Weyl's theory in an L^2-basis Gauss quadrature of the spectral density

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When a complete orthonormal square-integrable real basis set $\{\chi_n\}$ can be found in which a model one-dimensional Hamiltonian H_0 is represented by an infinite symmetric tridiagonal matrix, analysis of the spectrum of H_0 leads to a close analogy of Weyl's theory of the Schrödinger equation. With H_0 tridiagonal, the Schrödinger equation becomes a three-term recursion relation in n instead of a differential equation. The Sturm-sequence polynomials $p_n(E)$ form the solution regular at $n=0$, while a second, Weyl's solution $q_n(E)$, is irregular. Then the resolvent $(E-H_0)^{-1}$ is proportional to $p_{n_<}q_{n_>}$. Furthermore, completeness implies the orthogonality of the p_n, and hence, that truncating to a finite basis generates a Gauss quadrature of the spectral density with abscissas at the eigenvalues of the truncated H_0, and just as in Weyl's theory, approximating the spectral density as a Stieltjes integral. By truncating the representation of any additional potential to a finite matrix, the theory can be extended in analogy to R-matrix theory to potential and even multichannel scattering, yielding an explicit construction of the Fredholm determinant, whose zeros locate the resonances and bound states. In addition, such an analysis reveals, at least in the basis sets in which H_0 is tridiagonal, how other L^2-function methods such as stabilization, Stieltjes imaging, and coordinate rotation work and how accurate they are.

I. INTRODUCTION

The usual approach to solving for the lowest few bound states of an atomic system entails transforming the Schrödinger differential equation into a linear-algebra eigenvalue problem by introducing a set of square-integrable (L^2) basis functions. Recently, several methods[1-8] have been developed which extract such information as resonance energies and widths and scattering cross sections from the same L^2-basis matrix representation of the Hamiltonian. While it is evident how a well-chosen L^2 basis can approximate a bound state, it is less clear how to obtain properties of the scattering continuum from a set of functions which vanish exponentially at large distances. In the first paper in this series[5] (hereinafter referred to as I), we showed that diagonalizing certain Hamiltonians having no bound states in certain L^2 bases in which the Hamiltonian matrix is tridiagonal generates a Gaussian quadrature[9,10] of the continuum having abscissas at the eigenvalues and weights related to the correctly normalized continuum wave functions. Here, we extend these results to any real symmetric tridiagonal Hamiltonian matrix, and in so doing illuminate connections with and thereby provide a particular justification of other L^2 methods.

Restricting the Hamiltonian to tridiagonal form means that the second-order differential Schrödinger equation is transformed into its direct discrete analogy—a three-term recursion relation. Since an understanding of scattering as a perturbation of the continuum requires both of the linearly independent solutions, the careful analysis introduced by Weyl[11] provides the best path for developing the analogy. Atkinson[12] has already followed this path to display the full parallelism of the two Sturm-Liouville boundary-value problems. Here, we apply his results where the continuous Sturm-Liouville differential equation is transformed into the discrete Sturm sequence by introducing an L^2 basis and concentrate on what happens to the scattering physics.

In Sec. II, we examine the representation of the spectrum in a finite L^2 basis to produce the Stieltjes-integral approximation to the spectral density on which Langhoff[8] based his Stieltjes imaging approach. In a finite basis, incidentally, limiting the Hamiltonian to tridiagonal form is no great restriction, for the standard method of diagonalizing an Hermitian matrix employs a Householder[13] tridiagonalization as its first step. Here the analogy between the finite-basis results and Weyl's theory on the finite interval could not be more complete.

The payoff comes, however, in Sec. III, where we consider the limit as the number of basis functions becomes infinite and the basis becomes complete. Since finding such a basis which renders the Hamiltonian tridiagonal is tantamount to solving the original differential equation exactly, the restriction to tridiagonal form is severe, but is warranted by the insight which it affords into how a finite portion of the basis can interpolate properties of the continuum. To no great surprise, the Stieltjes limit of the spectral density produces a weight function which rises abruptly at each bound state and smoothly in the continuum and with respect to which the Sturm-sequence polynomials are orthogonal, and suggests a direct analogy to Weyl's function.[11] Furthermore, the results justify the stabilization method,[1] Langhoff's Stieltjes imaging,[8] and Heller's derivative rule[4,5] as interpolation schemes for the finite bases and indicate how the rotated-coordinate method[2] circumvents satisfying the scattering boundary conditions. In addition to the radial kinetic energy in oscillator and Slater basis sets already discussed in I, we present, as further examples, an analysis of the harmonic and Morse[14] oscillators in the Appendix. The Coulomb Hamiltonian and its special properties will be treated in a subsequent paper.

As was shown in I, the restriction of H to tridiagonal form can fruitfully be relaxed by adding a potential V of finite rank—i.e., represented in a finite basis—to any infinitely tridiagonal H. A Householder reduction,[13] carried out in reverse order, then folds $H+V$ into an infinite tridiagonal form $\tilde{H}$ for which all the results of Sec. III hold. Following this idea in Sec. IV, we study the perturbation of the spectrum of H by the potential to yield the J-matrix method[6] of approximating the phase shift as well as an explicit expression for the Fredholm determinant as the ratio of the weight functions with respect to which the respective Sturm-sequence polynomials of $\tilde{H}$ and H are orthogonal. The parallel with the R-matrix theory[7] of fitting the logarithmic derivative at the boundary of the space in which the potential is represented is then evident.

Finally, in Sec. V, we discuss extensions to Coulomb and multichannel scattering as well as possible application in conjunction with the Schwinger method[3] and to the calculation of resonance phenomena and three-body scattering.

II. FINITE BASIS SET

Consider a set of real functions $\{\chi_n(r): n=0,1,2,\ldots,N-1\}$ which are square integrable on the interval $(0,\infty)$,[15] and, indeed, form a basis of $L^2(0,\infty)$ as the number of functions N goes to infinity. Assume, in addition, that the functions are orthonormal[16]:

$$\int_0^\infty dr\,\chi_n(r)\chi_{n'}(r)=\delta_{nn'}\,, \tag{1}$$

and most importantly, that the basis transforms the Hamiltonian operator into a real symmetric tridiagonal matrix:

$$H_{nn'}=\int_0^\infty dr\,\chi_n(r)H\chi_{n'}(r)=0\,,$$
$$\text{unless } n'=n,\ \text{or}\ n\pm1\,. \tag{2}$$

Expanding a solution of the Schrödinger equation, for example, the scattering solution, in the basis formally as

$$\psi^+(r,E)=\sum_{n=0}^{\infty}\chi_n(r)\psi_n^+(E) \tag{3}$$

transforms the differential equation into a three-term recursion relation:

$$H_{n,n+1}\psi_{n+1}^+(E)+(H_{n,n}-E)\psi_n^+(E)+H_{n,n-1}\psi_{n-1}^+(E)=0\,. \tag{4a}$$

If the χ_n are chosen to mimic the regular behavior of the wave function dictated by the behavior of H at the left-hand boundary, the recursion will start with the boundary condition

$$H_{0,-1}\psi_{-1}^+(E)=0\,. \tag{4b}$$

While, as depicted by Hazi and Taylor, the expansion ansatz [Eq. (3)] should perform well for r not too large, the convergence behavior for representing a function which oscillates more or less rapidly depending on E at large r in terms of an L^2 basis will be highly nonuniform in n and E.

