=0}^{\infty}(-1)^m\frac{b_m(Y)}{m!}\left(\frac{t_\phi(H+\Delta)}{4}\right)^m, \quad (23)$$

where

$$b_m(Y)=i(4i)^m\int_0^{Y^2}d\tau\,\tau^m\exp(i\tau e^{i\phi}). \quad (24)$$

If $Y\sin\phi\gg1$ the expansions of Eqs. (18) and (23) are the same since $a_m(\infty)=m!b_m(\infty)$. However, if $Y\sin\phi$ is less than, or of the order of, unity the expansion of Eq. (18) converges far more rapidly owing to the additional factor of $m!$ in the denominator of the summand. Using the integral representation of Eq. (1) we obtain a relation between $G_{\rm int}(E)$ and $G_{\rm ext}(E)$ that is similar to Eq. (15), but with X replaced by

$$X=\exp(iY^2e^{i\phi})\exp[-it_0(H+\Delta)Y^2e^{i\phi}]. \quad (25)$$

The second exponential factor on the right side of Eq. (25) oscillates rapidly as Y varies; the shortest period of oscillation is roughly

$$\pi/[t_0(E_{\rm max}+\Delta)Y\cos\phi],$$

where $E_{\rm max}$ is the largest eigenvalue of H. Putting $Y\approx Y_0$ and using Eqs. (2) and (8) we can rewrite this period as, roughly,

$$\frac{\pi}{\cos\phi}\sqrt{\frac{\delta E}{E_{\rm max}+\Delta}}\sqrt{\frac{E+\Delta}{E_{\rm max}+\Delta}}.$$

In contrast, the regular Bessel functions on the right side of Eq. (14) oscillates with a shortest period that is roughly

$$\frac{2\pi}{\sqrt{\cos\phi}}\sqrt{\frac{E+\Delta}{E_{\rm max}+\Delta}}.$$

Since $\delta E/(E_{\rm max}+\Delta)\ll1$ the oscillation of X as Y varies is more rapid, and therefore potentially more troublesome, in Eq. (25) compared to Eq. (14).

III. APPLICATION AND RESULTS

The inclusive rate at which a continuous stationary or quasistationary process occurs, if $\mathcal{E}$ is the real positive energy of the system, is $-2\,{\rm Im}\,R(\mathcal{E}_+)$ where $\mathcal{E}_\pm=\mathcal{E}\pm i\eta$, where η is positive but infinitesimal, and where $R(E)$ is a Green function matrix element of the form

$$R(E)\equiv\langle\psi|G(E)|\psi\rangle. \quad (26)$$

To illustrate the effectiveness of the method described above, we have performed calculations of $R(\mathcal{E}_+)$ for two examples. Our first example is a hydrogen atom which is initially in the unperturbed ground state, represented by $|\psi_0\rangle$, and which ionizes after absorbing one photon of frequency ω. The rate for the atom to decay is obtained by putting $|\psi\rangle=V_+|\psi_0\rangle$ in Eq. (26), where V_+ is the one-photon absorption operator in the length gauge. Our second example is a particle which is incident from afar, initially in a plane-wave state represented by $|\psi_0\rangle$, and which scatters from a repulsive potential $W=1/(1+r)^4$ a.u. The scattering rate is obtained by putting $|\psi\rangle=W|\psi_0\rangle$ in Eq. (26). We represented $|\psi\rangle$ and $|\psi_0\rangle$ on a real basis composed of the functions

$$\sqrt{-2i\kappa}(2i\kappa r)^{l+1}e^{i\kappa r}L_n(2i\kappa r)Y_{lm}(\hat{\mathbf{x}}),$$

where $Y_{lm}(\hat{\mathbf{x}})$ is a spherical harmonic and where $L_n(x)$ is an ordinary Laguerre polynomial of degree n, with $\kappa=i|\kappa|$.

