L^2 discretizations of the continuum: Radial kinetic energy and Coulomb Hamiltonian

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The relationship between the matrix eigenvalues of the L^2 discretization of an operator with a continuous spectrum and Gaussian quadrature is discussed for the radial kinetic energy and for the attractive and repulsive Coulomb Hamiltonians. It is shown that discretization of the radial kinetic energy in a Laguerre- (Slater-) type basis gives a Gegenbauer quadrature, while discretization in an oscillator- (Gaussian-) type basis generates a Laguerre quadrature. Laguerre discretization of the Coulomb problem gives a Pollaczek quadrature in the repulsive case, and a new modified Pollaczek quadrature in the attractive case. The utility of these results is shown in applications to potential scattering and photoionization. Two numerical techniques for obtaining "equivalent quadrature" weights are discussed: a matrix method due to Gordon, and a very simple interpolatory method due to Heller.

I. INTRODUCTION

A matrix element of the form $\langle f|(z-H^0)^{-1}|f\rangle$, H^0 being the radial kinetic energy, will be analytic except for a branch cut, corresponding to the continuous spectrum of H^0, provided that the function f is sufficiently well behaved. We have previously shown[1,2] for the s-wave radial kinetic energy that construction of a matrix representation, $\bar{H}^0$, of H^0 in a finite set of square-integrable (L^2) functions of the form $re^{-\lambda r/2}L_n^1(\lambda r)$ gives a representation $\langle f|(z-\bar{H}^0)^{-1}|f\rangle$ which can be interpreted as a Gauss-Chebyschev quadrature representation of the actual matrix element. That is, the matrix eigenvalues of $\bar{H}^0$ can be interpreted as Chebyschev quadrature abscissas, and the difference in normalization between the L^2 eigenfunctions of H^0 and the continuum-normalized eigenfunctions of H^0 itself can be shown to be related to the corresponding Chebyschev quadrature weights. This realization allows the approximate matrix element, $\langle f|(z-\bar{H}^0)^{-1}|f\rangle$, which has discrete poles and residues, to be embedded[2,3] into an approximation which retains the cut structure of the actual matrix element. Thus, for example, $(z-\bar{H}^0)^{-1}$ may be used in the $z\to E+i\epsilon$ limit as part of the kernel of the s-wave Lippmann-Schwinger equation, allowing straightforward extraction of scattering information from calculations performed in an L^2 basis.[2] We refer to the quadrature generated by this L^2 discretization of H^0 as the "equivalent quadrature" generated by the basis.

It is the purpose of this paper to generalize this result to the interpretation of $(z-\bar{H}^0)^{-1}$ in the following cases:

$$H^0=H_l^0=-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r}, \tag{1.1}$$

where the basis used to define $\bar{H}_l^0$ is taken to be either a Laguerre-type (Slater) or oscillator-type (Gaussian) basis. In the second case

$$H^0=H_{l,\pm|Z|}^0=-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}\pm\frac{|Z|}{r} \tag{1.2}$$

and the basis is the Laguerre-type basis. That is, we generalize the techniques of Refs. 1 and 2 to higher partial waves and to the treatment of Coulomb interactions.

The plan of the paper is as follows. The idea of an equivalent quadrature is briefly reviewed in Sec. II, followed by discussion of the L^2 discretization of the radial kinetic energy in a Laguerre basis (Sec. III) and in an oscillator basis (Appendix A), where it is shown that the discretizations give rise to Gegenbauer and Laguerre quadratures, respectively. Applications to partial-wave potential scattering are given in Sec. III D. The Laguerre discretization of the Coulomb problem is treated in Sec. IV and shown to give rise to a Pollaczek quadrature (Appendix B) in the repulsive case, and a modified Pollaczek quadrature in the attractive case. Numerical results for Coulomb scattering and photoionization are given in Secs. IV B, IV D, and IV E. Section V contains discussions of two convenient numerical methods for construction of equivalent quadrature weights.

II. IDEA OF AN EQUIVALENT QUADRATURE

As disucssed in Ref. 1, for the case $H^0=-\frac{1}{2}d^2/dr^2$ matrix elements of the form $\langle f|(z-H^0)^{-1}|f\rangle$ can be well approximated by the discrete repre-

sentation $\langle f|(z-\bar{H}^0)^{-1}|f\rangle$, $\bar{H}^0$ being the matrix representation of H^0 in a finite L^2 basis set, provided that the function f is sufficiently well behaved. This is because $\langle f|(z-\bar{H}^0)^{-1}|f\rangle$ can be interpreted as a quadrature approximation to $\langle f|(z-H^0)^{-1}|f\rangle$, the particular quadrature depending on the choice of L^2 basis.

More specifically, we compare the spectral resolution

$$\langle f|(z-\bar{H}^0)^{-1}|f\rangle=\sum_{i=1}^{N}\frac{\langle f|\bar{\Psi}_{E_i^0}\rangle\langle\bar{\Psi}_{E_i^0}|f\rangle}{z-E_i^0}, \tag{2.1}$$

where

$$\bar{H}^0|\bar{\Psi}_{E_i^0}\rangle=E_i^0|\bar{\Psi}_{E_i^0}\rangle, \quad i=1,2,\ldots,N \tag{2.2}$$

and

$$\langle\bar{\Psi}_{E_i^0}|\bar{\Psi}_{E_j^0}\rangle=\delta_{ij}, \tag{2.3}$$

with the analogous expression

$$\langle f|(z-H^0)^{-1}|f\rangle=\int_0^\infty\frac{\langle f|\Psi_E\rangle\langle\Psi_E|f\rangle}{z-E}\,dE, \tag{2.4}$$

where

$$H^0|\Psi_{E^0}\rangle=E^0|\Psi_{E^0}\rangle \tag{2.5}$$

and

$$\langle\Psi_E|\Psi_{E'}\rangle=\delta(E-E'). \tag{2.6}$$

Provided that f is well approximated in the finite subspace which defines $\bar{H}^0$, we interpret Eq. (2.1) as a quadrature representation of Eq. (2.4) with abscissas E_i^0 and "equivalent quadrature" weights ω_i^{EQ} that is,

$$\sum_{i=1}^{N}\frac{|\langle f|\bar{\Psi}_{E_i^0}\rangle|^2}{z-E_i^0}\sum_{i=1}^{N}\frac{\omega_i^{\mathrm{EQ}}|\langle f|\Psi_{E_i^0}\rangle|^2}{z-E_i^0}. \tag{2.7}$$

Knowledge of the equivalent quadrature weights thus gives the difference in normalization between the δ-function-normalized eigenfunction of H^0 and the unit-normalized eigenfunctions of $\bar{H}^0$; from Eq. (2.7)

$$\frac{|\langle f|\bar{\Psi}_{E_i^0}\rangle|^2}{|\langle f|\Psi_{E_i^0}\rangle|^2}=\omega_i^{\mathrm{EQ}}, \tag{2.8}$$

which is an identity if f is exactly represented in the finite subspace. As discussed in Refs. 1–3, knowledge of the equivalent quadrature weights allows embedding of the approximation $\langle f|(z-\bar{H}^0)^{-1}|f\rangle$ into an interpolative approximation which retains the analytic structure of the actual matrix element $\langle f|(z-H^0)^{-1}|f\rangle$. This allows taking the $z\to E+i\epsilon$ limit, providing a useful technique for the solution of scattering problems.

The equivalent quadrature weights are most easily derived from explicit expansions of $|\bar{\Psi}_{E_i^0}\rangle$ and $|\Psi_{E_i^0}\rangle$ in the same L^2 basis. In Secs. III and IV we construct such expansions for the radial kinetic energy and Coulomb problems, and analyze the quadratures generated by discretization of these operators.

III. RADIAL KINETIC ENERGY: LAGUERRE BASIS

The radial kinetic energy

$$H_l^0=-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2} \tag{3.1}$$

can be analytically diagonalized in the (nonorthogonal) basis of L^2 Laguerre-type functions[4,5]

$$\phi_n(r)=\langle r|\,\phi_n\rangle=(\lambda r)^{l+1}e^{-\lambda r/2}L_n^{2l+1}(\lambda r), \quad n=0,1,2,\ldots,N-1 \tag{3.2}$$

both in the case where N is finite and when $N=\infty$. In the finite case $\bar{H}^0$ will have discrete eigenvalues and L^2 eigenfunctions; in the infinite case $\bar{H}^0$ will have a continuous spectrum and δ-function-normalized eigenfunctions. Comparison of the normalization in these two cases will yield the equivalent quadrature weights for the finite-dimensional case. The parallel analysis of the discretization of the radial kinetic energy in an oscillator basis is outlined in Appendix A.