Now, just as with the differential equation, the boundary condition [Eq. (4b)] selects one of the two possible basic solutions which is propagated by Eq. (4a) in n, one more condition is needed to fix the normalization. Since the normalization of the scattering solution depends on the behavior at the other end of the interval—a concept rather difficult to define in terms of the formal expansion [Eq. (3)]—we follow the usual practice with the differential equation to define a regular solution $p_n(E)$, by setting

$$p_0(E)=1 \text{ and } H_{0,-1}p_{-1}=0\,, \tag{5}$$

and defer the normalization to Sec. III. From the recursion equation (4a) and these bounday conditions,[17] $p_n(E)$ is clearly a polynomial of degree n in

E, known up to a factor dependent on n as the Sturm-sequence[13] polynomial.

Applying a boundary condition at some finite $n=N$ defines, just as for the finite interval in r for the differential equation, an eigenvalue problem in E. To keep the development parallel with Weyl's theory, we follow Atkinson[12] and examine the boundary condition

$$p_n(E)+\tan\beta\, H_{N,N-1}p_{N-1}(E)=0\ , \tag{6}$$

where β is some fixed angle in $[-\pi/2,\pi/2]$.[18] Green's identity then relates the values at the boundaries with the integral—here, sum—of the squares of the values in between; examining $\sum p_n(E)p_n(E')$ yields the Christoffel identity

$$(E-E')\sum_{n=0}^{N-1} p_n(E)p_n(E')=H_{N,N-1}[p_N(E)p_{N-1}(E')-p_N(E')p_{N-1}(E)]\ , \tag{7a}$$

with the on-shell limit,

$$\sum_{n=0}^{N-1} p_n^2(E)=H_{N,N-1}(p'_N p_{N-1}-p_N p'_{N-1})\ , \tag{7b}$$

and the complex-energy case

$$\sum_{n=0}^{N-1} |p_n(E)|^2(2i\ \mathrm{Im}E)=H_{N,N-1}[p_N(E)p_{N-1}(E^*)-p_N(E^*)p_{N-1}(E)]\ , \tag{7c}$$

where E^* is the complex conjugate of E and $p_n(E^*)$ of $p_n(E)$.

The fact that the right-hand side of Eq. (7a) plays the role the Wronskian plays in the theory of the differential equation becomes still more clear when we introduce a second polynomial solution of the recurrence relation $\bar{q}_n(E)$ which obeys the boundary conditions

$$\bar{q}_0(E)=0 \text{ and } H_{0,-1}\bar{q}_{-1}=-1\ . \tag{8}$$

Then, Green's theory gives

$$(E-E')\sum_{n=0}^{N-1} p_n(E')\bar{q}_n(E)=H_{N,N-1}[\bar{q}_N(E)p_{N-1}(E')-\bar{q}_{N-1}(E)p_N(E')]-1\ , \tag{9a}$$

while for $E'=E$,

$$H_{n,n-1}(\bar{q}_n p_{n-1}-\bar{q}_{n-1}p_n)=1\ . \tag{9b}$$

To be sure, the parallel with the Wronskian of the two solutions of a Sturm-Liouville differential equation is not quite in the traditional form; what we have called the regular solution p_n starts in Eq. (5) with what corresponds to unit value and zero derivative, while the second solution $\bar{q}_n$ starts in the opposite way.

Extracting the consequences of imposing the boundary value of Eq. (6) at finite N on the Christoffel identities, Eq. (7a), then completes the analogy with Weyl's theory of the finite interval. In addition to establishing various separation properties of the eigenvalues $E_j^N(\beta)$, depending on N and β, including what is known as the Hylleraas-Undheim theorem,[19] Atkinson[12] derives two types of orthogonality closely related to the orthonormality and completeness of the solutions of the Schrödinger equation. These are most readily understood when the recursion equation (4) is combined with the initial boundary conditions (5) into the truncated matrix equation,

$$\begin{bmatrix} H_{00}-E & H_{0,1} & 0 & 0 & 0 \\ H_{1,0} & H_{1,1}-E & H_{1,2} & 0 & 0 \\ 0 & H_{2,1} & H_{2,2}-E & 0 & 0 \\ 0 & 0 & 0 & H_{N-2,N-2}-E & H_{N-2,N-1} \\ 0 & 0 & 0 & H_{N-1,N-2} & H_{N-1,N-1}-\tan\beta\, H_{N,N-1}^2-E \end{bmatrix} \begin{bmatrix} p_0(E) \\ p_1(E) \\ p_2(E) \\ p_{N-2}(E) \\ p_{N-1}(E) \end{bmatrix}$$

$$= \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -H_{N-1,N}p_N(E)+\tan\beta\, H_{N,N-1}p_{N-1}(E) \end{bmatrix} . \quad (10)$$

Hence, the values of $E_j^N(\beta)$ fulfilling the boundary condition in Eq. (6) are the eigenvalues of the truncated Hamiltonian matrix, $H^N(\beta)$ on the left-hand side, while the $p_n(E_j^N)$ clearly form the components of the eigenvector. Setting E to one eigenvalue and E' to another in Eq. (7a) and using the separation of the eigenvalues leads in the usual way, to the orthogonality of the eigenvectors and allows the definition of orthornormal eigenvector components,

$$\psi_{nj}^N(\beta)=p_n(E_j^N)(w_j^N)^{1/2} , \quad (11)$$

obeying

$$\sum_{n=0}^{N-1} \psi_{ni}^N\psi_{nj}^N=\delta_{ij} , \quad (12)$$

where the normalization factor is simply the Christoffel weight,[10]

$$w_j^N(\beta)=1\Big/\sum_{n=0}^{N-1} p_n^2(E_j^N(\beta)) . \quad (13)$$

The second type of orthogonality, which corresponds to the completeness of the eigenvectors in the truncated function space, follows from the first,[12] giving

$$\sum_{j=1}^{N} \psi_{nj}^N\psi_{n'j}^N=\sum_{j=1}^{N} w_j^N p_n(E_j^N)p_{n'}(E_j^N)=\delta_{nn'} . \quad (14)$$

This is nothing more than a Gaussian quadrature[10,12] of the resolution of the identity.

To prepare the passage to the large-N limit, it is useful to cast these properties of the solutions in the language of Stieltjes integrals. Atkinson[12] defines the spectral function $\rho_\beta^N(E)$ as a nondecreasing right-continuous function with jumps at each eigenvalue equal to the corresponding Christoffel weight:

$$\rho_\beta^N(E)=\begin{cases} \displaystyle\sum_{0<E_j\le E} w_j^N(\beta), & E\ge 0 \\ \displaystyle -\sum_{E<E_j\le 0} w_j^N(\beta), & E>0 . \end{cases} \quad (15)$$

Then, the completeness orthogonality in Eq. (14) can be cast as the Stieltjes integral:

$$\int_{-\infty}^{\infty} d\rho_\beta^N(E)p_n(E)p_{n'}(E)=\delta_{nn'} . \quad (16)$$

Moreover, it is now straightforward to construct the spectral resolution of the resolvent of $H^N(\beta)$ as

$$G_{nn'}^N(E;\beta)=\sum_j \psi_{nj}^N\psi_{n'j}^N/(E-E_j^N)=\int_{-\infty}^{\infty} d\rho_\beta^N(E')p_n(E')p_{n'}(E')/(E-E') . \quad (17)$$