Results are shown in Table I for the cross section (rate per unit intensity of incident flux) for one-photon ionization of a hydrogen atom over a range of frequencies extending from just above threshold to 1 a.u. above threshold. We chose Δ to be 0.5 a.u.—the binding energy of the hydrogen atom. The calculations were repeated for various values of the phase ϕ and for four or five basis sizes. While we made no attempt to choose the optimal value of the basis wave number κ we did increase $|\kappa|$ with increasing frequency ω of the light; the positive energy eigenvalues of $S^{-1}H$ extend to a characteristic value of $|\kappa|^2/2$, and so $|\kappa|$ should be increased as the photoelectron energy E increases. Unfortunately, no advantage is accrued from the explicit E independence of the most demanding part of the calculation of $G_{\rm int}(E)$—the computation of powers $(H+\Delta)$—once the basis, and hence H, changes with E. We deleted either one or two eigenvectors of H, those with the largest eigenvalues—which, as noted above, improves the convergence of the expansion of $G_{\rm int}(E)$; the typical number of powers of $(H+\Delta)$ that must be included in this expansion is about 30. The Padé approximant for $G_{\rm ext}(E)$ was constructed from the first 50 terms (typically) in the expansion of $X/(1+X)$ in powers of X using the epsilon algorithm [10]. We increased Y from 1.0 in steps of 0.5, and ϕ from 0° in steps of 5°, and selected those values of Y (always less than Y_0) and ϕ for which the Padé approximant was best converged.

In the seventh column of Table I we show the contribution $\sigma_{\rm int}$ to the cross section from just $G_{\rm int}(E)$, ignoring $G_{\rm ext}(E)$. Our estimates of the full cross section σ with $G_{\rm ext}(E)$ included, are shown in the eighth column, and the exact results are shown in the last column [11]. Evidently the correction due to $G_{\rm ext}(E)$ is significant, particularly at higher frequencies; yet the estimates of σ obtained using the largest basis have converged to at least five places of accuracy, or almost five when $\omega=0.51$ a.u. Note that $Y_0>1$ for all basis sets, as desired, and although the inequality of Eq. (9) was intended only as a guide it is in fact always satisfied [12]. Note too that, in general, the best value of Y decreases more often than not as the basis size increases, and the best value of ϕ tends to be quite large for $n_{\rm bas}=20$, but decreases rapidly as the basis size increases.

TABLE I. Cross section σ for ionization of a hydrogen atom by a photon of frequency ω. A real basis of size $n_{\rm bas}$, and with wave number $i|\kappa|$ was used. The energy shift Δ was fixed to be 0.5 a.u., while the phase ϕ was varied. The temporal region was divided into two parts (see text) $0 \leqslant y < Y$ and $y > Y$, and a Padé approximant was used for $y > Y$. The contribution to the cross section from the region $y < Y$ is $\sigma_{\rm int}$, whereas σ also includes the contribution from the region $y > Y$. The exact cross sections are shown in the last column.

ω (a.u.)	$n_{\rm bas}$	$\lvert\kappa\rvert$ (a.u.)	Y_0	Y	ϕ (deg)	$\sigma_{\rm int}$ (Mb)	σ (Mb)	$\sigma_{\rm exact}$ (Mb)
0.51	20	0.4	8.9	5.0	30	5.43	5.83	5.97972805
0.51	30	0.4	12.1	3.0	10	3.47	6.034	5.97972805
0.51	40	0.4	16.4	6.0	0	6.68	5.9759	5.97972805
0.51	50	0.4	13.6	5.5	0	6.72	5.97943	5.97972805
0.70	20	0.5	4.4	3.5	40	3.41	2.5394	2.53123550
0.70	30	0.5	5.4	4.5	5	5.21	2.5275	2.53123550
0.70	40	0.5	6.2	4.0	5	4.44	2.53146	2.53123550
0.70	50	0.5	5.5	2.5	5	3.55	2.531203	2.53123550
1.10	20	1.7	2.5	2.0	20	3.15	0.7124	0.70932895
1.10	30	1.7	3.4	2.0	5	3.69	0.70953	0.70932895
1.10	40	1.7	4.7	1.5	0	3.01	0.7093233	0.70932895
1.50	20	2.0	3.1	2.5	10	3.78	0.2876	0.28839435
1.50	30	2.0	3.8	2.0	0	4.09	0.28852	0.28839435
1.50	40	2.0	4.3	1.5	0	3.10	0.2883953	0.28839435

