New L^2 approach to quantum scattering: Theory

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By exploiting the soluble infinite tridiagonal (Jacobi)-matrix problem generated by evaluating a zeroth-order scattering Hamiltonian H_0 in a certain L^2 basis set, we obtain phase shifts, wave functions, etc., which are exact for a full Hamiltonian H in which only the potential V is approximated. Only bound-bound (L^2) matrix elements of the Hamiltonian and finite matrix manipulations are needed. The method is worked out here for s-wave scattering using Laguerre basis functions. Kato improvement of the results and necessary generalizations to many channels are treated.

I. INTRODUCTION

In atomic and nuclear scattering, it is often desirable to use Slater (Laguerre) or oscillator (Hermite) basis functions. This paper is the first of several in which we present a new method for performing scattering calculations entirely with square-integrable (L^2) functions. We develop techniques in which we attempt to take full advantage of the analytic properties of a given Hamiltonian and also of the L^2 basis which is used to describe the wave function. Specifically, in what follows, we develop the basic theory using Laguerre-type basis functions appropriate for s-wave scattering. In the following paper,[1] we will apply the method to electron-hydrogen elastic s-wave scattering below the $n=2$ threshold, and to inelastic radial-limit scattering calculations above and below the ionization threshold.

Our basic approach is to treat an uncoupled Hamiltonian H_0 exactly in the space spanned by the complete L^2 basis. The remaining part of the Hamiltonian (i.e., the potential) is approximated to some desired degree of accuracy, V^{approx}, such that the resulting Hamiltonian H_0+V^{approx} is also exactly soluble in the complete L^2 space. Phase shifts and cross sections can then be extracted from the resulting wave function ψ_E. This wave function has the desirable property of being an exact solution to a well-defined scattering Hamiltonian. If V^{approx} is a good representation of the exact potential, and if second-order accuracy is desired, then ψ_E may be considered as a trial wave function in the standard variational formulas.

By an exact solution χ_E to the Hamiltonian H_0+V, we mean of course,

$$(H_0+V-E)|\chi_E\rangle=0. \tag{1.1}$$

In a space of complete L^2 functions $\{\phi_n\}$, where χ_E is expanded as $\chi_E=\sum_0^\infty b_n\phi_n$, Eq. (1.1) is equivalent to

$$\langle\phi_m|(H_0+V-E)|\chi_E\rangle=0 \tag{1.2}$$

for all $m=0,1,2,\ldots\infty$. For most potentials considered in scattering theory, it will not be possible to satisfy Eq. (1.2).

However, consider the basis set $\{\phi_m\}_{m=0}^\infty$ such that

$$\phi_m(r)=(\lambda r)e^{-\lambda r/2}L_m^1(\lambda r), \tag{1.3}$$

where λ is a scaling parameter. In Sec. II A, we show that by writing $\chi_E^0=\sum_0^\infty b_n^0\phi_n$, the similar equation

$$\langle\phi_m|(H_0-E)|\chi_E^0\rangle=0, \quad m=0,1,\ldots,\infty \tag{1.4}$$

where $H_0=-\frac{1}{2}d^2/dr^2$, leads to a soluble Jacobi-matrix problem for the b_n^0's. The properties of the Jacobi matrix representation of H_0 in the L^2 basis play a central role in our method. For this reason we call our approach the Jacobi (or J-) matrix method.

In Sec. II B, we construct a solution ψ_E for

$$\langle\phi_m|(H_0+V^N-E)|\psi_E\rangle=0, \quad m=0,1,\ldots,\infty \tag{1.5}$$

where V^N is an $N\times N$ matrix representation of V in the set $\{\phi_n\}$, thus achieving the goal of obtaining an exact solution to the Hamiltonian with an approximating potential. In Sec. III, we employ this wave function as a trial function in the Kato variational formula.[2] In Sec. IV, the necessary extension to multichannel scattering is developed. In Sec. V, a brief discussion is presented.

II. POTENTIAL SCATTERING

A. The unperturbed Hamiltonian H_0

Our task in this section is to determine the coefficients b_n^0 of the expansion of χ_E^0 in Eq. (1.4) in terms of our basis set $\{\phi_n\}$. Substituting the expansion for χ_E^0 in Eq. (1.4) results in an infinite matrix problem for the set $\{b_n^0\}$:

$$J \cdot b^0 = 0, \tag{2.1}$$

where J is the matrix

$$\begin{aligned} J_{nm} &= \int_0^\infty \phi_n(r)\left(-\frac{1}{2}\frac{d^2}{dr^2} - E\right)\phi_m(r)\,dr, \\ &= (-1/\lambda)(n+1)(m+1)(E+\tfrac{1}{8}\lambda^2) \\ &\quad \times (2x\delta_{n,m} - \delta_{n,m-1} - \delta_{m,m+1}), \end{aligned} \tag{2.2}$$