The spectral resolution of the Green's matrix is often hard to compute and, hence, rarely of practical interest, however. What is needed is an analogy to the greater-lesser product of a regular solution and an irregular solution which fulfills a condition at the right-hand boundary. To this purpose, we introduce what corresponds to Weyl's solution[11] in terms of its spectral resolution as

$$q_n^{(N)}(E;\beta)=\int d\rho_\beta^{(N)}(E')p_n(E')/(E'-E)=\sum_{j-1}^{N} w_j^{(N)}(\beta)p_n(E_j^{(N)}(\beta))/(E_j^{(N)}-E)\ . \tag{18}$$

Using the orthogonality property in Eq. (16) in conjunction with the second solution q_n yields further relations suggesting the correct behavior as N goes to infinity. First, $\bar{q}_n$ can be expressed as the Stieltjes integral

$$\bar{q}_n(E)=\int d\rho_\beta^{(N)}(E')[p_n(E')-p_n(E)]/(E'-E)\ , \tag{19}$$

since both sides satisfy the recursion equation (4) with the initial conditions of Eq. (8). Thus, comparing Eqs. (18) and (19),

$$q_n^{(N)}(E;\beta)=\bar{q}_n(E)+q_0^{(N)}(E;\beta)p_n(E)\ , \tag{20}$$

which displays that this Weyl's solution obeys the recursion equation (4) starting with Weyl's function,[11] $q_0(E,\beta)$, and with

$$-H_{0,-1}q_{-1}^{(N)}(E;\beta)=1\ . \tag{21}$$

From the integral representation in Eq. (18), on the other hand, it follows that at the other end of the interval in n, Weyl's solution obeys

$$q_N^{(N)}(E;\beta)+\tan\beta\, H_{N,N-1}q_{N-1}^{(N)}(E;\beta)=0\ , \tag{22}$$

at least whenever E is not an eigenvalue, whereas Eqs. (20) and (9a) can be used at the eigenvalues to extract the correct nonzero limit at each eigenvalue. This allows Weyl's function to be expressed with the help of Eqs. (20) and (22) as

$$q_0^{(N)}(E;\beta)=-[\bar{q}_N(E)+\tan\beta\, H_{N,N-1}\bar{q}_{N-1}(E)]/[p_N(E)+\tan\beta\, H_{N,N-1}p_{N-1}(E)]\ . \tag{23}$$

Equation (23) suggests that as the spectrum grows dense in the large-N limit, the zeros and poles of $q_n(E;\beta)$ will coalesce into a cut along the continuous spectrum with one branch in each half k plane going to zero with increasing n. This is best seen by examining the circle in the complex plane conformally mapped by Eq. (23) for $q_0(E;\beta)$ for fixed complex energy as beta varies from $-\pi/2$ to $\pi/2$. Because the boundary condition in Eq. (22) is real, $q_n(E^*;\beta)$ is the same as $[q_n(E;\beta)]^*$, which causes the Wronskian in the form of Eq. (9b) of q_N and its complex conjugate to vanish. This, with the help of Green's identity, leads to the radius of the circle as

$$r^{(N)}(E)=\left[\sum_{n=0}^{N-1}|p_n(E)|^2\right]^{-1} \tag{24}$$

and an analogous relation for the imaginary part of Weyl's function:

$$\mathrm{Im}q_0^{(N)}(E;\beta)=\mathrm{Im}(E)\sum_{n=0}^{N-1}|q_n^{(N)}(E;\beta)|^2\ . \tag{25}$$

Since the radii in Eq. (24) of the circle on which the values of Weyl's function lie form a nondecreasing sequence in N, the sum on the right-hand side remains bounded for complex energy.

Finally, by adding and subtracting $p_{n_<}(E)$ in the integrand of Eq. (17) and using the orthogonality and completeness of the polynomials, the resolvent matrix can be cast in the form familiar for Green's functions:

$$G_{nn'}^{(N)}(E;\beta)=-q_{n_>}^{(N)}(E;\beta)p_{n_<}(E)\ , \tag{26}$$

where $n_>$ and $n_<$ are the greater and lesser of n and n', respectively. With the above Stieltjes representations of the spectral function $\rho_\beta(E)$, Weyl's solution $q_n(E;\beta)$, and the Green's matrix $G_{nn'}(E;\beta)$, the stage is set for passing to the infinite-N limit.

III. INFINITE BASIS SET

Now we let the number of basis functions grow without bound, but still assume that the Hamiltonian matrix remains tridiagonal. First we follow Atkinson[12] to develop the limiting behavior of the functions introduced in Sec. II and then explore what this says about the representation of the physical wave function in the L^2 basis.

Atkinson[12] proceeds by using the boundedness of the spectral function implicit in the orthogonality

integral in Eq. (16) to show that a limiting spectral function $\rho_\beta(E)$ exists for each β and that it has the property of Gaussian quadrature, i.e., the sum using abscissas and weights of degree N exactly reproduces the integral of $d\rho_\beta(E)$ times a polynomial of degree up to $2N-1$. Furthermore, if the radius of the circle in Eq. (24) shrinks to zero because the sum in the denominator diverges, a unique, β independent, limit $\rho(E)$ exists for the spectral function. We shall see below that this limit-point case is the one of interest in conjunction with the expansion of the physical wave function. Then Weyl's function, and hence Eq. (20), q_n obtain limiting values for each energy representable by the integral[20]

$$q_n(E)=\int d\rho(E')p_n(E')/(E'-E)\ . \tag{27}$$

This is still a Stieltjes integral, for only where the spectrum becomes dense will the step function $\rho_\beta(E)$ coalesce into a smoothly increasing function.

Let us now examine these results in the light of what is known about the physical wave function. Since its expansion coefficients in Eq. (3) obey the same recursion Eq. (4a) with the same vanishing of the -1 term in Eq. (4b) as the polynomials, they can only differ by an energy-dependent, but n-independent factor. Indeed, to fulfill the initial condition of the polynomials in Eq. (5) requires

$$\psi_n^+(E)=\psi_0^+(E)p_n(E)\ , \tag{28}$$

where $1/\psi_0$ plays the role of the Jost function[19] connecting the regular with the physical solution and proscribing the initial condition of the physical wave function in n, rather than r. Moreover, taking matrix elements of the completeness relation and assuming an energy δ-function normalization of the scattering wave function reveals the orthogonality of the expansion coefficients:

$$\int\!\!\!\!\!\!-\, dE\ \psi_n^+(E)\psi_{n'}^-(E)=\delta_{nn'}\ , \tag{29}$$

where $\int\!\!\!\!\!\!-$ indicates an integral from 0 to ∞ over the continuous spectrum and a sum over the bound states,

$$\psi(r;n_b)=\sum_{n=0}^{\infty}\chi_n(r)\psi_n(n_b) \tag{30}$$

in which each term takes the form[19]

$$\psi_n(n_b)\psi_{n'}(n_b)=-2\pi i\operatorname*{Res}_{E\to E_{n_b}}[\psi_n^+(E)\psi_n^-(E)]\ . \tag{31}$$

Yet, comparing Eqs. (28) and (29) with Eq. (16) and its unique limit implies an explicit relation between $\psi_0(E)$ and the spectral function:

$$d\rho/dE=|\,\psi_0^+(E)\,|^2\ , \tag{32a}$$

which is smooth for positive energies, but at each bound state has steps

$$\rho_{n_b}=-2\pi i\operatorname*{Res}_{E\to E_{n_b}}[\psi_0^+(E)\psi_0^-(E)]\ . \tag{32b}$$

Note again the analogy between the Jost function and $1/\psi_0$, this time in terms of a spectral density.[19]

Thus, the equivalent quadrature concept introduced by Rescigno *et al.*[4] and developed for special cases without bound states in I is more general; it merely requires the completeness of the bound and scattering states and a tridiagonal Hamiltonian in a complete orthonormal basis. Furthermore, it can immediately be put to work to explain how other L^2 methods work.