We now consider s-wave scattering from a $1/(1+r)^4$ potential [13]. This potential is repulsive and therefore supports no bound states. In fact, even the attractive potential $-1/(1+r)^4$ does not support bound states. Hence we set Δ, which is one measure of the strength of the potential, to zero. Scattering from a $1/(1+r)^4$ potential was studied earlier by Rescigno *et al.* [14] using a generalization of the exterior complex scaling procedure [15]. They also used a real basis, similar to the one we used here but with the ordinary Laguerre polynomial $L_n(x)$ replaced by the associated Laguerre polynomial $L_n^{(2)}(x)$. However, in their study the potential was truncated at a finite distance. Some of their results [16], obtained using 10, 20, and 30 basis functions, with the potential truncated at $r=35$ a.u., are shown in the eighth column of Table II, labeled RBBM; their results obtained using 100 basis functions are shown in the last column, labeled RBBM/100. Our results are shown in the sixth and seventh columns, and were obtained in a similar fashion to those shown in Table I except that the Padé approximant for $G_{\rm ext}(E)$ was constructed from the first 30 terms (typically) in the power series in X and ϕ was increased from 0° in steps of 10°. Our estimates of σ obtained with a basis size of 30 have converged to four places at the two highest values of the momentum, i.e., $p=0.35$ and $p=0.55$ a.u., but have converged perhaps to only three places at $p=0.15$ a.u. At $p=0.15$ roundoff error became uncontrollable when we increased the basis size beyond 30. Nevertheless, the discrepancy in the fourth figure between our results obtained with a basis size of 30 and the RBBM/100 results at $p=0.15$ a.u. might be due to the truncation of the potential in the RBBM method; the error in truncation is likely to be more serious at smaller p, and indeed the discrepancy at $p=0.15$ a.u. be-

TABLE II. Cross section in a.u. for s-wave scattering from the potential $1/(1+r)^4$ a.u. by a particle of mass 1 a.u. incident with momentum p. The notation is the same as in Table I. The energy shift Δ was set to zero. In the ninth column we show results (RBBM) taken from Ref. [14]; these results were obtained using 10, 20, or 30 basis functions in conjunction with an exterior complex scaling technique, and with the potential truncated at $r=35$ a.u. In the last column we show results (RBBM/100) obtained using the same technique but with 100 basis functions.

p (a.u.)	$n_{\rm bas}$	$\lvert\kappa\rvert$ (a.u.)	Y_0	Y	ϕ (deg)	$\sigma_{\rm int}$	σ	RBBM	RBBM/100
0.15	10	0.2	1.5	1.00	70	6.19	1.76	0.07	2.0777
0.15	20	0.3	2.1	1.00	0	3.09	2.109	2.70	2.0777
0.15	30	0.3	2.6	1.00	0	2.76	2.0814	2.104	2.0777
0.35	10	0.6	1.8	1.50	40	2.07	1.098	2×10^{-5}	1.0308
0.35	20	0.7	2.1	1.00	0	1.12	1.006	1.02	1.0308
0.35	30	0.7	2.6	1.00	0	1.11	1.0315	1.026	1.0308
0.55	10	1.1	1.6	1.50	50	1.01	0.621	5×10^{-6}	0.58248
0.55	20	0.8	2.6	1.00	50	0.522	0.575	0.726	0.58248
0.55	30	0.8	3.1	1.50	0	0.546	0.58253	0.5445	0.58248

tween the RBBM/100 results obtained by truncating the potential at 25 and 35 a.u appears in the third figure.