A. Finite Laguerre basis

The eigenvalues and eigenvectors of $\bar{H}^0$, the matrix representation of the radial kinetic energy in the subspace spanned by the N functions $\{\phi_n(r)\}_{n=0}^{N-1}$, are determined by solution of the matrix problem

$$\bar{H}_l^0|\bar{\Psi}_{E_i^0}\rangle=E_i^0|\bar{\Psi}_{E_i^0}\rangle, \tag{3.3}$$

where

$$|\Psi_{E_i}\rangle=\sum_{n=0}^{N-1}a_n(E_i^0)|\,\phi_n\rangle. \tag{3.4}$$

The expansion coefficients a_n and eigenvalues E_i^0 are determined by the requirement that

$$\langle\,\phi_m|(H_l^0-E_i^0)|\,\bar{\Psi}_{E_i}\rangle=0, \quad m=0,1,\ldots,N-1 \tag{3.5}$$

which reduces to the conditions[4]

$$2x(l+1)b_0-b_1=0, \tag{3.6a}$$

$$2x(m+l+1)b_m-(m+2l+1)b_{m-1}-(m+1)b_{m+1}=0, \tag{3.6b}$$

$$2x(N+l)b_{N-1}-(N+2l)b_{N-2}=0 \tag{3.6c}$$

on the coefficients

$$b_n(E)=\frac{\Gamma(n+2l+2)}{n!}a_n(E), \tag{3.7}$$

where x is the kinematical factor

$$x=x(E)=\frac{E-\lambda^2/8}{E+\lambda^2/8}. \tag{3.8}$$

Equations (3.6a) and (3.6b) are the recursion relations satisfied by the Gegenbauer[5] (ultraspherical) polynomials $C_m^{l+1}(x)$. The condition (3.6c) is also satisfied by these polynomials provided that $C_N^{l+1}(x)=0$. This latter condition is in effect the boundary condition that determines the discrete spectrum of $\bar{H}_l^0$ in the finite-dimensional space. The eigenvalues are thus given by

$$E_i^0=\frac{\lambda^2}{8}\frac{1+x_i^N}{1-x_i^N}, \tag{3.9}$$

where x_i^N is the ith zero of the Nth-order ultraspherical polynomials. The corresponding eigenfunctions

$$|\bar{\Psi}_{E_i^0}\rangle=A_i\sum_{n=0}^{N-1}\frac{n!}{\Gamma(n+2l+2)}C_n^{l+1}(x_i^N)|\phi_n\rangle \tag{3.10}$$

form an orthonormal set provided that

$$A_i^2=\lambda(1+x_i^N)\frac{\Gamma(N+2l+1)}{(N!)(N+2l+1)}[C_{N-1}^{l+1}(x_i^N)]^{-2}. \tag{3.11}$$

As may be shown by application of the Christoffel-Darboux relation appropriate to the ultraspherical polynomials[6]

$$(X-Y)\sum_{k=0}^{P}\frac{k!(k+m+1)}{\Gamma(k+2l+2)}C_k^{l+1}(X)C_k^{l+1}(Y)=\frac{1}{2}\frac{(P+1)!}{\Gamma(P+2l+2)}\,C_P^{l+1}(X)C_{P+1}^{l+1}(Y)-C_{P+1}^{l+1}(X)C_P^{l+1}(Y). \tag{3.12}$$

B. Infinite Laguerre basis

In the space spanned by the complete discrete set $\{\phi_n(r)\}_{n=0}^{\infty}$ the expansion coefficients $b_n(E)$ satisfy Eqs. (3.6a) and (3.6b) for $m=0,1,2\ldots$, and the boundary condition of Eq. (3.6c) does not come into play. $\bar{H}^0$ thus has a continuous spectrum in the basis and

$$|\Psi_E\rangle=B_l(E)\sum_{n=0}^{\infty}\frac{n!}{\Gamma(n+2l+2)}C_n^{l+1}(x)|\phi_n\rangle. \tag{3.13}$$

The continuum normalization factor $B(E)$ is determined by the requirement that

$$\langle r|\Psi_E\rangle=\langle r|\chi_E\rangle\equiv\left(\frac{2}{k\pi}\right)^{1/2}(kr)j_l(kr), \tag{3.14}$$

where

$$\langle\chi_E|\chi_{E'}\rangle=\delta(E-E'),\quad E=\tfrac{1}{2}k^2 \tag{3.15}$$

in the sense that the moments

$$\langle\gamma_m|\Psi_E\rangle=\langle\gamma_m|\chi_E\rangle,\quad m=0,1,2,\ldots,\infty, \tag{3.16}$$

where $\{\gamma_m\}_{n=0}^{\infty}$ is the set of functions biorthogonal[7] to the nonorthogonal $\{\phi_n\}_{n=0}^{\infty}$. In the present case, the γ_m are explicitly given as

$$\langle r|\gamma_m\rangle=\frac{m!}{\Gamma(m+2l+2)}\frac{\langle r|\phi_m\rangle}{r}. \tag{3.17}$$

Equation (3.16) now becomes

$$B_l(E)\frac{m!}{\Gamma(m+2l+2)}C_m^{l+1}(x)=\frac{m!}{\Gamma(m+2l+2)}\langle\gamma_m|\chi_E\rangle \tag{3.18}$$

which, on performing the integral $\langle\gamma_m|\chi_E\rangle$, gives

$$B_l(E)=\left(\frac{2}{\pi k}\right)^{1/2}2^l(l!)(1-x^2)^{(l+1)/2}. \tag{3.19}$$

C. Laguerre equivalent quadrature

Knowledge of the normalization coefficients A_i and $B(E)$ now allows elucidation of the relationship between $\langle f|(z-H_l^0)^{-1}|f\rangle$ and the discretized approximation $\langle f|(z-\bar{H}_l^0)^{-1}|f\rangle$.

From Sec. II

$$\langle f|(z-\bar{H}_l^0)^{-1}|f\rangle=\sum_{i=1}^{N}\frac{\langle f|\bar{\Psi}_{E_i^0}\rangle\langle\bar{\Psi}_{E_i^0}|f\rangle}{z-E_i^0} \tag{3.20}$$

and

$$\langle f|(z-H_l^0)^{-1}|f\rangle=\int_0^{\infty}dE\,\frac{\langle f|\Psi_E\rangle\langle\Psi_E|f\rangle}{z-E}, \tag{3.21}$$

respectively. The fact that the discrete approximation has poles at E_i^0's which are related to the zeros of the Gegenbauer (ultraspherical) polynomials suggests that Eq. (3.20) represents a Gegenbauer quadrature approximation to Eq. (3.21), provided that

$$|f\rangle=\sum_{n=0}^{N-1}C_n|\gamma_n\rangle$$

(i.e., if $|f\rangle$ can be exactly expressed in the N-dimensional subspace biorthogonal to $\{\phi_n\}_{n=0}^{N-1}$).
To show this, we transform the integration interval $[0,\infty]$ to $[-1,+1]$ via the transformation $x=(E-\frac{1}{8}\lambda^2)/(E+\frac{1}{8}\lambda^2)$, appropriate to the analysis of Sec. III A, and simultaneously approximate the integral by a quadrature with abscissas at x_i^N and unknown quadrature weights ω^{EQ}:

$$\langle f|(z-H_l^0)^{-1}|f\rangle=\int_0^{\infty}dE\,\frac{\langle f|\Psi_E\rangle\langle\Psi_E|f\rangle}{z-E} \tag{3.21}$$

$$=\int_{-1}^{+1}dx\,\frac{dE}{dx}\frac{|\langle f|\Psi_E\rangle|^2}{z-E(x)} \tag{3.22}$$

$$\cong \sum_{i=1}^{N} \omega_i^{\mathrm{EQ}} \frac{dE}{dx} \frac{|\langle f|\Psi_{E(x)}\rangle|^2}{z-E(x)}\bigg|_{x=x_i^N}, \tag{3.23}$$

where

$$E(x)=\tfrac{1}{8}\lambda^2(1+x)/(1-x). \tag{3.24}$$

The equivalent quadrature weights implicit in the approximation of Eq. (3.20) may now be determined by equating the residues at the poles of Eqs. (3.20) and (3.23), giving

$$\omega_i^{\mathrm{EQ}}\left(\frac{dE}{dx}|B(E(x))|^2\right)_{x=x_i^N}=|A_i|^2. \tag{3.25}$$