Over ten years ago, Hazi and Taylor[1] discovered that pseudostate eigenfunctions closely reproduce the form of the scattering wave function up to an overall normalization out to quite large radii, even away from resonance eigenvalues. By comparing the jth pseudostate,

$$\psi_j^{(N)}(r;\beta)=\sum_{n=0}^{N-1}\chi_n(r)\psi_{nj}^{(N)}(\beta)\ , \tag{33}$$

to the scattering wave function evaluated at the jth pseudostate eigenvalue with the help of Eqs. (11) and (28) we see that

$$\psi^+(r;E_j^{(N)}(\beta))=\psi_0^+(E_j^{(N)}(\beta))[w_j^{(N)}(\beta)]^{-1/2}\psi_j^{(N)}(r;\beta)+\sum_{n=N}^{\infty}\chi_n(r)\psi_n^+(E_j^{(N)}(\beta))\ . \tag{34}$$

If, as is usually the case, the large values of n only become important with large r, this explicitly demonstrates the behavior which Hazi and Taylor[1] experienced and displays the renormalization relating pseudostate and true continuum wave functions.

Next, we can see that the Stieltjes imaging[8] approach of Langhoff is a natural one. There it is assumed that the first several energy moments of bound-free oscillator strengths $f(E)\propto|\,\langle i\,|\,O_{\rm dip}\,|\,\psi^\dagger(E)\rangle\,|^2$, where $i\rangle$ is

the bound state and $O_{\rm dip}$, the dipole operator, are correctly given by a sum over pseudostates. This is certainly true in light of Eq. (34) and the quadrature property of the spectral function, assuming that $\langle i \mid O_{\rm dip}$ is well approximated by a few basis functions. The fact that the method is completed by generating quadrature abscissas and weights from the moments to construct a Stieltjes histogram representation of the integrated oscillator strength as a spectral function is no surprise in light of the argument in Sec. II above.

In I, we discussed the basis for the derivative rule introduced by Heller[4] for forming the renormalization factor in Eq. (34) more directly than by Stieltjes imaging. We extend that argument here to the more general boundary condition in Eq. (6). In the limit as E approaches the positive real axis from above, $q_n(E)$ in Eq. (27) splits into a principal-value integral and an imaginary part:

$$q_n^+(E)=q_n(E+i0)=\mathscr{P}\int d\rho(E')p_n(E')/(E'-E)+i\pi p_n(E)d\rho/dE\ . \tag{35}$$

If we then define

$$\xi_\beta^{(N)}(E)=\arg[q_n^+(E)+\tan\beta\, H_{N,N-1}q_{N-1}^+(E)] \tag{36}$$

and use the separation of the eigenvalues to help pin down the multivaluedness of this definition, we can require that ξ advances by π from one pseudostate eigenvalue to another:

$$\xi_\beta^{(N)}(E_j^{(N)}(\beta))=j\pi\ . \tag{37}$$

When the derivative of this function of E is evaluated at the eigenvalues, we obtain, after some algebra using Eqs. (7b), (13), and (20),

$$\left.\frac{d\xi_\beta^{(N)}}{dE}\right|_{E_j^{(N)}(\beta)}=\pi\left.\frac{d\rho}{dE}\right|_{E_j^{(N)}(\beta)}\frac{1}{w_j^{(N)}(\beta)}\ , \tag{38}$$

which is just π over the square of the renormalization factor, in light of Eq. (32a). This justifies Heller's conjecture and Yamani's[4] numerical experience that for moderately large N just about any smooth interpolation of Eq. (37) allows a good approximation of the desired derivative. Clearly, the parameter β could be used to move the pseudostate eigenvalues between the zeros of p_N and p_{N-1} along the continuous spectrum to an energy of interest.

For the bound states, on the other hand, the Hylleraas-Undheim theorem[19] forbids forcing the lowest zeros of the Sturm-sequence polynomials below the lowest true bound states. As the true eigenvalue is approached, however, the corresponding weight tends towards the step in the spectral function, for using that the norm of the bound-state wave function in Eq. (30) is one, in conjunction with Eqs. (31), (32b), and (28), gives

$$\rho_{n_b}=\left[\sum_{n=0}^{\infty}p_n^2(E_{n_b})\right]^{-1}\ , \tag{39}$$

which is evidently the limiting behavior of the Christoffel weight $w_j(\beta)$, in Eq. (13) as $N\to\infty$, and $E_j(\beta)\to E_{n_b}$.

Next, we ask about the significance of Weyl's solution of the recursion relation $q_n(E)$, as an expansion coefficient by defining

$$Q(r;E)=\sum_{n=0}^{\infty}\chi_n(r)q_n(E)\ . \tag{40}$$

Taking matrix elements of $H-E$ operating on this function reveals that it does not satisfy the Schrödinger equation, for the initial condition in Eq. (8) with the recursion equation (4) implies

$$(H-E)Q(r;E)=\chi_0(r)\ . \tag{41}$$

Using the Green's function expressed as

$$G(r,r';E)=-\chi(r_>;E)\psi_{\rm reg}(r_<;E) \tag{42}$$

as a product of Weyl's solution and the regular solution[11] indicates that, at large r,

$$Q(r;E)\sim\chi(r;E)\int_0^\infty dr'\psi_{\rm reg}(r';E)\chi_0(r') \tag{43}$$

or that $Q(r;E)$ behaves asymptotically like Weyl's solution. The possibility of adding an additional term to the solution of the inhomogeneous equation (41) containing the regular solution is removed by noting that in the limit-point case only $\chi(r;E)$ is square integrable at complex energy[11] and the norm of $Q(r;E)$ is bounded then as well, as is evident from Eq. (25). Thus, p_n and q_n are the n-space analogs of the regular and Weyl's solutions, but are not the expansion coefficients of these solutions in the basis set. Since the spectral density of $\psi_{\rm reg}(r;E)$ and $\rho(E)$, or equivalently, the Jost function and $1/\psi_0$, have the same points of increase, however, they differ very little, while $Q(r;E)$ is modified only enough from Weyl's solution to be regular in the origin, and hence expandable in the basis as well as ideal for use in the Kohn variational principle.[19]

Finally, we note that in the infinite basis, the resolvent matrix obtains the limiting form of Eq. (26);

$$G_{nn'}(E)=-q_{n_>}(E)p_{n_<}(E) . \quad (44)$$

For n and n' less than N, this can be expressed as the finite-basis approximation in Eq. (26) and a correction term following from Eq. (20) and its limiting form as

$$G_{nn'}(E)=G_{nn'}^{(N)}(E;\beta) -p_n(E)p_{n'}(E)[q_0(E)-q_0^{(N)}(E;\beta)] . \quad (45)$$

Although the correction term subtracts off the pseudostate poles in $G_{nn'}$ to restore the correct poles and residues at the bound states and the branch cut along the positive real axis, it is clearly much less important at energies away from these singularities. This property lies at the basis of the rotated-coordinate method,[2] where the branch cut is rotated away from the real axis to make $q_0(E;\beta)$ closely approximate $q_0(E)$ at physical energies, and, hence, to allow using the finite-basis Green's matrix without correction, albeit at the cost of working with a complex symmetric, rather than Hermitian, H. We will discuss this in a future paper on the calculation of resonances with L^2 methods.