where $x = (E-\frac{1}{8}\lambda^2)/(E+\frac{1}{8}\lambda^2)$. Note that J is an infinite tridiagonal (Jacobi) matrix. Equation (2.1) is thus a three-term recursion relation for the s_n's [where $b_n^0 = s_n/(n+1)$] of the form

$$2xs_n - s_{n-1} - s_{n+1} = 0, \quad \text{for } n \geq 1, \tag{2.3a}$$

with the initial relation

$$2xs_0 - s_1 = 0, \quad \text{for } n = 0. \tag{2.3b}$$

Equation (2.3a), being a second-order difference equation, naturally has two linearly independent solutions. However, Eq. (2.3b) provides a boundary condition and thereby completely determines the s_n's. Equation (2.3a) is the recursion relation satisfied by the Chebyschev polynomials,[3] and Eq. (2.3b) gives us those polynomials of the second kind. Therefore, we may write

$$s_n = \sin(n+1)\theta, \tag{2.4}$$

where $\cos\theta = x = (E-\frac{1}{8}\lambda^2)/(E+\frac{1}{8}\lambda^2)$. $s_n/\sin\theta$ is then an nth-order polynomial in x. A similar analysis of H_0 in the basis $\{\phi_n\}$ has been provided by Schwartz.[4] The expression for χ_E^0 then becomes

$$\begin{aligned} \langle r|\chi_E^0\rangle &= \sum_{n=0}^\infty \frac{s_n}{n+1}\phi_n(r) \\ &= \sum_{n=0}^\infty \frac{\sin(n+1)\theta}{n+1}\phi_n(r). \end{aligned} \tag{2.5}$$

Since we have now solved Eq. (1.4) exactly in the basis set, it is not surprising that the s_n's are simply the expansion coefficients of $\sin kr$ (with $E = \frac{1}{2}k^2$) in terms of the ϕ_n's.[5] Note that although we have used a discrete (L^2) basis, H_0 nonetheless has a continuous spectrum. This stems from the fact that the set $\{\phi_n\}$ is infinite and complete in r on $[0,\infty]$.

For the purpose of Sec. II B, we will require an independent solution to the three-term recursion relation (2.3a). Specifically, we wish to find a set $\{c_n\}$ such that the function

$$\tilde{C}(r) = \sum_{n=0}^\infty \frac{c_n}{n+1}\phi_n(r)$$

behaves as $\cos kr$ when $r \to \infty$. Since the c_n's form an independent solution to (2.3a), they satisfy the following equation:

$$2xc_n - c_{n-1} - c_{n+1} = 0, \quad n \geq 1 \tag{2.3c}$$

with the boundary condition

$$2xc_0 - c_1 = \beta \neq 0. \tag{2.3d}$$

It is easy to verify, because β is nonvanishing, that the differential equation satisfied by $\tilde{C}(r)$ is

$$(H_0 - E)\tilde{C}(r) = -\beta(E+\tfrac{1}{8}\lambda^2)e^{-\lambda r/2}. \tag{2.6}$$

By employing the Green's function $g(r,r') = (2\sin kr_< \cos kr_>)/k$ it can be readily shown that the solution to (2.6) is

$$\begin{aligned} \tilde{C}(r) &= -\frac{2\beta}{k}\left(E+\frac{\lambda^2}{8}\right) \\ &\quad \times \left[\left(\int_0^r \sin kr'\, e^{-\lambda r'/2}\,dr'\right)\cos kr \right. \\ &\quad \left. + \left(\int_r^\infty \cos kr'\, e^{-\lambda r'/2}\,dr'\right)\sin kr\right], \end{aligned}$$

which, upon carrying out the integration, reduces to

$$\tilde{C}(r) = -\beta(\cos kr - e^{-\lambda r/2}). \tag{2.7}$$

The requirement that $\tilde{C}(r) \to \cos(kr)$ as $r \to \infty$ means that $\beta = -1$. With this value for β, it is easily verified that $c_n = -\cos(n+1)\theta$ satisfies Eqs. (2.3c) and (2.3d). Therefore $\tilde{C}(r)$ now reads

$$\begin{aligned} \tilde{C}(r) &= \cos kr - e^{-\lambda r/2} \\ &= -\sum_{n=0}^\infty \frac{\cos(n+1)\theta}{n+1}\phi_n(r). \end{aligned} \tag{2.8}$$

Note the interesting property that $\tilde{C}(r)$ behaves regularly at the origin.