Using Eqs. (3.11) and (3.18) and solving Eq. (3.25) for ω_i^{EQ} we find

$$\omega_i^{\mathrm{EQ}}=\omega_i^N/\rho(x_i), \tag{3.26}$$

where

$$\omega_i^N=\frac{\pi}{2^{2l}(l!)^2}\frac{\Gamma(N+2l+1)}{N!}\left(C_{N-1}^{l+1}(x)\frac{d}{dx}C_N^{l+1}(x)\right)^{-1}\bigg|_{x=x_i^N} \tag{3.27}$$

and

$$\rho_l(x)=(1-x^2)^{l+1/2}. \tag{3.28}$$

$\rho_l(x)$ is the weight function which generates the Gegenbauer polynomials of index l and the ω_i^N are indeed the appropriate weights for performing the quadrature

$$\int_{-1}^{+1}\rho_l(x)p(x)\,dx=\sum_{i=0}^{N-1}\omega_i^N p(x_i^N), \tag{3.29}$$

which is exact if $p(x)$ is a polynomial of degree $2N-1$ or less.

We conclude by noting that we have shown that for suitably restricted L^2 functions $|f\rangle$ the Laguerre discretization of the radial kinetic energy produces a Gauss-Gegenbauer (Gauss-ultraspherical) quadrature approximation to matrix elements of the corresponding Green's function. If $|f\rangle$ is a more general L^2 function, the discretization produces an approximation to such a quadrature.

D. Application of Laguerre discretization technique to elastic scattering

As discussed in Ref. 2, elastic-scattering phase shifts may be computed from the L^2 discretized Green's function $(z-\bar{H}_l^0)^{-1}$ via construction of the partial-wave Fredholm determinant, provided that the equivalent quadrature weights are known. The analysis of Sec. III C gives the required weights explicitly for all l. As an application we consider s-, p-, and d-wave scattering from the attractive exponential potential $V=-V_0e^{-\gamma r}$ with $V_0=5$ and $\gamma=1.0$. Typical results are given in Table I. Details of the construction of the Fredholm determinant and the appropriate dispersion correction are analogous to those of Ref. 2. The more general dispersion-correction integral needed for higher partial waves is given by

$$C(x_0)=P\int_{-1}^{+1}\frac{(1-x^2)^{+1/2}}{E(x_0)-E(x)}\,dx$$

$$=\frac{4\sqrt{\pi}}{\lambda^2}\frac{\Gamma[l+(3/2)]}{\Gamma(l+2)}\times{}_2F_1[-2l-2,1;-l-\tfrac{1}{2};\tfrac{1}{2}(1-x_0)], \tag{3.30}$$

which is a polynomial of degree $2l+2$.

IV. RADIAL COULOMB HAMILTONIAN: LAGUERRE BASIS

A. Laguerre discretization of repulsive Coulomb Hamiltonian

The spectrum of the radial-partial-wave Coulomb Hamiltonian

$$H_l^0(|Z|)=-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}+\frac{|Z|}{r} \tag{4.1}$$

is easily analyzed in the Laguerre basis of Eq. (3.2) as the additional term Z/r is diagonal in the basis, and thus the analysis is, in some ways, similar to that of the radial kinetic energy in the Laguerre basis.

In the finite basis $\{\phi_n\}_{n=0}^{N-1}$ the coefficients $b_n(E_i^0)$

TABLE I. s-, p-, and d-wave phase shifts (mod π) for scattering from the potential $V=-5e^{-r}$ which has two bound states $l=0$, one bound state for $l=1$, and no bound states for higher l. Calculations were performed via the techniques of Ref. 2 with the equivalent quadrature weights of Sec. III C. Results are shown for 10, 20, 30, and 40 Laguerre-type basis functions, for the scale parameters $\lambda=2.0$.

	k (a.u.)	$N=10$	$N=20$	$N=30$	$N=40$	Exact
$l=0$	0.25	1.759	1.745	1.744	1.743	1.743
	0.50	0.8957	0.8939	0.8919	0.8898	0.8903
	0.75	0.3290	0.3264	0.3242	0.3206	0.3218
	1.00	2.722	3.044	3.041	3.037	3.038
$l=1$	0.25	0.0067	0.0028	0.0022	0.0019	0.0014
	0.50	3.007	2.995	2.994	2.993	2.992
	0.75	2.735	2.727	2.725	2.724	2.723
	1.00	2.486	2.466	2.463	2.462	2.460
$l=2$	0.25	0.0320	0.0304	0.0298	0.0296	0.0291
	0.50	0.5462	0.5414	0.5400	0.5395	0.5385
	0.75	1.304	1.296	1.294	1.293	1.292
	1.00	1.502	1.491	1.488	1.487	1.485

in the expansion

$$|\bar{\Psi}_{E_i^0}(|Z|)\rangle\rangle = \sum_{n=0}^{N-1} \frac{n!}{\Gamma(n+2l+2)} b_n(E_i^0)|\phi_n\rangle \tag{4.2}$$

are determined by the relations

$$2[(l+1+2Z/\lambda)x - 2Z/\lambda]b_0 - b_1 = 0\,, \tag{4.3a}$$

$$2[(m+l+1+2Z/\lambda)x - 2Z/\lambda]b_m - (m+2l+1)b_{m-1} - (m+1)b_{m+1} = 0\,, \quad 2 \le m \le N-2 \tag{4.3b}$$

$$2[(N+l+2Z/\lambda)x - 2Z/\lambda]b_{N-1} - (N+2l)b_{N-2} = 0, \tag{4.3c}$$

where

$$x = \frac{E - \lambda^2/8}{E + \lambda^2/8}\,.$$

The first two relations are the recursion relations satisfied by the Pollaczek[8,9] polynomial (the Pollaczek polynomials are defined in Appendix B),

$$P_n^{l+1}(x,|Z|) = \frac{\Gamma(n+2l+2)}{n!\,\Gamma(2l+2)} e^{in\theta} \times {}_2F_1(-n, l+1-i\gamma; 2l+2; 1-e^{-2i\theta}), \tag{4.4}$$

where

$$\gamma = -\frac{|Z|}{k}\,, \quad x = \cos\theta\,.$$

It is interesting to note that

$$P_n^{l+1}(x,0) = C_n^{l+1}(x)\,. \tag{4.5}$$

The Pollaczek polynomials are orthogonal on the interval $[-1,+1]$ with weight function

$$\rho(x) = (2^{2l+1}/\pi)e^{(2\theta-\pi)\gamma}(1-x^2)^{l+1/2}|\,\Gamma(l+1+i\gamma)|^2\,. \tag{4.6}$$

The last equation of (4.3) tells us that

$$P_N^{l+1}(x;|Z|) = 0\,. \tag{4.7}$$

Therefore the discrete spectrum of H^0 in the finite space is given by

$$E_i = \frac{\lambda^2}{8}\frac{1+x_i^N}{1-x_i^N}\,, \tag{4.8}$$

where x_i^N is the ith zero of $P_N(x,|Z|)$. For the repulsive case the zeros of $P_N(x,|Z|)$ lie in the interval $[-1,+1]$, corresponding to the fact that we would expect that the discrete eigenvalues of $\bar{H}_i^0(|Z|)$ would lie in the interval $(0,\infty)$ in the case of a finite discretization.