IV. ADDITION OF A POTENTIAL OF FINITE RANK: *J*-MATRIX METHOD

While the results of Sec. III have merit in the understanding they lend to how L^2 scattering methods work, they require finding a complete basis in which the Hamiltonian of interest is tridiagonal—a feat tantamount to solving the Schrödinger equation directly. Indeed, the known examples mentioned in the introduction are just those Hamiltonians for which the analytic solution can be looked up in textbooks. These cases are very much of use, however, as zeroth-order solutions to be perturbed by an additional potential to be approximated in an appropriate way. In this section, we study the perturbation of the spectrum of such a Hamiltonian by a potential of finite rank in the basis set. This results in the J-matrix method[6]—J referring to the Jacobi, or tridiagonal, form of the Hamiltonian matrix—introduced by Heller and Yamani and discussed in I.

We approximate a potential $V(r)$ of interest by

$$V_{nn'}=\int_0^\infty \chi_n V \chi_{n'} dr = 0 \text{ for } n \text{ or } n' > N-1 , \quad (46)$$

and the total Hamiltonian by

$$\tilde{H}_{nn'}=H_{nn'}+V_{nn'} , \quad (47)$$

where the zeroth-order Hamiltonian $H_{nn'}$ is tridiagonal. By performing a Householder[13] transformation starting at $N-1$ and working down to 0, $\tilde{H}$ can be brought to infinite tridiagonal form and all the results of Sec. III apply. (We write the functions of interest for $\tilde{H}$ with a tilde to distinguish them from those corresponding to H.) In performing the tridiagonalization, it is important to recall that the Householder method so applied transforms the first $N-2$ basis functions χ_n, among one another to effect the tridiagonalization. What is of interest here, however, is how the solutions for H are altered by the potential V. The development brings us to the basis-set analogy of Jost-function[19] theory for a potential of finite range, or R-matrix theory.[7]

By also taking the $E-i0$ limit in Eq. (35), we can write the regular solution at scattering energies in terms of the two branches of Weyl's solution at scattering energies in terms of the two branches of Weyl's solution as

$$p_n=(q_n^+-q_n^-)/2\pi i\frac{d\rho}{dE} . \quad (48)$$

This can be put in a more familiar form in terms of the physical wave function by introducing a Jost solution,

$$e_n^\pm=q_n^\pm/\psi_0^\pm , \quad (49)$$

to give, using Eq. (28),

$$\psi_n^+=i(e_n^- - Se_n^+)/2\pi , \quad (50)$$

where

$$S=\psi_0^+/\psi_0^- . \quad (51)$$

This all fits eminently well with the usual relation between Weyl's solutions[11] and the incoming and outgoing Jost solutions as well as the interpretation of $1/\psi_0$ as the Jost function and S having unit modulus with twice the negative of the argument of the Jost function. Indeed, using Eqs. (28), (44), and (49), the resolvent matrix can be written in its usual form as

$$G_{nn'}^\pm(E)=-e_{n_>}^\pm(E)\psi_{n_<}^\pm(E) . \quad (52)$$

To connect the solutions with and without the potential, we simply require that the solutions with boundary conditions for large n, the Jost solutions, be identical outside the range of the potential:

$$\tilde{e}_n(E)=e_n(E) \text{ for } n > N-1 . \quad (53)$$

This means that the physical solution for $\tilde{H}$ takes the form

$$\tilde{\psi}_n^+(E)=i(e_n-Se_n^+)=\psi_n^+-Te_n^+ \quad \text{for } n>N-1 , \tag{54}$$

where T is the relative transition operator appropriate to the additional potential V. As presented in the previous J-matrix papers,[6,5] matrix partitioning then yields the exact solution for the wave function and for T in terms of the known solutions for H and the inner-space part of $\tilde{H}$. We review those results here with the more general truncation $\tilde{H}^{(N)}(\beta)$ depicted in Eq. (10).[21]

For $n<N$, the Schrödinger equation takes the form

$$\sum_{n'=0}^{N-1}[H^{(N)}(\beta)-E\delta_{nn'}]\tilde{\psi}_{n'}^+ +\delta_{n,N-1}H_{N-1,N}[\tilde{\psi}_N^+ +\tan\beta H_{N,N-1}\tilde{\psi}_{N-1}^+]=0 , \tag{55}$$

while for $n>N-1$, the three-term recursion in Eq. (4a) holds and is fulfilled by Eq. (54), and extends its validity to $n=N-1$. Equation (55) can be solved using the truncated resolvent $G_{nn'}^{(N)}(\beta)$ to give

$$\tilde{\psi}_n^+ =G_{n,N-1}^{(N)}H_{N-1,N}(\tilde{\psi}_N^+ +\tan\beta H_{N,N-1}\tilde{\psi}_{N-1}^+) . \tag{56}$$

Requiring that both Eqs. (54) and (56) hold at the function-space boundary, equivalently in the spirit of the R-matrix method, using Eq. (28) to equate what corresponds to the logarithmic derivatives,

$$\frac{\tilde{H}_{N,N-1}p_{N-1}}{\tilde{p}_N+\tan\beta H_{N,N-1}p_{N-1}} =\frac{H_{N,N-1}(e_{N-1}^- -\tilde{S}e_{N-1}^+)}{e_N^- -\tilde{S}e_N^+ +\tan\beta H_{N,N-1}(e_{N-1}^- -\tilde{S}e_{N-1}^+)} \tag{57}$$

to give, using Eqs. (49) and (51),

$$\tilde{S}=S(q_N^-\tilde{p}_{N-1}-q_{N-1}^-\tilde{p}_N)/(q_N^+\tilde{p}_{N-1}-q_{N-1}^+\tilde{p}_N) , \tag{58}$$

or

$$T=(\psi_0^+)^2(p_N\tilde{p}_{N-1}-p_{N-1}\tilde{p}_N)/(q_N^+\tilde{p}_{N-1}-q_{N-1}^+\tilde{p}_N) . \tag{59}$$

Putting the results for S back into Eq. (54) for

$$\tilde{\psi}_N+\tan\beta H_{N,N-1}\tilde{\psi}_{N-1}$$

and using Eq. (28) then gives the ratio of the Jost functions for H and $\tilde{H}$, in a mixed basis notation incorporating the Householder transformation as

$$D_\pm(E)=\psi_0^\pm/\tilde{\psi}_0^\pm=H_{N,N-1}(q_N^\pm\tilde{p}_{N-1}-q_{N-1}^\pm\tilde{p}_N) . \tag{60}$$

The fact that this ratio is also the Fredholm determinant,[19]

$$D_\pm(E)=\det(1-G_\pm V) , \tag{61}$$

follows rigorously after some algebra exploiting the lower-triangular structure of G_+V outside the inner space because of Eq. (46) to reduce to the determinant of an N-dimensional matrix.

While it is evident that the phase shift $\delta(E)$ is the phase of $D_-(E)$ (Ref. 19) in consonance with Eq. (58), it is even more illuminating to use the phase of the Fredholm determinant in conjunction with Weyl's solutions for H and $\tilde{H}$. Using Eqs. (49), (53), and (60),

$$\tilde{q}_n^\pm(E)=q_n^\pm(E)/D_\pm(E) \quad \text{for } n>N ; \tag{62}$$

hence, using Eq. (36),

$$\tilde{\xi}_\beta^{(N)}(E)=\xi_\beta^{(N)}(E)+\delta(E) . \tag{63}$$

This suggests extracting the phase shift solely from a finite basis by comparing the spacing of the pseudostate eigenvalues of H and $\tilde{H}$ using Heller's derivative rule, Eqs. (37) and (38).