B. Adding an approximating potential

One way to introduce an approximation to V is to truncate the representation of V in the basis $\{\phi_n\}$ to an $N \times N$ matrix; we call this new potential V^N:

$$\begin{aligned} V_{nm}^N &= \int_0^\infty \phi_n(r)V(r)\phi_m(r)\,dr, \quad n,m \leq N-1 \\ &= 0, \qquad \text{otherwise.} \end{aligned} \tag{2.9}$$

Our task is to solve

$$\langle \phi_m | (H_0 + V^N - E) | \psi_E \rangle = 0, \quad m = 0, 1, \ldots, \infty \tag{2.10}$$

where $\psi_E = \sum_{n=0}^{\infty} d_n \phi_n(r)$. Schematically, these equations look like

$$\begin{array}{c} \\ 0 \\ \vdots \\ (N-1) \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccc} 0 & \cdots & (N-1) & \cdots \end{array} \\ \left[\begin{array}{cc|c} X\,X\,X\,X\,X\,X & & \\ X\,X\,X\,X\,X\,X & & \\ X\,X\,X\,X\,X\,X & & 0 \\ X\,X\,X\,X\,X\,X & & \\ X\,X\,X\,X\,X\,X & & \\ X\,X\,X\,X\,X\,X & X & \\ \hline & X\,X & X\,X \\ & & X\,X\,X \\ & & X\,X\,X \\ 0 & & X\,X\,X \\ & & 0 \end{array}\right] \end{array} \left[\begin{array}{c} d_0 \\ d_1 \\ \vdots \\ d_{N-1} \\ d_N \\ \vdots \end{array}\right] = \left[\begin{array}{c} 0 \\ 0 \\ \vdots \end{array}\right] \tag{2.11}$$

These equations can be solved in a number of ways. For example, one may use a matrix partitioning technique similar to Feshbach's method,[6] treating the infinite Jacobi "tail" of the matrix by folding it in as an optical potential. However, we approach the problem from a different viewpoint, noting that V^N couples only the first N functions ϕ_m, $m = 0, 1, \ldots, N-1$, to each other. Thus outside the space spanned by these N basis functions, we expect the sine-like and the cosine-like solutions, derived in Sec. II A, to be valid. Therefore we write our solution as

$$\psi_E = \tilde{\Phi} + \tilde{S} + t\tilde{C}, \tag{2.12}$$

where $\tilde{\Phi} = \sum_{n=0}^{N-1} \tilde{a}_n \phi_n$, $\tilde{S}$ is the sine-like expansion χ_E^0 of Eq. (2.5), and $\tilde{C}$ is the cosine-like solution of Eq. (2.8). The unknown coefficient t, then, corresponds to the tangent of the phase shift caused by V^N. Since the $\tilde{a}_n$'s are yet to be determined, we can absorb the first N terms in the expansion of $\tilde{S}$ and $\tilde{C}$ into the $\tilde{a}_n$'s, writing

$$\psi_E = \Phi + S + tC, \tag{2.13}$$

where

$$\Phi(r) = \sum_{n=0}^{N-1} a_n \phi_n(r), \tag{2.14a}$$

$$S(r) = \sum_{n=N}^{\infty} \frac{s_n}{n+1} \phi_n(r) = \sum_{n=N}^{\infty} \frac{\sin(n+1)\theta}{n+1} \phi_n(r), \tag{2.14b}$$

$$C(r) = \sum_{n=N}^{\infty} \frac{c_n}{n+1} \phi_n(r) = -\sum_{n=N}^{\infty} \frac{\cos(n+1)\theta}{n+1} \phi_n(r). \tag{2.14c}$$

The two forms (2.12) and (2.13) for ψ_E are, of course, equivalent, but (2.13) is more convenient.

We now proceed to verify that the $(N+1)$ unknowns $\{a_n, t\}$ are sufficient to determine an exact solution to the Hamiltonian $H_0 + V^N$. Equation (2.10) imposes a restriction on ψ_E for each m, $m = 0, 1, \ldots, \infty$. We group these restrictions into four cases: first, the $N-1$ conditions arising from $m = 0, 1, \ldots, N-2$; second, the case for $m = N-1$; third, the condition for $M = N$; and last, the remaining set of conditions arising from $m = N+1, N+2, \ldots, \infty$.