The Christoffel-Darboux relation satisfied by the Pollaczek polynomial is

$$(x-y)\sum_{k=0}^{P} \frac{k!(k+l+1+2z/\lambda)}{\Gamma(k+2l+2)} P_k^{l+1}(x,|Z|)P_k^{+1}(y,|Z|) = \frac{1}{2}\frac{(p+1)!}{\Gamma(p+2l+2)}\,[P_p^{l+1}(x,|Z|)P_{p+1}^{l+1}(y,|Z|) - P_{p+1}^{l+1}(x,|Z|)P_p^{l+1}(y,|Z|)]\,. \tag{4.9}$$

Using this relation, one can easily show that the orthonormal eigenfunctions are given by

$$|\bar{\Psi}_{E_i^0}\rangle = A_i \sum_{n=0}^{N-1} \frac{n!}{\Gamma(n+2l+2)} P_n^{l+1}(x_i^N,|Z|)|\,\phi_n\rangle\,, \tag{4.10}$$

where A_i has the value

$$A_i^2 = \frac{\lambda}{1-x_i^N}\frac{\Gamma(N+2l+2)}{N!(N+2l+1)}\left(P_{N-1}^{l+1}(x_i^N,|Z|\,\frac{d}{dx}P_N^{l+1}(x,|Z|)\Big|_{x=x_i^N}\right)^{-1}\,. \tag{4.11}$$

In the infinite basis $\{\phi_n\}_{n=0}^{\infty}$ the spectrum is continuous and

$$|\Psi_E\rangle = B_l(E)\sum_{n=0}^{\infty} \frac{n!}{\Gamma(n+2l+2)} P_n^{l+1}(x,|Z|)|\,\phi_n\rangle\,. \tag{4.12}$$

The continuum normalization factor $B(E)$ is now determined as in Sec. III by the requirement

$$B_l(E)\frac{1}{\Gamma(m+2l+2)} P_m^{l+1}(x,|Z|) = \langle\gamma_m|\,\chi_E\rangle\,, \tag{4.13}$$

where[10]

$$\langle r|\chi_E\rangle = \left(\frac{2}{\pi k}\right)^{1/2}\frac{1}{2}(2kr)^{l+1}e^{ikr}e^{\pi\gamma/2}\frac{|\Gamma(l+1-i\gamma)|}{\Gamma(2l+2)}$$

$$\times {}_1F_1(l+1-i\gamma;2l+2;-2ikr) \tag{4.14}$$

is the Coulomb wave function and the $\{\gamma_m\}$ are the functions biorthogonal to the $\{\phi_n\}$,

$$\langle r|\gamma_m\rangle = \frac{m!}{\Gamma(m+2l+2)}\frac{\langle r|\phi_m\rangle}{r}\,. \tag{4.15}$$

On performing the integral occurring in Eq. (4.13), we have

$$B_l(E) = \left(\frac{2}{\pi k}\right)^{1/2}2^l|\Gamma(l+1-i\gamma)|(1-x^2)^{(l+1/2)}e^{(\theta-\pi/2)\gamma}\,, \tag{4.16}$$

which reduces to the result of Eq. (3.18) in the case that $Z=0$.

The quadrature implicit in the finite discretization of Eq. (4.2) is now determined by repetition of the arguments of Sec. III C: Using Eqs. (4.11) and (4.16) we find

$$\omega_i^{\mathrm{EQ}} = \omega_i^P/\rho^P(x_i)\,, \tag{4.17}$$

where

$$\omega_i^P = \frac{2\Gamma(N+2l+1)}{N!} \times\left(P_{N-1}^{l+1}(x_i^N,|Z|)\frac{d}{dx}P_N^{l+1}(x,|Z|)\Big|_{x=x_i^N}\right)^{-1} \tag{4.18}$$

and

$$\bar\rho^P(x) = \frac{2^{2l+1}}{\pi}e^{(2\theta-\pi)\gamma}(1-x^2)^{(l+1/2)}|\Gamma(l+1+i\gamma)|^2\,, \tag{4.19}$$

with $x=\cos\theta$ and $\gamma=-|Z|/k$. $\rho^P(x)$ is the Pollaczek weight function and ω_i^P are the Pollaczek weights for the quadruature,

$$\int_{-1}^{+1}\rho^P(x)p(x)\,dx = \sum_{i=0}^{N-1}\omega_i^P p(x_i^N)\,, \tag{4.20}$$

which is exact if $p(x)$ is a polynomial of degree $2N-1$ or less.

We conclude this subsection by noting that we have shown that discretization of the repulsive Coulomb Hamiltonian in a finite Laguerre basis generates a Gauss-Pollaczek quadrature representation of the actual operator.

B. Application to elastic Coulomb scattering in repulsive case

For the case of a repulsive Coulomb potential plus a "short-range" potential of arbitrary or indefinite sign, the phase shift $\delta_l^c(E)$, relative to the pure Coulomb phase $\arg\Gamma(l+1-i|Z|/k)$, may be determined from the relationship

$$D_l^c(E+i\epsilon) = |D_l^c(E+i\epsilon)|\,e^{-i\delta_l^c(E)}\,, \tag{4.21}$$

where $D_l^c(z)$ is the Coulomb Fredholm determinant

$$D_l^c(z) = \det\left(\frac{z-H_l^0(|Z|)-V}{z-H_l^0(|Z|)}\right)\,, \tag{4.22}$$

V being the short-range potential. If $H_l^0(|Z|)$ and $H_l^0(|Z|)+V$ are discretized in a finite Laguerre basis, the phase $\delta_l^c(E)$ may be determined by the techniques of Refs. 1 and 2. Results for Coulomb scattering from the short-range separable potential

$$V = -4\pi(\tfrac{1}{2}\alpha)|u\rangle\langle u|\,, \tag{4.23a}$$

where

$$u(r) = e^{-r}/r\,, \tag{4.23b}$$

are given in Table II for several expansion sizes and energies. In this case the dispersion correction integral which arises in the analysis of Table II is

$$C_{l,Z}(x_0) = P\int_{-1}^{+1}\frac{\rho^P(x)}{E(x_0)-E(x)}\,dx = \Gamma(2l+2)\frac{4(1-x_0)}{\lambda^2}\left[\frac{1}{l+1+(2|Z|/\lambda)}+2(1-x_0)\mathrm{Re}\left(\frac{e^{i\theta_0}}{l+1+i\gamma_0}\,{}_2F_1(-l+i\gamma_0,1;l+2+i\gamma_0;e^{2i\theta_0})\right)\right]\,, \tag{4.24}$$

where

$$\gamma_0 = -\frac{|Z|}{k_0} = -\frac{|Z|}{\lambda}\left(\frac{1-x_0}{1+x_0}\right)^{1/2}\,,\quad E=\tfrac{1}{2}k^2\,,$$

$\rho^P(x)$ is the Pollaczek weight function (Appendix B), and again $E(x)=\frac{1}{8}\lambda^2(1+x)/(1-x)$. We note that the particular Gauss-hypergeometric function appearing in Eq. (4.24) is easily evaluated using the continued-fraction representation discussed by Wall.[11]

C. Laguerre discretization of attractive Coulomb Hamiltonian

In the case of the attractive Coulomb Hamiltonian, $H^0(-|Z|)$, the recursion relations of Eqs. (4.3a) and (4.3b) determine the discrete eigenvalues of $\bar H^0(-|Z|)$ in a finite Laguerre subspace. The formal solution of the recursion scheme is given by the polynomials

$$P_N^{l+1}(x,-|Z|) \tag{4.25}$$

TABLE II. Coulomb phase shift [relative to $\arg\Gamma(l+1-i\gamma)$] for scattering from a $Z=1$ repulsive Coulomb potential plus the short-range potential of Eq. (4.23) for $l=0$, with $\alpha=20$. Results are given for several different expansion sizes and for two different values of the scale parameter λ.

k (a.u.)	$N=8$ $\lambda=2.0$	$N=10$ $\lambda=2.0$	$N=14$ $\lambda=2.0$	$N=14$ $\lambda=3.2$	Exact
0.25	3.1407	π	π	π	π
0.50	3.0534	3.134 83	3.135 719	3.135 719	3.135 730 92
1.00	2.6563	2.662 28	2.662 208 03	2.662 208 98	2.662 208 46
1.50	1.9845	1.980 39	1.980 469 5	1.980 470 09	1.980 470 88

and the discrete eigenvalues given by the zeros defined by

$$P_N^{l+1}(x_i^N, -|Z|)=0, \quad i=0,1,2\ldots,N-1 \qquad (4.26)$$

and the eigenvalues are thus $E_i^0=\frac{1}{8}\lambda^2(1+x_i^N)/(1-x_i^N)$ The $P_n^{l+1}(x,-|Z|)$ are not the Pollaczek polynomials of Sec. IV A and Appendix B, in that the x_i corresponding to the bound states of $\bar{H}^0(-|Z|)$ lie outside the interval $[-1,+1]$ and thus are *not* the zeros of the polynomials generated by a positive weight function on the interval $(-1,+1)$.[12] We refer to these more general polynomials, defined by the recursion of Eqs. (4.3a) and (4.3b), for $Z<0$ as the "attractive Coulomb-Pollaczek" (ACP) polynomials.