In the same spirit, we can define a finite-basis-set approximation to the Fredholm determinant using Eq. (29) and its limit in Eq. (60) as

$$D^{(N)}(E;\beta)=H_{N,N-1}[q_N^{(N)}(E;\beta)\tilde{p}_{N-1} -q_{N-1}^{(N)}(E;\beta)\tilde{p}_N] \tag{64}$$

to give

$$D_\pm(E)=D^{(N)}(E;\beta)+[q_0^\pm(E)-q_0^{(N)}(E;\beta)](p_N\tilde{p}_{N-1}-\tilde{p}_Np_{N-1}) . \tag{65}$$

Not surprisingly, Eq. (64) can be simplified using the boundary condition in Eq. (22) to give the finite-basis approximation to the Fredholm determinant as the ratio of the determinant of the truncated $E-\tilde{H}$ to that of $E-H$, or

$$D^{(N)}(E;\beta)=(\tilde{p}_N+\tan\beta H_{N,N-1}\tilde{p}_{N-1})/(p_N+\tan\beta H_{N,N-1}p_{N-1}) . \quad (66)$$

Similar to the finite-basis representation of the resolvent, $D^{(N)}(E;\beta)$ has zeros and poles as pseudostates instead of the correct multivalued structure of $D(E)$, but, vide Eq. (65) and the discussion after Eq. (45), if the singularities are rotated away from the real axis into the complex plane, it should give a rapidly convergent approximation.

V. DISCUSSION

We have now exploited the analogy which Atkinson[12] displayed between a Sturm-Liouville differential equation and a Sturm-Liouville three-term recursion to develop a Weyl's theory of the recursion and follow the consequence of introducing an L^2 basis to transform the Schrödinger differential equation into a three-term recursion. The results illustrate directly in terms of basis sets the discovery of Hazi and Taylor,[1] and how the equivalent quadrature and Stieltjes imaging methods work, and shed some light on how rotating the coordinates into the complex plane[2] allows an entirely L^2 approximation of continuum properties. While this has been demonstrated explicitly for a number of physically interesting model Hamiltonians, including the radial kinetic and Coulomb operators previously[4–6] and the harmonic and Morse oscillators in the Appendix here, it seems reasonable to postulate that the relations between the solutions for H and $\tilde{H}$ developed in Sec. IV should provide a good approximation scheme for other cases for which a basis making H infinitely tridiagonal is difficult to construct.[22] Work on an extension to block-tridiagonal Hamiltonian matrices is in progress.

So far, the discussion has been limited to potential scattering. The extension to multichannel scattering in the close-coupling formalism with a finite number of discrete target pseudostates has been carried out[6] for the J-matrix theory and applied with success to the photodetachment of H^-.[6] While truncating the potential to an $N\times N$ matrix in the J-matrix method falsifies the high-energy behavior, and hence the Born approximation, the exact representation of the resolvent of the model H can be used in another way with the variationally stable Schwinger procedure. As explicated by McKoy *et al.*,[3] the Schwinger method in an L^2 basis uses matrix elements of the potential between the inner and outer spaces in addition to the inner-inner terms included in the J-matrix approximation. Indeed, the Schwinger method follows directly from approximating the potential matrix by

$$V^{\rm app}_{nn}=\sum_{m=0}^{N-1}\sum_{m'=0}^{N-1}V_{nm}(V^{(N)})^{-1}_{mm'}V_{m'n'} , \quad (67)$$

where $V^{(N)}$ is the $N\times N$ truncation of the potential, to give an expression for the T matrix which depends on the inverse of the $N\times N$ matrix

$$D_{nn'}(E)=V_{nn'}-(VGV)_{nn'} . \quad (68)$$

An examination of that dependence reveals that the Fredholm determinant for $V^{\rm app}$ is, in close analogy to Eq. (61), just the ratio of N-dimensional determinants $\det_N(D)/\det_N(V)$. If the basis set and potential allow a stable recursive calculation of the inner-outer matrix elements needed in addition to $G_{nn'}(E)$ to converge the construction of $D_{nn'}$ in Eq. (68), this provides a feasible computational method of adding an approximation to the potential to the known tridiagonal model H which is both variationally stable and gives the correct Born behavior.

The above discussion of treating the many-channel problem in terms of an infinite tridiagonal H for one degree of freedom combined with a pseudostate representation of the target suggests going one step further, however. Evidently the unbound pseudostates represent the three-body breakup[14] continuum in the same way as the one-dimensional pseudostates represent the two-body continuum in this way. Perhaps some basis-set analogy of the Fadeev formalism will be necessary, as well as multidimensional generalizations along the lines discussed by Atkinson.[12]

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APPENDIX: NEW EXAMPLES OF EQUIVALENT QUADRATURE

As we mentioned in the Introduction, basis sets in which the Hamiltonian is tridiagonal to infinite order are known for several special cases. In I, we discussed the radial kinetic energy in both an oscillator and a Slater

basis, as well as the radial Coulomb Hamiltonian. We leave a further discussion of the Coulomb case to a later paper, and give, as two new examples, the radial harmonic oscillator and the Morse potential.

1. Radial harmonic oscillator

In appropriate units where $\hbar$ and the effective mass are chosen equal to 1, the three-dimensional harmonic oscillator has the Hamiltonian

$$H=-\tfrac{1}{2}d^2/dr^2+L(L+1)/2r^2+Kr^2/2\ , \tag{A1}$$

with $r\in(0,\infty)$. In the Laguerre-polynomial[9] basis

$$\chi_n(r)=[2\lambda\Gamma(n+1)/\Gamma(n+L+3/2)]^{1/2}e^{-\lambda^2r^2/2}(\lambda r)^{L+1}L_n^{L+1/2}(\lambda^2r^2),\quad n=0,1,\ldots \tag{A2}$$

which is orthonormal with respect $r\in(0,\infty)$, H is symmetric tridiagonal with nonzero elements,

$$H_{n,n-1}=[n(n+L+1/2)]^{1/2}(\lambda^4-K)/2\lambda^2,\ H_{n,n}=(2n+L+3/2)(\lambda^4+K)/2\lambda^2\ . \tag{A3}$$

Taking a hint from the Pollaczek polynomials[9,4] and verifying with the known Gaussian relations[9] between continuous hypergeometric functions, the solution of the three-term recursion equation (4) obeying the regular boundary condition in Eq. (5) can be expressed as the polynomial in E,

$$p_n(E)=[\Gamma(n+L+3/2)/\Gamma(n+1)\Gamma(L+3/2)]^{1/2}(-\xi)^{\mp n}{}_2F_1(-n,(L+3/2\pm\epsilon)/2;L+3/2;-\xi^{\pm2})\ , \tag{A4}$$

where

$$\xi=(\lambda^2-K^{1/2})/(\lambda^2+K^{1/2})$$

and

$$\epsilon=E/K^{1/2}\ . \tag{A5}$$

A second solution, obeying $H_{0,-1}q_{-1}=-1$, can be obtained from the analytic continuation of the hypergeometric function in $p_n(E)$ as

$$\begin{aligned}q_n(E)=&[\Gamma(n+L+3/2)\Gamma(n+1)/\Gamma(L+3/2)K]^{1/2}[\Gamma((L+3/2-\epsilon)/2)/2\Gamma(n+1+(L+3/2-\epsilon)/2)]\\&\times(1-\xi^2)^{L+3/2}(-\xi)^n{}_2F_1(n+L+3/2,(L+3/2-\epsilon)/2;n+1+(L+3/2-\epsilon)/2;\xi^2)\ ,\end{aligned} \tag{A6}$$

which is a meromorphic function[9] of E with its poles at the singularities of the Γ function in the numerator at

$$E_{\bar n}=(2\bar n+L+3/2)K^{1/2},\quad \bar n=0,1,2,\ldots\ . \tag{A7}$$

These energies are, of course, the exact eigenvalues of the radial harmonic oscillator.