The first case leads to the $N-1$ equations

$$\sum_{n=0}^{N-1} (J_{mn} + V_{mn}^N) a_n = 0, \quad m = 0, 1, \ldots, N-2. \tag{2.15a}$$

In case two, we have the equation

$$\sum_{n=0}^{N-1} (J_{N-1,n} + V_{N-1,n}^N) a_n + \left(J_{N-1,N} \frac{c_N}{N+1} \right) t = -J_{N-1,N} \frac{s_N}{N+1}. \tag{2.15b}$$

In case three, V^N is no longer operative. We consequently get

$$J_{N,N-1} a_{N-1} + \left(J_{N,N} \frac{c_N}{N+1} + J_{N,N+1} \frac{c_{N+1}}{N+2} \right) t = -\left(J_{N,N} \frac{s_N}{N+1} + J_{N,N+1} \frac{s_{N+1}}{N+2} \right),$$

which, upon using the three-term recursion relation satisfied by both c_n and s_n, reduces to

$$J_{N,N-1}a_{N-1} - J_{N,N-1}(c_{N-1}/N)\,t = J_{N,N-1}(s_{N-1}/N). \tag{2.15c}$$

So far we have $(N+1)$ equations in $(N+1)$ unknowns. It would seem that we are left with an infinite number of equations arising from case four with no corresponding unknowns. Therefore, if we claim that $\psi = \Phi + S + tC$ is an exact solution for $H_0 + V^N$, then the remaining case-four equations, for $m = N+1, N+2, \ldots, \infty$, must be automatically satisfied. Fortunately, this is the case, because

$$\langle \phi_m | (H_0 + V^N - E) | \tilde{\Phi} + \tilde{S} + t\tilde{C} \rangle = \langle \phi_m | (H_0 - E) | S + tC \rangle \tag{2.16}$$

if $m \geq N+1$. Equation (2.16) follows from the fact that V^N is defined to be zero in this region of Hilbert space, and because $(H_0 - E)$ is tridiagonal in the basis $\{\phi_n\}$, and therefore does not connect the N terms in the expansion of $\tilde{\Phi}$ or the first N terms in the expansion of $\tilde{S}$ and $\tilde{C}$ with ϕ_m for $m > N+1$. Furthermore, for each $m \geq N+1$ the right-hand side of Eq. (2.16) leads to the three-term recursion relation (2.3a) and (2.3c) for the coefficients s_n's and c_n's. Therefore the right-hand side of Eq. (2.16) vanishes identically. Thus, we now have exactly $(N+1)$ equations to determine the $(N+1)$ unknowns $\{t, a_n\}$. Hence the form (2.13) for ψ_E is indeed capable of giving an exact solution to (2.10).

Equations (2.15) can be written in matrix form as

$$\left[\begin{array}{ccc|c} (J+V)_{0,0} & \cdots & (J+V)_{0,N-1} & 0 \\ (J+V)_{1,0} & \cdots & (J+V)_{1,N-1} & 0 \\ \vdots & & \vdots & \vdots \\ (J+V)_{N-1,0} & \cdots & (J+V)_{N-1,N-1} & 0 \\ \hline 0 & \cdots & J_{N,N-1} & -J_{N,N-1}c_{N-1}/N \end{array}\right] \left[\begin{array}{c} a_0 \\ a_1 \\ \vdots \\ a_{N-1} \\ \hline t \end{array}\right] = \left[\begin{array}{c} 0 \\ 0 \\ \vdots \\ 0 \\ \hline J_{N,N-1}s_{N-1}/N \end{array}\right] \tag{2.17}$$

Notice that the large $N \times N$ block of the coefficient matrix is composed of the matrix elements of $(H_0 + V^N - E)$ in the first N Laguerre basis functions. To perform a calculation, we need merely augment this $N \times N$ matrix with the extra row and column shown and with the right-hand side driving term. Equation (2.17) can be immediately solved for t by standard techniques. An illuminating formula for $\tan\delta = t$ can be obtained by prediagonalizing the inner $N \times N$ matrix $(H_0 + V^N - E)_{nm}$ with the energy-independent transformation Γ, where

$$[\tilde{\Gamma}(H_0 + V^N - E)\Gamma]_{nm} = (E_n - E)\delta_{n,m}. \tag{2.18}$$