As long as

$$(n+l+1)-2|Z|/\lambda>0, \quad n=0,1,2\ldots$$

the ACP polynomials can be generated from a positive weight function, defined in this case on the interval $[-\xi,+1]$, with

$$-\xi<-\frac{1}{1-2|Z|/\lambda}\,.$$

We quote two theorems which will partially characterize the weight function.

Theorem S [Szego[13]]: Let $d\alpha(x)$ be a distribution on the finite segment $[a,b]$ and let $\{p_n(x)\}$ denote the associated orthonormal set of polynomials. Let $[a',b']$ be a subinterval of $[a,b]$ such that $\int_{a'}^{b'} d\alpha(x)>0$. Then if n is sufficiently large, every polynomial $p_n(x)$ has at least one zero in $[a',b']$.

Theorem HU (Hylleraas-Undheim)[14]: If the eigenvalues λ_i of an N-dimensional matrix representation $\bar{M}$ of an Hermitian operator M are ordered

$$\bar{\lambda}_1\leq\bar{\lambda}_2\leq\cdots\bar{\lambda}_i\cdots\leq\bar{\lambda}_N\,,$$

then $\lambda_i\leq\bar{\lambda}_i$, where λ_i is the ith lowest eigenvalues of M itself (i.e., $\lambda_1\leq\lambda_2\leq\cdots\lambda_i\cdots$).

Theorem S combined with theorem HU implies that the weight function which generates the polynomials whose zeros approximate the eigenvalues of Hermitian operator will reflect the spectrum of that operator in that $\alpha(x)$ will only increase at those (real) values of x which are in the spectrum of the operator. In the present case this implies that the positive weight function $\rho^{\mathrm{ACP}}(x)$ which generates the ACP polynomials will be of the form

$$d\alpha(x)=\rho^{\mathrm{ACP}}(x)\,dx=\begin{cases}\rho(x)\,dx, & x\in[-1,+1] \qquad (4.27a)\\ \sum_{i=1}^{\infty}\rho_i\delta(x-x_i^B), & x\in[-1,+1] \qquad (4.27b)\end{cases}$$

$\rho(x)$ being a positive weight function, continuous on $[-1,+1]$, ρ_i being positive real numbers,

$$x_n^B=\frac{E_n^B-\lambda^2/8}{E_n^B+\lambda^2/8}\,, \quad n=1,2,\ldots \qquad (4.28a)$$

and

$$E_n^B=-\tfrac{1}{2}|Z|^2(1/n^2)\,, \qquad (4.28b)$$

E_n^B being the Coulomb bound states.

For the analysis of the discretization of the continuous spectrum of $H_l(-|Z|)$ only values of $\rho^{\mathrm{ACP}}(x)$ on $[-1,+1]$ are needed, and we have, following the analysis of Sec. IV A,

$$\omega_i^{\mathrm{EQ}}=\frac{\omega_i^{\mathrm{ACP}}}{\rho^P(x_i,-|Z|)}, \quad x_i\in[-1,+1] \qquad (4.29)$$

where

$$\omega_i^{\mathrm{ACP}}=\frac{2\Gamma(N+2l+1)}{N!}\left(P_{N-1}^{l+1}(x_i,-|Z|)\frac{d}{dx}P_N^{l+1}(x-|Z|)\Big|_{x=x_i}\right)^{-1} \qquad (4.30)$$

and

$$\rho^P(x,-|Z|)=\frac{1}{\pi}2^{2l+1}e^{(2\theta-\pi)\frac{|Z|}{k}}(1-x^2)^{l+1/2}|\Gamma(l+1+i\gamma)|^2\,. \qquad (4.31)$$

$\rho^P(x, -|Z|)$ is the continuation of $\rho^P(x)$, the Pollaczek weight function, from positive to negative Z. The results of Eqs. (4.24) and (4.30) follow from the Christoffel-Darboux formulas for the $P_n^{l+1}(x, -|Z|)$, which follow directly from the recursion scheme, Eq. (4.3). We conclude that $\rho_{(x)}^{\mathrm{ACP}} = \rho^P(x, -|Z|)$, $x \in [-1, +1]$. The ρ_i of Eq. (4.27b) are not determined by this informal analysis, but are not needed for extraction of scattering information from L^2 discretization of the attractive Coulomb problem.

D. Photoeffect in hydrogen

The cross section σ_{ph} for the photoionization of the hydrogen atom is proportional to the quantity $|\langle \phi_k(r)|D(r)|C_1(r,k)\rangle\rangle|^2$, where $D(r)$ is the dipole operator and $C_1(r,k)$ is the appropriate p-wave Coulomb wave function normalized to a δ function of the energy scale. We have

$$|\langle \phi_k(r)|D(r)|C_1(r,k_i)\rangle\rangle|^2 \omega_i^{\mathrm{EQ}} \left(\frac{dE}{dx}\right)_{x=x_i^0} = |\langle \phi_k(r)|D(r)|\bar{\Psi}_{E_i^0}(-|Z|)\rangle\rangle|^2, \quad (4.32)$$

$\bar{\Psi}_{E_i}(-|Z|)$ being the unit normalized discrete eigenfunction of $\bar{H}_l^0(-|Z|)$, the discretized attractive Coulomb Hamiltonian. Knowledge of $\bar{\Psi}_{E_i}(-|Z|)$ and the equivalent quadrature weights thus allows computation of σ_{ph} from calculations performed entirely in an L^2 basis, complementing the analytic continuation results of Broad and Reinhardt.[15] Cross sections determined using Eq. (4.32) at the E_i^0's, followed by rational interpolation, give the results of Table III. These results confirm that, over that part of coordinate space spanned by the function $D(r)|\phi_k(r)\rangle\rangle$, the essential difference between $|C_1(r,k_i)\rangle\rangle$ and $|\bar{\Psi}_{E_i^0}(-|Z|)\rangle\rangle$ is a normalization factor, which is indeed given by the equivalent quadrature weight of Eq. (4.29).

E. Application to elastic Coulomb scattering in attractive case

For the case of an attractive Coulomb potential plus a short-range potential $V(r)$, the phase $\delta_l^C(E)$, relative to $\arg\Gamma(l+1-i\gamma)$, may be determined from the partial-wave Fredholm determinant

$$D_l^C(z) = \det\{[z - H_l^0(-|Z|) - V(r)]/[z - H_l^0(-|Z|)]\} \quad (4.33)$$

as

$$D_l^C(E + i\epsilon) = |D_l^C(E + i\epsilon)|\, e^{-i\delta_l^C(E)}. \quad (4.34)$$

As $H_l^0(-|Z|)$ has bound states, the dispersion relation for the determinant is of the form

$$D_l^C(z) = 1 + \sum_i \frac{a_i}{z - E_i^B} + \int_0^\infty \frac{A(E)\,dE}{z - E}, \quad (4.35)$$

where the a_i are the residues at the (simple) bound-state poles at E_i^B. An approximate determinant, arising from the L^2 discretization of $H_l^0(-|Z|)$ and $H_l^0(-|Z|) + V$, will have the form

$$D^{\mathrm{Approx}}(z) = \det(\{z - [\bar{H}_l^0(-|Z|) + \bar{V}]\}/\{z - [\bar{H}_l^0(-|Z|)]\}) = \prod_{i=1}^N \frac{z - E_i}{z - E_i^0} = 1 + \sum_i \frac{\gamma_i}{z - E_i^{0,B}} + \sum_j \frac{\Gamma_j}{z - E_j^{0,C}}. \quad (4.36)$$

The γ_i are the residues at the approximate bound-state energies $E_i^{0,B}$ ($E_i^{0,B} < 0$) and the sum

$$\sum_j \frac{\Gamma_j}{z - E_j^{0,C}}$$

gives a quadrature approximation to the integral appearing in Eq. (4.35) ($E_i^{0,C} > 0$). To obtain scattering information from the discretized approximation of Eq. (4.36), we take the $E + i\epsilon$ limit using the equivalent quadrature of Eq. (4.29) with appropriate dispersion correction terms to obtain

TABLE III. Photoionization cross sections for ground-state atomic hydrogen as computed by diagonalization of the $Z = 1$ attractive Coulomb Hamiltonian discretized in a Laguerre basis with $\lambda = 1.5$. Results with $N = 8$, 9, 10, and 15 are compared with the exact result.