IV. FINAL REMARKS

We have described a method for calculating full- and half-collision rates by representing the resolvent on a real discrete basis without concern for the asymptotic boundary conditions. While we have demonstrated the effectiveness of this method for one-particle systems, it remains to be seen whether it can be usefully applied to more complicated systems. When the system contains three or more particles, and one or more channels is closed, the projection operator P_{open} must be invoked. We conclude this paper with a brief outline of a technique for constructing and employing P_{open} in the case where the system contains two electrons and a nucleus, e.g., a helium atom. This technique is independent of the coordinate system; independent-particle coordinates would allow a much simpler construction of the projection operator, but are unsuitable for accurately accounting for correlation.

Let us label the electrons by the numbers 1 and 2. We regard the nucleus, whose atomic number is Z, as infinitely heavy and at rest. Consider the group of channels in which, asymptotically, one of the electrons, say electron 2, is free while the other electron, i.e., electron 1, remains *bound* in a state of the residual one-electron system whose energy is less than some real negative cutoff value E_c. Let $P_1(E_c)$ be the operator which projects onto this subspace. Introducing the null operator 0_2 for electron 2, the two electrons inhabit the subspace spanned by those eigenvectors of the nonsymmetric Hamiltonian

$$H_1 \equiv -\frac{1}{2}\nabla_1^2 - \frac{Z}{r_1} + 0_2 \tag{27}$$

that have eigenvalues less than E_c. The exact eigenvalue spectrum of H_1 is the spectrum of a hydrogenlike ion with atomic number Z, with one difference: the spectrum of H_1 is infinitely degenerate owing to the inclusion of 0_2, whose eigenvalues are all zero. The operator $P_1(E_c)$ projects onto the subspace spanned by those eigenvectors of H_1 with eigenvalues less than E_c, and can be expressed as

$$P_1(E_c) = \frac{1}{2\pi i}\oint_{\mathcal{C}} dE\, G_1(E), \tag{28}$$

where $G_1(E) = (E - H_1)^{-1}$ and where $\mathcal{C}$ is any counterclockwise contour which encloses those poles of $G_1(E)$ that correspond to the bound states of the residual one-electron system with energy eigenvalues less than E_c. (The contour $\mathcal{C}$ must exclude the other bound-state poles as well as the cut along the positive real energy axis.) Equation (28) can be verified by expressing $G_1(E)$ in terms of its spectral decomposition and performing the integration over E using Cauchy's residue theorem. It is convenient to choose $\mathcal{C}$ to be the boundary of the closed sector $\pi - \beta \leqslant |\arg(E - E_c)| \leqslant \pi$, where β is a fixed angle in the range $0 < \beta < \pi$; thus $\mathcal{C}$ consists of the two straight lines $E = E_c + s e^{\pm i(\pi - \beta)}$, where $0 \leqslant s < \infty$, joined at infinity by an arc. The integration over the infinite arc can be performed immediately to give

$$P_1(E_c) = \frac{\beta}{\pi} - \frac{1}{2\pi i}\int_0^\infty ds [e^{-i\beta} G_1(E_c - e^{-i\beta}s) - e^{i\beta} G_1(E_c - e^{i\beta}s)]. \tag{29}$$

We will not pursue the evaluation of this integral here as this will be taken up elsewhere [17]; suffice it to say that we have found the most suitable value of β to be $\pi/2$.

To calculate the rate $\Gamma(E, E_c)$ for a continuous stationary or quasistationary process in which one electron remains bound with an energy less than E_c, while the other electron is liberated, we cannot simply insert $P_1(E_c)$ into the matrix element for $R(E)$ on the right side of Eq. (26) since $P_1(E_c)$ projects onto a subspace spanned by eigenvectors of H_1, not H. Rather, we can use the different expression [18]

$$\Gamma(E, E_c) = -4\,\mathrm{Im}\langle \psi | P_1(E_c) G(E) | \psi \rangle - 2\langle \psi | G^\dagger(E)[P_1(E_c), iW_{12}] G(E) | \psi \rangle, \tag{30}$$

where W_{12} is the interaction between electrons and $[P_1(E_c), W_{12}]$ is the commutator of the projection operator with this interaction. The second term on the right side of Eq. (30) accounts for final-state correlation (the inclusion of i in the commutator ensures it is Hermitian). The commutator falls off with increasing distance of the free electron at least as fast as an inverse square in open channels.