Augmenting Γ to be the $(N+1) \times (N+1)$ matrix

$$\Gamma_A = \begin{pmatrix} \Gamma & 0 \\ 0 & 1 \end{pmatrix} \tag{2.19}$$

and applying it to Eq. (2.17), we obtain

$$t = \tan\delta = \frac{[\sin N\theta/N] + r(E)J_{N,N-1}[\sin(N+1)\theta/(N+1)]}{[\cos N\theta/N] + r(E)J_{N,N-1}[\cos(N+1)\theta/(N+1)]}, \tag{2.20}$$

where $r(E) = \sum_{m=0}^{N-1} \Gamma^2_{N-1,m}/(E_m - E)$. In arriving at (2.20), we have used the fact that $s_n = \sin(n+1)\theta$ and $c_n = -\cos(n+1)\theta$. Note that the entire energy dependence of the phase shift is given analytically by Eq. (2.20). It is interesting that at the N Harris eigenvalues[7] E_m, $\tan\delta$ becomes simply

$$\tan\delta(E_m) = \tan(N+1)\theta(E_m). \tag{2.21a}$$

Also at the $N-1$ points E_μ, where $r(E_\mu) = 0$, we have

$$\tan\delta(E_\mu) = \tan N\theta(E_\mu). \tag{2.21b}$$

III. KATO CORRECTION

The results of Sec. II are sufficient for obtaining the exact solution ψ_E and the exact $\tan\delta = t$ for the Hamiltonian $H_0 + V^N$ at energy E. Compared to the wave function and the phase shift for the exact Hamiltonian $H_0 + V$, ψ_E and t in general contain first-order errors. However, we may reduce these errors to second order by employing ψ_E as a trial function in the Kato[2] formula. If we write ψ_t for ψ_E of Eq. (2.12) and $\tan\delta_t$ for $\tan\delta$ of Eq. (2.20), then the Kato formula reads

$$\tan\delta_s = \tan\delta_t - \frac{2}{k}\int_0^\infty \psi_t(E - H)\psi_t\, dr, \tag{3.1}$$

where $\tan\delta_s$ is the stationary result.

Since $(H_0 + V^N - E)\psi_t = 0$, we can write the last equation as

$$\tan\delta_s = \tan\delta_t + (2/k)\langle\psi_t|(V - V^N)|\psi_t\rangle,$$
$$\equiv \tan\delta_t + (2/k)\langle\psi_t|V^R|\psi_t\rangle. \quad (3.2)$$

Equation (3.2) is just the distorted-wave Born formula, where V^N is the distorting potential and V^R is the perturbation which has been excluded from the calculation of $\tan\delta_t$. In order to perform the integral in Eq. (3.2), bound-free and free-free matrix elements of the potential are required. An approximation to the Kato correction (3.2) which involves only bound-bound matrix elements of V is considered in the next paper.[1]

IV. MANY-CHANNEL SCATTERING

In this section, we extend the previous potential scattering formulas to allow collision with targets possessing internal states. Basically we will be treating the close-coupling equations, employing an s-wave Laguerre set to describe the projectile wave function in each channel. As in the close-coupling formalism, we can treat exchange by the addition of a nonlocal potential.

Assuming the target possesses coordinates which we collectively call ρ, the Schrödinger equation for the many-particle wave function Θ reads

$$\left(H_T(\rho) - \frac{1}{2}\frac{\partial^2}{\partial r^2} + V(\rho, r) - E\right)\Theta = 0. \quad (4.1)$$

In the above equation, H_T is the given target Hamiltonian, r is the projectile coordinate, and $V(\rho, r)$ is the interaction with the target constituents. We assume that the target Hamiltonian posses a discrete set of L^2 eigenfunctions χ_α such that

$$H_T\chi_\alpha = E_\alpha\chi_\alpha, \quad \alpha = 1, \ldots, \infty. \quad (4.2)$$

If the target has a dense or continuous spectrum, the method of pseudotarget states may be employed.[8] This is done in the following paper for the case of electron-hydrogen scattering.

As in the one-particle case, we will not be able to solve Eq. (4.1) for Θ exactly in the Hilbert space which is spanned by the set

$$\{|\chi_\alpha\rangle|\phi_n^{(\alpha)}\rangle\}, \quad \alpha = 1, \ldots, \infty,$$
$$n = 0, 1, \ldots, \infty. \quad (4.3)$$

The functions $\{\phi_n^{(\alpha)}\}$ are the s-wave Laguerre set

$$\phi_n^{(\alpha)}(r) = (\lambda_\alpha r)e^{-\lambda_\alpha r/2}L_n^1(\lambda_\alpha r). \quad (4.4)$$

Here we have allowed the projectile basis to be channel-dependent through the scaling parameter λ_α. We again truncate V by defining an approximate potential $\tilde{V}$ which has the matrix elements

$$\tilde{V}^{\alpha\alpha'}_{nn'} \equiv \langle\chi_\alpha\phi_n^{(\alpha)}|V(\rho, r)|\chi_{\alpha'}\phi_n^{(\alpha')}\rangle \quad (4.5)$$

for $\alpha, \alpha' \leq N_c$ and $n \leq N_\alpha - 1$, $n' \leq N_{\alpha'} - 1$. We define $\tilde{V}^{\alpha\alpha'}_{nn'} \equiv 0$ otherwise. The number N_α is the truncation limit in the channel α and N_c is the total number of channels which are allowed to couple.