Photon energy (a.u.)	$N=8$	$N=9$	$N=10$	$N=15$	Exact
0.51	0.209 64	0.213 62	0.213 598	0.213 540 06	0.213 540 01
0.55	0.174 73	0.174 34	0.174 388	0.174 392 14	0.174 392 16
0.60	0.138 63	0.137 82	0.137 834	0.137 830 51	0.137 830 50
0.65	0.110 98	0.110 83	0.110 807	0.110 804 99	0.110 804 90
0.70	0.090 09	0.090 41	0.090 390	0.090 392 075	0.090 392 081

$$\mathrm{Re}\, D^{\mathrm{approx}}(E_0+i\epsilon)=1+\sum_i \frac{\gamma_i}{z-E_i^{0,B}}+\sum_j \frac{\omega_j^{\mathrm{EQ}} A^{\mathrm{approx}}(E_j^{0,c})(dE/dx)_{x=x_j^0}}{E_0-E_j^{0,c}}$$

$$+\frac{A(E_0)(dE/dx)_{x=x_0}}{f(x_0)}\left(P\int_{-1}^{+1}\frac{f(x)\,dx}{E_0-E(x)}-\sum_j \frac{\omega_j^{\mathrm{EQ}} f(x_j)}{E_0-E_j^{0,c}}\right), \tag{4.37a}$$

$$\mathrm{Im}\, D^{\mathrm{approx}}(E_0+i\epsilon)=-i\pi A^{\mathrm{approx}}(E_0), \tag{4.37b}$$

where, as appropriate to Eq. (4.3), $E(x)=\frac{1}{8}\lambda^2(1+x)/(1-x)$, and thus $dE/dx=\frac{1}{4}\lambda^2(1-x^2)^{-1}$. The $A^{\mathrm{approx}}(E_j^{0,c})$ are obtained by

$$A^{\mathrm{approx}}(E_j^{0,c})=\Gamma_j\left[\omega_j^{\mathrm{EQ}}\left(\frac{dE}{dx}\right)_{x=x_j^0}\right]^{-1} \tag{4.38}$$

and the $A^{\mathrm{approx}}(E_0)$ by interpolation. We note that the dispersion correction of Eq. (4.37a) is a generalization of those discussed in Refs. 2 and 3, in that

$$P\int_{-1}^{+1}\frac{\rho(x)\,dx}{E_0-E(x)} \tag{4.39}$$

has been replaced by the often more tractable integral

$$P\int_{-1}^{+1}\frac{f(x)\,dx}{E_0-E(x)}, \tag{4.40}$$

where $f(x)$ is restricted only by the requirements that the principal-value integral of Eq. (4.40) exist, and that the Lipschitz condition

$$\left|A(E)\frac{dE}{dx}f(x_0)-f(x)A(E_0)\left(\frac{dE}{dx}\right)_{x=x_0}\right|<C|E-E_0| \tag{4.41}$$

be satisfied in the neighborhood of E_0, for some positive constant C.

Results for scattering from the potential V of Eq. (4.23), in addition to a unit attractive Coulomb potential, are given in Table IV for a variety of basis sets. The function $f(x)$ was taken to be $(1-x^2)^{1/2}$, making evaluation of the dispersion correction integral identical to the $l=0$ case of Eq. (4.23).

V. APPROXIMATE DETERMINATION OF QUADRATURE WEIGHTS

Once the equivalent quadrature weights have been formally determined, numerical values must still be obtained. As in most cases the evaluation of the weights in terms of high-order polynomials and their derivatives is a numerically ill-conditioned problem, we discuss two straightforward numerical methods for determining the weights. The first is a modification of the numerically stable method of Gordon,[16] appropriate to the case where the recursion scheme for generating the polynomials is known. The second, introduced by Heller, is an exceedingly simple technique for determining equivalent quadrature weights, $w_i/\rho(x_i)$, from an interpolation of the abscissas.

A. Modified Gordon method

Gordon[16] has given a numerically stable method for obtaining Gaussian weights from the power moments u_k of a positive weight function $\rho(x)$. The method involves a continued-fraction transformation of the u_k to obtain quantities a_k, which may be used to construct a well-conditioned matrix problem for construction of the quadrature abscissas and weights. In the case that the three-term recursion generating the orthogonal polynomials is known, the determination of quadrature weights may be reduced to a stable-matrix problem, equivalent to that of Gordon, without explicit construction or knowledge of the u_k, or a_k, except for $k=0$.

The recursion scheme

$$\bar{P}_{n+1}=(a_n+xb_n)\bar{P}_n-c_n\bar{P}_{n-1} \tag{5.1}$$

may be written in the more symmetric form

$$xP_n=r_{n-1}P_{n-1}+s_nP_n+r_nP_{n+1}, \tag{5.2}$$

where $\bar{P}_n=t_nP_n$, t_n being independent of x. Equation (5.2) is equivalent to the matrix equation

TABLE IV. Coulomb s-wave phase shifts for scattering from the spherically symmetric separable potential $V=-4\pi(\frac{1}{2}\alpha)u(r)u(r')$, $u(r)=e^{-\gamma r}/r$, in addition to a unit attractive Coulomb potential. Results are given for expansion sizes $N=10$, 20, 30 for $\alpha=20$ and the scale parameter $\lambda=2.2$. The construction of the Coulomb Fredholm determinant and the approximate dispersion technique used to take the $E+i\epsilon$ limit are discussed in the text.

k (a.u.)	$N=10$	$N=20$	$N=30$	Exact
0.50	0.4785	0.4752	0.4738	0.4735
1.00	0.4579	0.4555	0.4558	0.4556
2.00	0.3867	0.3838	0.3841	0.3840
3.00	0.3165	0.3121	0.3125	0.3123
5.00	0.2154	0.2081	0.2087	0.2085

$$\overline{M}A = xA, \tag{5.3}$$

where $\overline{M}$ is the symmetric tridiagonal matrix,

$$M_{i,i} = s_i, \tag{5.4a}$$

$$M_{i,i+1} = M_{i+1,i} = r_i, \tag{5.4b}$$

and $A_i = P_i$. The matrix $\overline{M}$, which is identical to the matrix constructed from the a_k by Gordon, may be diagonalized by the unitary transformation

$$\tilde{\Gamma}\overline{M}\Gamma = \overline{\Lambda}, \tag{5.5}$$

$\overline{\Lambda}$ is the diagonal matrix whose elements give the quadrature abscissas,

$$x_i = \Lambda_{ii}, \tag{5.6}$$

and the weights are given by

$$\omega_i = (\Gamma_{1,i})^2 a_0, \tag{5.7}$$

where $a_0 = u_0 = \int_a^b \rho(x)\,dx$ is the zeroth moment of the weight function. In terms of the ω_i the equivalent quadrature weights are given as $\omega_i^{\mathrm{EQ}} = \omega_i/\rho(x_i)$.