There is a single second solution just because the completely discrete spectrum does not create a branch cut. Indeed, by using the series expansion for the ${}_2F_1$ for q_0 in Eq. (A6) as well as the three-term recursion equation (4), the second solution can be expressed in the spectral representation,

$$q_n(E)=\sum_{\bar n=0}^{\infty}\rho_{\bar n}p_n(E_{\bar n})/(E_{\bar n}-E)\ , \tag{A8}$$

where

$$\rho_{\bar n}=(1-\xi^2)^{L+3/2}\xi^{2\bar n}\Gamma(\bar n+L+3/2)/\Gamma(L+3/2)\Gamma(\bar n+1) \tag{A9}$$

is the step at each bound state which defines the spectral function. Furthermore, by examining the integral of the Green's matrix given by Eq. (4a) along a very large circle in the complex energy plane centered at the origin, we obtain the orthogonality with respect to the spectral function:

$$\oint dE\,G_{nn'}(E)=\sum_{\bar n=0}^{\infty}\rho_{\bar n}p_n(E_{\bar n})p_{n'}(E_{\bar n})=\delta_{nn'}\ . \tag{A10}$$

The only physical states are the bound states $\psi_{\bar{n}}(r)$, which can be expanded in the basis set as

$$\psi_{\bar{n}}(r)=\sum_{n=0}^{\infty}\chi_n(r)\psi_{n\bar{n}}\ , \tag{A11}$$

where, as expected,

$$\psi_{n\bar{n}}=(\rho_{\bar{n}})^{1/2}p_n(E_{\bar{n}})\ . \tag{A12}$$

At the special choice of $\lambda^4=K$, H becomes diagonal, and all the formulas collapse correctly to their limiting values (with $\psi_{nn'}=\delta_{nn'}$), so that $\psi_n=\chi_n$ and $G_{nn'}=\delta_{nn'}/(E_n-E)$.

On the other hand, in the limit as $K\to 0$, which means $\epsilon\to\infty$ and $\xi\to 1$, the spectrum becomes dense, and the continuum of the radial kinetic energy described in I is reconstructed. The singularities in the hypergeometric functions in Eqs. (A4) and (A6) then flow together to form confluent hypergeometric functions[9]: for p_n, the Laguerre polynomial,

$$p_n(E)=(-1)^n[\Gamma(n+1)\Gamma(L+3/2)/\Gamma(n+L+3/2)]^{1/2}L_n^{L+1/2}(x)\ , \tag{A13}$$

where $x=2E/\lambda^2$, and for $q_n(E)$ either of two branches:

$$q_n^{\pm}(E)=\frac{2}{\lambda^2}\left[\frac{\Gamma(n+L+3/2)\Gamma(n+1)}{\Gamma(L+3/2)}\right]^{1/2}(-1)^n(x_{\pm})^{L+1/2}\psi(n+L+3/2;L+3/2;x_{\pm})\ , \tag{A14}$$

where $x_{\pm}=-(x\pm 0)$, while the steps of the spectral function coalesce into the positive weight function,

$$d\rho/dE=2e^{-x}x^{L+1/2}/\lambda^2\Gamma(L+1/2)\ , \tag{A15}$$

with respect to which the p_n are orthonormal. The physical solution is then

$$\psi(r;E)=\sum_{n=0}^{\infty}\chi_n(r)(d\rho/dE)^{1/2}p_n(E)$$
$$=r^{1/2}J_{L+1/2}(kr)=(2/\pi k)^{1/2}u_L(kr)\ , \tag{A16}$$

the energy δ-function normalized Riccati-Bessel function.[19]

2. Morse oscillator

As is well known,[14] the one-dimensional $[x\in(-\infty,\infty)]$ Morse potential,

$$V(x)=Ae^{-2x}-Be^{-x}\ , \tag{B1}$$

admits exact solution of the Schrödinger equation,

$$[-\tfrac{1}{2}d^2/dx^2+V(x)]\psi(x,E)=E\psi(x,E)\ , \tag{B2}$$

by transforming to the new variable

$$z=(8A)^{1/2}e^{-x}\ . \tag{B3}$$

The solutions can be expressed in terms of Whittaker functions[9] of z and depend on the parameters $b=B/(2A)^{1/2}$ and k, from $E=k^2/2$. There is one regular solution,

$$\varphi(x,E)=z^{-1/2}W_{b,ik}(z)\ , \tag{B4}$$

which dies rapidly as $x\to-\infty$ and two irregular solutions,

$$f_{\pm}(x,E)=z^{-1/2}M_{b,\mp ik}(z)\ , \tag{B5}$$

which behave as $\exp[\pm i(px-\delta)]$, where $\delta=\ln[(8A)^{1/2}]$, as $x\to\infty$. The energy–δ-function–normalized, physical scattering solution can then be written in the usual way as

$$\psi^{+}(x,E)=(2k/\pi)^{1/2}\varphi(x,E)/L_{+}(E)\ , \tag{B6}$$

where the Jost function $L_{+}(E)$ is defined as the Wronskian between the regular solution and the plus or minus irregular solution and has the value here:

$$L_{\pm}(E)=\Gamma(1\mp 2ik)/\Gamma(1/2-b\mp ik)\ . \tag{B7}$$

In the usual way,[19] the zeros of $L_{+}(E)$ in the upper-half k plane locate solutions regular at $-\infty$ which also die exponentially at ∞, i.e., bound states. From Eq. (B7), it is clear that the bound states are located where the argument of the Γ function in the denominator is a negative integer, or,

$$k_{\bar{n}}=i(b+1/2-\bar{N}+\bar{n}) , \tag{B8}$$

where the number of bound states $\bar{N}$ is the largest integer still less than $b+1/2$, so that $k_{\bar{n}}$ lies on the positive imaginary axis. The $E_{\bar{n}}=k_{\bar{n}}^2/2$ are numbered in order of increasing binding energy ($-E_{\bar{n}}$). The unit normalized bound states are then obtained from the residue of the scattering solutions[19] at $E_{\bar{n}}$ in terms of Laguerre polynomials as

$$\psi_{\bar{n}}(x)=[-2\pi i \lim_{E\to E_{\bar{n}}} \psi^+(x,E)\psi^-(x,E)(E-E_{\bar{n}})]^{1/2}$$

$$=\left[\frac{(2b-2\bar{N}+2\bar{n}+1)\Gamma(\bar{N}+\bar{n})}{\Gamma(2b-\bar{N}+1-\bar{n})}\right]^{1/2} e^{-z/2}z^{b+1/2-\bar{N}+\bar{n}}L_{\bar{N}-\bar{n}}^{2b+1-2\bar{N}+2\bar{n}}(z) . \tag{B9}$$

Having this complete description of the solutions as functions of x and E, we ask if there is an L^2-basis set in which the Hamiltonian operator in Eq. (B2) is tridiagonal. Such a basis indeed exists, in the form of normalized Laguerre polynomials multiplied with the square root of their weight function as

$$\chi_n(x)=[\Gamma(n+1)/\Gamma(n+2\beta+1)]^{1/2}e^{-z/2}z^{\beta+1/2}L_n^{2\beta}(z), \quad n=0,1,\ldots . \tag{B10}$$

The only nonzero elements of H in this basis are then

$$H_{n,n}=-[n+(\beta+1/2)^2 +(b-\beta-n-1)(2n+2\beta+1)]/2 \tag{B11}$$

and

$$H_{n,n-1}=H_{n-1,n}=(b-\beta-n)[n(n+2\beta)]^{1/2}/2 . \tag{B12}$$

Together with the completeness of the bound and scattering states, this infinite tridiagonal form for H means that all the results of Sec. III hold about the Gaussian quadrature of the spectrum generated by introducing the basis set.