To determine an S matrix, we will need N_0 independent solutions Θ_α of Eq. (4.1), where N_0 is the number of open channels. In the same spirit as in the single-channel case, we expand Θ_α as

$$\Theta_\alpha = \Phi_\alpha + \frac{\chi_\alpha S_\alpha}{\sqrt{k_\alpha}} + \sum_{\alpha'=1}^{N_c}\frac{R_{\alpha\alpha'}\chi_{\alpha'}C_{\alpha'}}{\sqrt{k_{\alpha'}}},$$
$$\alpha = 1, \ldots, N_0. \quad (4.6)$$

The quantities k_α are the channel momenta $k_\alpha = (2|E_\alpha - E|)^{1/2}$, where E_α is the channel energy appearing in Eq. (4.2). Analogous to the one-channel case, the S_α's and C_α's for open channels (see below for closed channels) are

$$S_\alpha = \sum_{n=N_\alpha}^{\infty}\frac{\sin(n+1)\theta_\alpha}{n+1}\phi_n^{(\alpha)},$$
$$C_\alpha = -\sum_{n=N_\alpha}^{\infty}\frac{\cos(n+1)\theta_\alpha}{n+1}\phi_n^{(\alpha')}; \quad (4.7)$$
$$\theta_\alpha = \cos^{-1}[(k_\alpha^2 - \tfrac{1}{4}\lambda_\alpha^2)/(k_\alpha^2 + \tfrac{1}{4}\lambda_\alpha^2)].$$

The internal function Φ_α is given by

$$\Phi_\alpha = \sum_{\alpha'=1}^{N_c}\sum_{n=0}^{N_{\alpha'}-1} a^\alpha_{\alpha' n}\chi_{\alpha'}\phi_n^{(\alpha)}. \quad (4.8)$$

The $a^\alpha_{\alpha' n}$'s are the expansion coefficients to be determined. The number of these coefficients is $\sum_{\alpha'=1}^{N_c} N_{\alpha'}$. The remaining unknowns $R_{\alpha\alpha'}$ are of course the elements of a reactance matrix which may be used to determine the S matrix as

$$S = (1 + i[R])(1 - i[R])^{-1}, \quad (4.9)$$

where $[R]$ is the $N_0 \times N_0$ open channel part of R.

The sum in (4.6) should formally be extended to infinity, but since $\tilde{V} \equiv 0$ for any channel $\alpha > N_c$, $R_{\alpha\alpha'}$ vanishes for α or $\alpha' > N_c$. Actually the sum need only be over open channels. But if we do things this way, we place the burden of describing the exponentially decaying closed-channel asymptotic behavior on the internal function Φ_α. Near the threshold of channel $\alpha' = N_0 + 1$, however, the decay will be so slow that Φ_α will be incapable of properly describing the asymptotic behavior. Fortunately, we can allow the sum to include the closed channels up to N_c because we can find functions $C_\alpha(r)$ that can describe the asymptotic behavior in the closed channels in the same way that $C_\alpha(r)$ and $S_\alpha(r)$ do for open channels. The proper asymptotic form in a closed channel α is $e^{-|k_\alpha|r}$. A function which has this asymptotic form can be obtained by combining the expressions for $\tilde{S}_\alpha$ and $\tilde{C}_\alpha$ for imaginary $ik_\alpha = i(2|E_\alpha - E|)^{1/2}$.

The resulting function and its expansion in terms of the basis set is given by

$$\tilde{C}_\alpha(r) = e^{-k_\alpha r} - e^{-\lambda_\alpha r/2} = \sum_{n=0}^{\infty} \frac{(-1)^n e^{-(n+1)\eta_\alpha}}{n+1} \phi_n^{(\alpha)} \tag{4.10a}$$

for $k_\alpha \leq \lambda_\alpha/2$ and where

$$\eta_\alpha = \cosh^{-1}\left|\frac{k_\alpha^2 + \lambda_\alpha^2/4}{k_\alpha^2 - \lambda_\alpha^2/4}\right|.$$

For $k_\alpha > \lambda_\alpha/2$ the formula reads

$$\tilde{C}_\alpha(r) = \sum_{n=0}^{\infty} \frac{e^{-(n+1)\eta_\alpha}}{n+1} \phi_n^{(\alpha)}. \tag{4.10b}$$

The form (4.10b) is really not needed, since for $k_\alpha > \lambda_\alpha/2$ the decay is rapid enough to be described by Φ_α.