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APPENDIX: CONNECTION OF SERIES AND INTEGRAL REPRESENTATIONS

The series representation of the resolvent, Eq. (3), can be written compactly as

$$G(E) = t_\phi e^{-b}\left(\frac{1}{a} + 2ib\mathcal{S}(a,b)\right), \tag{A1}$$

where $b = t_\phi H$, $a = t_\phi E$, and

$$\mathcal{S}(a,b) \equiv \sum_{n=1}^{\infty} \mathcal{I}_n(a)\frac{L_{n-1}^{(1)}(2b)}{n}. \tag{A2}$$

In this appendix we show that the integral representation of $G(E)$, i.e., Eq. (5), can be obtained by resumming the series representation.

We make use of the following integral representation [19] of $L_n^{(1)}(2b)$:

$$L_n^{(1)}(2b) = \frac{2e^{2b}}{n!\sqrt{2b}}\int_0^\infty dy\, e^{-y^2} y^{2n+2} J_1(y\sqrt{8b}). \tag{A3}$$

Writing $\xi=(\tau+i)/(\tau-i)$, we first reexpress the series form of $\mathcal{S}(a,b)$ as

$$\mathcal{S}(a,b)=\int_0^\infty d\tau\, e^{ia\tau}\sum_{n=1}^{\infty}\xi^n\frac{L_{n-1}^{(1)}(2b)}{n} \tag{A4}$$

$$=2\frac{e^{2b}}{\sqrt{2b}}\int_0^\infty d\tau\, e^{ia\tau}\int_0^\infty dy\, e^{-y^2}J_1(y\sqrt{8b})\sum_{n=1}^{\infty}\xi^n\frac{y^{2n}}{n!} \tag{A5}$$

$$=2\frac{e^{2b}}{\sqrt{2b}}\int_0^\infty d\tau\, e^{ia\tau}\int_0^\infty dy\, e^{-y^2}J_1(y\sqrt{8b})(e^{\xi y^2}-1). \tag{A6}$$

Incidentally, this last equation can be used to quickly verify Eq. (A1); using [19]

$$\int_0^\infty dy\, e^{-qy^2}J_1(y\sqrt{8b})=\frac{1}{2\sqrt{2b}}(1-e^{-2b/q}), \tag{A7}$$

Eq. (A6) becomes

$$\mathcal{S}(a,b)=\frac{1}{2b}\int_0^\infty d\tau\, e^{ia\tau}(1-e^{(1-i\tau)b}) \tag{A8}$$

$$=-i\frac{e^b}{2b}\left[\frac{1}{a-b}-\frac{e^{-b}}{a}\right], \tag{A9}$$

and substituting this last expression for $\mathcal{S}(a,b)$ into the right side of Eq. (A1) we confirm Eq. (A1).

To proceed with the derivation of the integral representation we return to Eq. (A6). We put $\xi=1+2i/(\tau-i)$, write

$$\int_0^\infty d\tau\, e^{ia\tau}(e^{\xi y^2}-1)=-\frac{i}{a}+e^{y^2}\int_0^\infty d\tau\, e^{ia\tau}e^{2iy^2/(\tau-i)}, \tag{A10}$$

transform from τ to $\tau+i$, divide the integral on the right side of Eq. (A10) into two integrals, one over the interval $[-i,0]$, the other over $[0,\infty]$, and use, for Re $p>0$ and Re $q\geqslant 0$,

$$\int_0^\infty d\tau\, e^{-p\tau-q/(4\tau)}=\sqrt{\frac{q}{p}}K_1(\sqrt{pq}), \tag{A11}$$

to give

$$\int_0^\infty d\tau\, e^{ia\tau}(e^{\xi y^2}-1)=-\frac{i}{a}+e^{y^2-a}\left[y\sqrt{\frac{8}{a}}K_1(y\sqrt{e^{-i\pi}8a})+\int_{-i}^0 d\tau\, e^{ia\tau}e^{2iy^2/\tau}\right]. \tag{A12}$$