B. Heller derivative method

In his thesis Heller[17,18] suggested that the equivalent quadrature weights could be directly calculated by considering the function $f(\xi)$ which "smoothly" interpolates the ordered (increasing) abscissas x_i obtained directly from the diagonalization of the discretized operator in the sense that

$$f(\xi)\big|_{\xi=i} = x_i. \tag{5.8}$$

In terms of $f(\xi)$ the conjecture is that

$$\omega^{\mathrm{EQ}} = \frac{\omega_i}{\rho(x_i)} = \left.\frac{df(\xi)}{d\xi}\right|_{\xi=i}. \tag{5.9}$$

For the case of the s-wave radial kinetic energy this may be explicitly verified, as the zeros of the Chebyschev polynomials of the second kind are given explicitly by[19,20]

$$X_i^N = -\cos\left(\frac{i+1}{N+1}\right)\pi;\quad i = 0, 1, 2\ldots, N-1 \tag{5.10}$$

thus

$$f(\xi) = -\cos\frac{(\xi+1)}{N+1}\pi \tag{5.11}$$

and

$$\left.\frac{df(\xi)}{d\xi}\right|_{\xi=i} = \frac{\pi}{N+1}\sin\frac{(i+1)}{N+1}\pi, \tag{5.12}$$

which is indeed the appropriate weight for the Chebyschev equivalent quadrature as

$$\omega_i^{\mathrm{Ch}} = \frac{\pi}{N+1}\sin^2\frac{(i+1)}{n+1}\pi \tag{5.13a}$$

and

$$\rho^{\mathrm{Ch}}(x_i^N) = (1-x_i^2)^{1/2} = \sin\frac{(i+1)\pi}{N+1}. \tag{5.13b}$$

In general the interpolatory function $f(\xi)$ is not known and must be obtained approximately. Results of high accuracy have been obtained using pointwise rational fraction fits and spline fits, using as input the fact that $f(\xi) = x_i$ for integer values of ξ. Results of application of the derivative method to determination of equivalent quadrature weights are given in Tables V and VI, where they are compared with the results obtained by the technique of Sec. II A. The derivative method gives remarkably accurate weights, even for low-order quadratures where the interpolation of the x_i is less well determined. We note that, as the derivative method does not require specification of the weight function $\rho(x)$, it can be used in situations where the analyses of the present paper cannot or have not been carried out. The major requirement for application is that the abscissas x_i are rea-

TABLE V. Equivalent quadrature weights $w_i/\rho(x_i)$ calculated by the stable-matrix technique of Sec. V A and by the Heller derivative technique (w_i^{deriv}) of Sec. V B, with an N-point rational interpolation. Results are given for the Laguerre discretization of the $l = 2$ radial kinetic energy with $\lambda = 1.0$ and expansion sizes 10 and 14. Similar results were obtained for other l and λ values.

E_i^0	$w_i/\rho(x_i)$	w_i^{deriv}
	$N = 10$	
6.429 277 94E − 03	1.152 317 07E − 01	1.151 216 68E − 01
1.686 112 50E − 02	1.633 692 09E − 01	1.633 795 22E − 01
3.338 428 78E − 02	2.025 637 66E − 01	2.025 608 17E − 01
5.868 024 95E − 02	2.300 833 56E − 01	2.300 852 53E − 01
9.767 181 04E − 02	2.442 625 97E − 01	2.442 589 73E − 01
1.599 745 10E − 01	2.442 625 97E − 01	2.442 589 71E − 01
2.662 735 78E − 01	2.300 833 56E − 01	2.300 852 52E − 01
4.680 345 46E − 01	2.025 637 66E − 01	2.025 608 17E − 01
9.266 878 67E − 01	1.633 692 09E − 01	1.633 795 22E − 01
2.430 288 46E + 00	1.152 317 07E − 01	1.151 216 69E − 01
	$N = 14$	
3.688 083 89E − 03	6.798 041 69E − 02	6.797 745 57E − 02
9.459 437 55E − 03	9.843 581 94E − 02	9.843 592 32E − 02
1.811 566 80E − 02	1.258 562 70E − 01	1.258 562 58E − 01
3.037 624 29E − 02	1.490 454 22E − 01	1.490 454 25E − 01
4.736 190 00E − 02	1.671 752 00E − 01	1.671 751 98E − 01
7.084 113 41E − 02	1.796 185 16E − 01	1.796 185 18E − 01
1.036 781 31E − 01	1.859 484 73E − 01	1.859 483 96E − 01
1.507 068 06E − 01	1.859 484 73E − 01	1.859 484 72E − 01
2.205 639 45E − 01	1.796 185 16E − 01	1.796 185 17E − 01
3.299 065 28E − 01	1.671 752 00E − 01	1.671 751 98E − 01
5.143 822 45E − 01	1.490 454 22E − 01	1.490 454 25E − 01
8.625 130 48E − 01	1.258 562 70E − 01	1.258 562 57E − 01
1.651 789 54E + 00	9.843 581 94E − 02	9.843 592 64E − 02
4.236 617 29E + 00	6.798 041 69E − 02	6.797 740 00E − 02

TABLE VI. Equivalent quadrature weights calculated by the matrix technique of Sec. VA, $w_i/\rho(x_i)$ and by the Heller derivative method of Sec. VB (w_i^{deriv}) for the $Z=-1$ attractive Coulomb problem with $l=2$. Results are given for $\lambda=2.5$ for expansion sizes $N=10$ and $N=14$. Only those $E_i^{0,c}$ which correspond to the discretized continuum are given.

$E_i^{0,c}$ (>0)	$w_i/\rho(x_i)$	w_i^{deriv}
	$N=10$	
7.291 431 39E −02	2.181 750 63E −01	2.182 268 60E −01
2.026 450 54E −01	2.610 614 99E −01	2.610 539 17E −01
4.082 264 32E −01	2.845 997 47E −01	2.846 023 37E −01
7.424 090 48E −01	2.883 229 05E −01	2.883 212 70E −01
1.320 484 66E +00	2.726 561 67E −01	2.726 579 36E −01
2.432 877 86E +00	2.391 632 73E −01	2.391 599 44E −01
5.002 793 05E +00	1.906 153 85E −01	1.906 275 88E −01
1.361 418 31E +01	1.312 736 89E −01	1.311 467 30E −01
	$N=14$	
1.545 845 11E −02	1.244 938 82E −01	1.244 874 24E −01
7.759 901 27E −02	1.580 119 21E −01	1.580 120 50E −01
1.670 264 09E −01	1.838 418 25E −01	1.838 418 21E −01
2.932 047 97E −01	2.018 265 52E −01	2.018 265 50E −01
4.719 762 90E −01	2.116 901 88E −01	2.116 901 89E −01
7.304 568 68E −01	2.132 990 05E −01	2.132 990 03E −01
1.117 513 97E +00	2.067 578 06E −01	2.067 578 07E −01
1.728 073 26E +00	1.924 452 57E −01	1.924 452 55E −01
2.766 769 64E +00	1.710 221 41E −01	1.710 221 51E −01
4.749 930 32E +00	1.434 272 86E −01	1.434 272 46E −01
9.287 347 82E +00	1.108 828 29E −01	1.108 841 91E −01
2.440 826 40E +01	7.508 637 80E −02	7.507 579 75E −02

sonably evenly spaced, allowing interpolative approximation of $df(\xi)/d\xi$.

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APPENDIX A: RADIAL KINETIC ENERGY IN AN OSCILLATOR BASIS

The radial kinetic energy H_l^o may be analytically diagonalized in the L^2 basis of oscillator functions

$$\phi_n(r)=\langle r\,|\,\phi_n\rangle=(\lambda r)^{l+1}e^{-\lambda^2r^2/2}L_n^{l+1/2}(\lambda^2r^2) \tag{A1}$$

in both the finite and infinite cases, in direct analogy with the Laguerre case discussed in Sec. III.