We wish to show that Θ of Eq. (4.6) is capable of describing the exact solution for the problem

$$\left(H_T - \frac{1}{2}\frac{\partial^2}{\partial r^2} + \tilde{V} - E\right)\Theta_\alpha = 0. \tag{4.11}$$

We demand that all projections by $\langle \chi_\beta \phi_n^{(\beta)}|$ from the left vanish:

$$\langle \chi_\beta \phi_n^{(\beta)}| \left(H_T - \frac{1}{2}\frac{\partial^2}{\partial r^2} + \tilde{V} - E\right)|\Theta_\alpha\rangle = 0. \tag{4.12}$$

We need not consider the χ_β's for $\beta > N_c$, for in this case it is easy to show that the left-hand side of (4.12) is identically zero. Consider now a typical projection for $\beta < N_c$. It can readily be written as

$$\left\langle \phi_m^{(\beta)} \middle| -\frac{1}{2}\frac{\partial^2}{\partial r^2} - (E - E_\beta) \middle| \sum_{n=0}^{N_\beta - 1} a_{\beta n}^{\alpha} \phi_n^{(\beta)} + \frac{S_\alpha \delta_{\alpha\beta}}{k_\alpha^{1/2}} + \frac{R_{\alpha\beta} C_\beta}{k_\beta^{1/2}} \right\rangle + \sum_{\alpha'=1}^{N_c} \left\langle \phi_m^{(\beta)} \middle| V^{\beta\alpha'} \middle| \sum_{n=0}^{N_{\alpha'}-1} a_{\alpha' n}^{\alpha} \phi_n^{(\alpha')} \right\rangle = 0. \tag{4.13}$$

We will not consider the four cases for m as is done in the single-channel case, but show instead that for $m > N_\beta$ the left-hand side of (4.13) also vanishes identically. First, the potential term vanishes by the definition of $\tilde{V}$ for $m > N_\beta$. Second, $[-\frac{1}{2}(\partial^2/\partial r^2) - (E - E_\beta)]$ is tridiagonal in the $\{\phi^{(\beta)}\}$. Thus, there will be no overlap between $\phi_m^{(\beta)}$ and the first N_β functions $\phi_n^{(\beta)}$. Then (4.13) becomes

$$\left\langle \phi_m^{(\beta)} \middle| -\frac{1}{2}\frac{\partial^2}{\partial r^2} - (E - E_\beta) \middle| \frac{S_\alpha \delta_{\alpha\beta}}{k_\alpha^{1/2}} + \frac{R_{\alpha\beta} C_\beta}{k_\beta^{1/2}} \right\rangle = 0. \tag{4.14}$$

But this is automatically true for $m > N_\beta$, in direct analogy with the single-channel case, because of the three-term recursion relation satisfied by the coefficients of S_β and C_β. The remainder of the equations; i.e., Eq. (4.13) for $m \leq N_\beta$, lead to the same number of conditions as there are unknowns. The totality of these equations can be organized in a similar fashion as done in the form (2.17), with the L^2 matrix elements of $\tilde{V}$ appearing in a large inner block. One extra row and column are added to this block for each channel $\alpha \leq N_c$. The right-hand side driving term and the solution "vector" containing the $a_{\beta n}^{\alpha}$'s and $R_{\alpha\alpha'}$'s have as many columns as open channels. The R matrix can then be obtained by solving the resulting linear equations. As before, the calculation may be facilitated by a prediagonalization of the inner block using an energy-independent transformation.

V. DISCUSSION

The comparison between the approach taken in this paper and the R-matrix method is considered first. In R-matrix theory,[9] Hilbert space is divided into two parts, an inner coordinate-space up to a radius A and the remaining space from A to infinity. In the present work and in the spirit of Feshbach's generalization of R-matrix theory,[6] we have divided the Hilbert space into two function spaces. We have an inner space consisting of those functions coupled by $V^N(\phi_n, n = 0, 1, \ldots, N-1)$, and an outer space in which the Hamiltonian is already solved and consists of the remaining functions $(\phi_n, n = N, \ldots, \infty)$. It is interesting to compare the Wigner R matrix which has the form

$$R(E) = \frac{1}{2}\sum_n \frac{[\psi_n(A)]^2}{E_n - E} = \sum_n \frac{\gamma_n^2}{E_n - E}$$

with what we have designated $r(E)$ in Eq. (2.20):

$$r(E) = \sum_n \frac{\Gamma_{N-1,n}^2}{E_n - E}.$$

If the set $\{\phi_n\}$ were orthogonal, $\Gamma_{N-1,n}$ would just be

$$\Gamma_{N-1,n} = \langle \phi_{N-1} | \psi_n \rangle.$$

Note that $\Gamma_{N-1,n}$ and γ_n are both the components of the wave function ψ_n at the boundary of their respective inner spaces.