Hence, from Eqs. (A6) and (A12) we have

$$\mathcal{S}(a,b)=2\frac{e^{2b}}{\sqrt{2b}}\int_0^\infty dy\, J_1(y\sqrt{8b})\times\left(-\frac{i}{a}e^{-y^2}+e^{-a}\int_{-i}^0 d\tau\, e^{ia\tau}e^{2iy^2/\tau}+\sqrt{\frac{8}{a}}e^{-a}yK_1(y\sqrt{e^{-i\pi}8a})\right). \tag{A13}$$

We now use

$$\frac{d}{dx}K_0(x)=-K_1(x), \tag{A14}$$

and

$$\frac{d}{dx}[xJ_1(x)]=xJ_0(x), \tag{A15}$$

and we integrate by parts as follows:

$$\int_0^\infty dy\, yK_1(\alpha y)J_1(\beta y)=-\frac{1}{\alpha}\int_0^\infty dy\, y\left(\frac{d}{dy}K_0(\alpha y)\right)J_1(\beta y) \tag{A16}$$

$$=\frac{\beta}{\alpha}\int_0^\infty dy\, yK_0(\alpha y)J_0(\beta y). \tag{A17}$$

Thereby we obtain

$$\mathcal{S}(a,b)=4i\frac{e^{2b-a}}{a}\int_0^\infty dy\, yK_0(y\sqrt{e^{-i\pi}8a})J_0(y\sqrt{8b})+2\frac{e^{2b}}{\sqrt{2b}}\int_0^\infty dy\, J_1(y\sqrt{8b})\times\left(-\frac{i}{a}e^{-y^2}+e^{-a}\int_{-i}^0 d\tau\, e^{ia\tau}e^{2iy^2/\tau}\right). \tag{A18}$$

Using Eq. (A7) to perform the integration over y in the second term on the right side of Eq. (A18) (after interchanging the order of the integrals over y and τ), we obtain (after performing the integration over τ)

$$\mathcal{S}(a,b)=4i\frac{e^{2b-a}}{a}\int_0^\infty dy\, yK_0(y\sqrt{e^{-i\pi}8a})J_0(y\sqrt{8b})+\frac{e^{2b}}{2ib}\left(\frac{e^{-a}-e^{-2b}}{a}+\frac{e^{-b}-e^{-a}}{a-b}\right). \tag{A19}$$

Substituting the right side of Eq. (A19) for $\mathcal{S}(a,b)$ into Eq. (A1) we arrive at Eq. (5) provided that $\Delta=0$; to incorporate a nonvanishing value of Δ we simply perform the simultaneous transformations $E\to E+\Delta$ and $H\to H+\Delta$, which leave $G(E)$ unchanged.

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[6] We define δE as the average of the separation from E of the two eigenvalues of H that are closest to E; those eigenvalues can be determined by, for example, inverse iteration [8].

[7] The following infinte series converges rapidly for typical values of Y:

$$a_m(Y)=\sum_{n=0}^{\infty}\frac{\zeta^n}{(n!)^2(2n+m+2)}\left(c_n+\frac{1}{2n+m+2}-\frac{1}{2}\ln\zeta Y^2\right)Y^{2n+m+2},$$

where $\zeta=e^{i(\phi-\pi)}/4$ and $c_n=c_{n-1}+(1/n)$, $n\geqslant 1$, with $-c_0$ equal to Euler's constant.

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$$\left(\frac{2^5\pi^2Z^6}{3c\omega^4}\right)\frac{e^{-4\gamma}\tan^{-1}(1/\gamma)}{1-e^{-2\pi\gamma}}.$$

[12] In the case where the system is complex it may not be worthwhile to calculate Y_0 due to the cost incurred in calculating δE.

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$$1/(1+r)^4=(1/6)\int_0^{\infty}ds\,s^3e^{-s}e^{-sr}.$$

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