In the finite basis $\{\phi_n(r)\}_{n=0}^{N-1}$

$$|\bar{\psi}_{E_i^0}\rangle=\sum_{n=0}^{N-1}\frac{n!}{\Gamma(n+l+3/2)}b_n(E_i^o)\,|\,\phi_n\rangle\ , \tag{A2}$$

the b_i being determined by the conditions

$$(l+\tfrac{3}{2}-x)b_0+b_1=0\ , \tag{A3a}$$

$$(2m+l+\tfrac{3}{2}-x)b_m+(m+l+\tfrac{1}{2})b_{m-1}+(m+1)b_{m+1}=0\ ,\quad m=2,\ldots,N-2 \tag{A3b}$$

$$(2N+l-\tfrac{1}{2}-x)b_{N-1}+(N+l-\tfrac{1}{2})b_{N-2}=0\ , \tag{A3c}$$

where Eq. (A3c) serves as the "boundary condition" analogous to that of Eq. (3.6c), and $x=2E/\lambda^2$. The first $N-1$ equations are identical to those satisfied by the Laguerre polynomials $L_m^{l+1/2}(x)$, provided we make the identification

$$b_m(E)\sim(-1)^mL_m^{l+1/2}(x)\ . \tag{A4}$$

The last equation is also satisfied by the same set of polynomials provided

$$L_N^{l+1/2}(x)=0\ . \tag{A5}$$

The eigenvalues of H^o in the finite space are therefore given by

$$E_i^o=\tfrac{1}{2}\lambda^2x_i^N\ , \tag{A6}$$

where x_i^N is the ith zero of $L_N^{l+1/2}(x)$. The eigenvector $|\bar{\Psi}_i\rangle$ corresponding to the eigenvalue E_i^o can now be written down as

$$|\bar{\Psi}_{E_i^0}\rangle=A_i\sum_{n=0}^{N-1}(-1)^n\frac{n!}{\Gamma(n+l+3/2)}L_n^{l+1/2}(x_i^N)\,|\,\phi_n\rangle\ . \tag{A7}$$

Using the Christoffel-Darboux relation

$$(x-y)\sum_{k=0}^{P}\frac{k!}{\Gamma(k+l+3/2)}L_k^{l+1/2}(x)L_k^{l+1/2}(y)=\frac{(P+1)!}{\Gamma(P+l+3/2)}\left[L_p^{l+1/2}(x)L_{p+1}^{l+1/2}(y)-L_{p+1}^{l+1/2}(x)L_p^{l+1/2}(y)\right]\ . \tag{A8}$$

We find the normalization constant

$$A_i^2=\frac{2\lambda x_i^N}{N!}\frac{\Gamma(N+l+1/2)}{(N+l+1/2)}\left[L_{N-1}^{l+1/2}(x_i^N)\right]^{-2}\ . \tag{A9}$$

In the infinite-dimensional case, $\{\phi_n\}_{n=0}^{\infty}$, the spectrum is continuous and

$$|\psi_E\rangle=B(E)\sum_{n=0}^{\infty}(-1)^n\frac{n!}{\Gamma(n+l+3/2)}L_n^{l+1/2}(x)\,|\,\phi_n\rangle\ . \tag{A10}$$

Again the continuum normalization function $B(E)$ is determined from the relation

$$\langle \gamma_n | \chi_E \rangle = (-1)^n \frac{n!}{\Gamma(n+l+3/2)} L_n^{l+1/2}(x) B(E), \quad \text{(A11)}$$

where, in this case,

$$|\gamma_m\rangle = \frac{1}{\lambda} \frac{n!}{\Gamma(m+l+3/2)} |\phi_n\rangle, \quad \text{(A12)}$$

and, as in Sec. III, $\langle r | \chi_E \rangle = (2/k\pi)^{1/2}(kr) j_l(kr)$. The continuum normalization factor is thus

$$B(E) = \frac{2}{\sqrt{k}} x^{(l+1)/2} e^{-x/2}, \quad \text{(A13)}$$

where again $E = k^2/2 = \lambda^2 x/2$.

The equivalent quadrature analysis of Sec. III C can now be carried out, giving

$$\omega_i^{\mathrm{EQ}} = \omega_i^{\mathrm{Lag}} / \rho(x_i), \quad \text{(A14)}$$

where

$$\omega_i^{\mathrm{Lag}} = \frac{\Gamma(N+l+1/2)}{N!} \left(L_{N-1}^{l+1/2}(x_i^N) \frac{d}{dx} L_N^{l+1/2}(x) \Big|_{x=x_i^N} \right)^{-1}, \quad \text{(A15)}$$

where $\rho(x) = x^{l+1/2} e^{-x}$ is the Laguerre weight function. The ω_k^{Lag} are the Gauss-Laguerre quadrature weights:

$$\int_0^\infty x^{l+1/2} e^{-x} p(x)\, dx = \sum_{i=1}^{N} \omega_i^{\mathrm{Lag}} p(x_i), \quad \text{(A16)}$$

which is exact if $p(x)$ is a polynomial of order $2N-1$ or less.

The dispersion correction integral

$$C_l(x_0) = \int_0^\infty \frac{\rho(x)}{E(x_0) - E(x)}\, dx \quad \text{(A17)}$$

is given by

$$C_l(x_0) = (2/\lambda^2)(-1)^{l+1} e^{-x_0} \gamma^*(-l-\tfrac{1}{2}, -x_0), \quad \text{(A18)}$$

where[21]

$$\gamma^*(a, x) = \frac{x^{-a}}{\Gamma(a)} \int_0^x e^{-t} e^{a-1}\, dt. \quad \text{(A19)}$$

APPENDIX B: POLLACZEK POLYNOMIALS

The polynomials $P_n^{l+1}(x, z)$ discussed in Sec. IV A in connection with the discretization of the repulsive Coulomb Hamiltonian are a special case of those introduced by Pollaczek[8] in the form $P_n^{\alpha}(x; a, b)$, where $a \geq |b|$. In the repulsive Coulomb case $a = -b = 2z/\lambda$ and the requirement that $a \geq |b|$ is equivalent to $z \geq 0$, which corresponds to the repulsive case.

Here we give the properties of $P_n^{\alpha}(x; z)$, while those of $P_n^{\alpha}(x; a, b)$ can be found in the literature.[9] $p_n^{\alpha}(x; z)$ may be defined by their generating series

$$\begin{aligned} H(x; z) &= (1 - te^{i\theta})^{-(\alpha - i\gamma)} (1 - te^{-i\theta})^{-(\alpha + i\gamma)} \\ &= (t^2 - 2xt + 1)^{-\alpha} \exp\left(i\gamma \ln \frac{1 - te^{i\theta}}{1 - te^{-i\theta}} \right) \\ &= (t^2 - 2xt + 1)^{-\alpha} \exp\left(-\frac{4z}{\lambda} (1 - x) \sum_{m=0}^{\infty} \frac{U_m(x)}{m+1} t^{m+1} \right) \\ &= \sum_{n=0}^{\infty} P_n^{\alpha}(x; z) t^n, \quad |t| < 1 \end{aligned} \quad \text{(B1)}$$

where $x = \cos\theta$, $\gamma = -(2z/\beta)[(1-x)/(1+x)]^{1/2}$, and $U_m(x)$ is the Chebyschev polynomial. Another way of defining the polynomials is recursively:

$$\begin{aligned} &P_{-1}^{\alpha}(x, z) = 0, \quad P_0^{\alpha}(x; z) = 1, \\ &(n+1) P_{n+1}^{\alpha} - 2[x(n + \alpha + 2z/\lambda) - 2z/\lambda] P_n^{\alpha} + (n + 2\alpha - 1) P_{n-1}^{\alpha} = 0, \end{aligned} \quad \text{(B2)}$$

and explicitly the polynomials are given by

$$P_n^{\alpha}(x; z) = \frac{\Gamma(n+2\alpha)}{n!\,\Gamma(2\alpha)} e^{in\theta} \times {}_2F_1(-n, \alpha - i\gamma; 2\alpha; 1 - e^{-2i\theta}), \quad \text{(B3)}$$

with the important special case

$$P_n^{\alpha}(x; 0) = C_n^{\alpha}(x). \quad \text{(B4)}$$

These polynomials are orthogonal on the interval $[-1, +1]$ with weight function

$$\rho^{\alpha}(x; z) = (1/\pi) 2^{2\alpha - 1} e^{(2\theta - \pi)\gamma} (1 - x^2)^{\alpha - 1/2} |\Gamma(\alpha + i\gamma)|^2 \quad \text{(B5)}$$

and the orthogonality relation is

$$\int_{-1}^{+1} P_n^{\alpha}(x; z) P_m^{\alpha}(x; z) \rho^{\alpha}(x, z)\, dx = \frac{\Gamma(n+2\alpha)}{n!} \frac{\delta_{n,m}}{(n + \alpha + 2Z/\lambda)}. \quad \text{(B6)}$$

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[20]M. Abramowitz and I. A. Stegun, in Ref. 5, Chap. 25.

[21]Reference 5, p. 260.