Recent work seems to indicate that the R-matrix method works best using eigenfunctions of the scattering H_0 as a basis.[10] In this basis, H_0 is of course diagonal, and may be treated exactly by the addition of the Buttle correction. In our basis set, H_0 is tridiagonal and is also treated exactly. Other types of basis sets can also be used in the R-matrix method. In general, however, the ability

to account for H_0 exactly is lost. The same is true in the present method, in the analogous situation when other basis functions not belonging to the tridiagonal set $\{\phi_n\}$ are used.

As in the R-matrix approach, we expect to find no Kohn-type pseudoresonances[11] appearing in computed cross sections. Because in some sense V^N uniformly approximates V, we expect ψ^N to uniformly approximate ψ as $N \to \infty$. A series of ever denser, but narrower pseudoresonances as found by Schwartz in this limit seems rather unlikely. This conjecture has been borne out by extensive calculations, some of which appear in the next paper.[1]

It is interesting to note that our truncated potential V^N leads to a separable kernel[12] in the T-matrix equation

$$T = V + VG^0 T.$$

It is easy to see that T possesses nonvanishing matrix elements only in the same L^2 subspace as that of V^N. This means that we can solve the finite matrix problem

$$T_{n'n} = V^N_{n'n} + \sum_{m,l=0}^{N-1} V^N_{n'm} G^0_{ml} T_{ln};$$

$$n' = 0, \ldots, N-1, \quad n = 0, \ldots, N-1. \tag{5.1a}$$

Then, the on-shell T matrix is obtained as

$$\sum_{n,n'=0}^{N-1} \langle E_0|n\rangle T_{nn'} \langle n'|E_0\rangle, \tag{5.1b}$$

where $|E_0\rangle$ is the properly normalized continuum eigenfunction of H_0. Compared to the approach taken in Secs. II–IV, the separable approach leads to a less convenient algorithm. The kernel of Eq. (5.1a) is energy dependent and must be regenerated, and the linear equations must be resolved, at each new value of the total energy.

Finally, we compare the Jacobi-matrix approach to the recently developed L^2 Fredholm techniques.[13–15] Both approaches enjoy the advantage of requiring only L^2 matrix elements of the potential. The L^2 Fredholm method employs the devices of analytic continuation,[13] dispersion correction,[14] and contour rotation.[15] These techniques can be viewed as supplying, in an approximate fashion, information about the continuous spectrum of H_0 which is not explicitly contained in a finite L^2 matrix representation. Unfortunately, the amount of information concerning H_0 that can be extracted decreases with the number of basis functions per channel, and this can cause difficulties when basis size is a restriction. On the other hand, approximate treatment of H_0 can be advantageous when for example channel threshold details are of no interest or are unwanted artifacts of particular models. In the J-matrix method, H_0 is accounted for exactly independent of basis size. Thus we start with a large part of the problem "diagonalized" and the full analytic structure of the S matrix is built into the problem, raising the hope that quite small basis sets will be sufficient for many problems. The analytic nature of the solutions allows variational corrections to be made and provides a solid footing for further theoretical work.

We now summarize the steps necessary to perform a calculation with the J-matrix method. First, the potential V^N (or $\tilde{V}$) is evaluated in the Laguerre basis set; and is then added to the $N \times N$ tridiagonal representation of $H_0 - E$. To this inner matrix we add one extra row and column, for each asymptotic channel, containing matrix elements of H_0 and the $\cos(n+1)\theta$ terms. The right-hand side "driving" terms are similarly constructed with the $\sin(n+1)\theta$ terms. The resulting linear equations can be solved efficiently if a prediagonalizing transformation Γ is applied to the inner matrix as in Sec. II. If desired, the matrix elements of $H_0 + V^N - E$ can be evaluated in the Slater set $(\lambda r)^n e^{-\lambda r/2}$, $n = 1, 2, \ldots, N$, since these are just transformed Laguerres. Then a different transformation Γ' will be necessary to prediagonalize the inner matrix.

In the following paper we apply the method presented here to s-wave electron-hydrogen scattering model. The generalization of the method to all partial waves for both Laguerre and Hermite basis sets has been derived and will be the subject of a future publication. The case where H_0 contains the term α/r (i.e., the Coulomb case) is also worked out for Laguerre sets.

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