As noted by Knapp and Diestler,[14] the Hamiltonian matrix separates further into two blocks with the special choice of $\beta=b-\bar{N}\in(-\frac{1}{2},\frac{1}{2})$, which causes $H_{N,N-1}$ in Eq. (B12) to vanish. Comparing Eqs. (B9) and (B10) for this choice of beta reveals that the first $\bar{N}$ basis functions, ψ_n, $n=0,1,\ldots,\bar{N}-1$, span exactly the same space as the $\bar{N}$ bound states. The remainder of the basis functions, ψ_n, $\bar{n}=\bar{N},\bar{N}+1,\ldots$, then span solely the space of the scattering states $\psi(x,E)$. This behavior is borne out in the explicit calculation of the expansion coefficients of the bound states,

$$\psi_{n\bar{n}}=\int_{-\infty}^{\infty} dx\, \chi_n(x)\psi_{\bar{n}}(x) , \tag{B13}$$

and of the scattering states,

$$\psi_n^+(E)=\int_{-\infty}^{\infty} dx\, \chi_n(x)\psi^+(x,E) , \tag{B14}$$

where it is found that $\psi_{n\bar{n}}=0$ for $n>N$ and $\psi_n(E)=0$ for $n<N$ and E not a bound-state energy.

Since when there is a bound state ($b>1/2$, $\bar{N}>0$), ψ_0 vanishes, the formulas in Sec. III must now be modified somewhat. For the continuum, $\psi_{\bar{N}}$ plays the role of ψ_0, with the higher coefficients given in analogy to Eq. (28) by

$$\psi_n^+(E)=\psi_N^+(E)p_\nu(E) , \tag{B15}$$

where $\nu=n-\bar{N}$ and

$$p_\nu(E)=\left[\frac{\Gamma(n+1)\Gamma(n+2\beta+1)}{\Gamma(\bar{N}+1)\Gamma(\bar{N}+2\beta+1)}\right]^{1/2} {}_3F_2(-\nu,\beta+\bar{N}+1/2+ik,\beta+\bar{N}+1/2-ik;2\beta+\bar{N}+1;1) \tag{B16}$$

is a polynomial[9] of degree ν in E, and

$$\psi_{\bar{N}}^+(E)=[2\pi k/\Gamma(\bar{N}+1)\Gamma(\bar{N}+2\beta+1)]^{1/2}\Gamma(\beta+\bar{N}+1/2-ik)/\Gamma(1-2ik)\cos(\beta+ik)\pi . \tag{B17}$$

Taking matrix elements of the completeness relation of the bound and scattering states in the basis set then yields two separate orthogonality relations. First, the expansion coefficients of the bound states are orthonormal, with

$$\sum_{\bar{n}=0}^{\bar{N}-1} \psi_{n\bar{n}}\psi_{n'\bar{n}}=\delta_{nn'} ; \tag{B18}$$

second, the polynomials $p_\nu(E)$ are orthogonal, with

$$\int_0^\infty d\rho(E;\bar{N},\beta)p_\nu(E)p_{\nu'}(E)=\delta_{\nu\nu'} \tag{B19}$$

with respect to the spectral function,

$$\frac{d\rho(E;\bar{N},\beta)}{dE}=\psi_{\bar{N}}^{\pm}\psi_{\bar{N}}^{-}=\frac{2^{\bar{N}}\sinh(2\pi k)}{\Gamma(\bar{N}+1)\Gamma(\bar{N}+2\beta+1)}\left|\frac{\Gamma(\beta+1/2+ik)}{\cos[(\beta+ik)\pi]}\right|^2\Pi_{\bar{N}}(E) , \tag{B20}$$

where $\Pi_{\bar{N}}(E)$ is the determinant of the bound block of $E-H$:

$$\Pi_{\bar{N}}(E)=\prod_{\bar{n}=0}^{\bar{N}-1}(E-E_{\bar{n}})=|\Gamma(\beta+\bar{N}+1/2+ik)/\Gamma(\beta+1/2+ik)|^2/2^{\bar{N}} . \tag{B21}$$

Weyl's solution is then defined as in Eq. (27) as

$$q_\nu(E)=\int_0^\infty d\rho(E';\bar{N},\beta)p_\nu(E')/(E'-E) , \tag{B22}$$

and has a branch cut along the positive real energy axis with discontinuity $2\pi i p_\nu(E)d\rho/dE$ as in Eq. (35). The resolvent matrix for the continuum block of H is then $G'_{\nu\nu}=-q_{\nu_>}p_{\nu_<}$ as in Eq. (44).

For the actual computation of the resolvent, it seems best to use Eq. (4a) to recur down to $q_0(E)$ and then to recur in the strength b of the attractive potential down in unit steps to a potential with no bound states, but the same value of beta. This can be implemented in terms of Eqs. (B20) and (B21) by

$$\frac{d\rho(E;\bar{N},\beta)}{dE}=2(E-E_{\bar{N}-1})\frac{d\rho(E;\bar{N}-1;\beta)}{dE}\Big/\bar{N}(\bar{N}+2\beta) , \tag{B23}$$

so that, using Eqs. (B19) and (B22),

$$q_0(E;\bar{N},\beta)=2[(E-E_{\bar{N}-1})q_0(E;\bar{N}-1;\beta)+1]/\bar{N}(\bar{N}+2\beta) . \tag{B24}$$

The integral to be evaluated numerically in Eq. (B22) for q_0 at $\bar{N}=0$ then has the somewhat simpler integrand containing $\rho(E;0,\beta)$. Indeed, in the case when b is an integer, i.e., $b=\bar{N}$ and $\beta=0$, the recursion ends at $b=0$, corresponding to the repulsive potential alone. The spectral function for this special case then has the simple form:

$$d\rho(E;0,0)/dE=2\pi\sinh(k\pi)/\cosh^2(k\pi) , \tag{B25}$$

and Weyl's function is the known polygamma function,[9]

$$q_0(E;0,0)=-2G^{(1)}(1/2-ik) . \tag{B26}$$

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[15]Orthornormality of the basis can be relaxed to tridiagonal overlap in certain cases. See, for example, in I the radial kinetic energy in a Slater basis.

[16]The semi-infinite interval is chosen here as a useful example. See the Appendix for an example on the doubly infinite interval.

[17]Omitting the special case that one of the $H_{N,N-1}$ vanishes, which can be studied separately (see Ref. 11).

[18]The factors $H_{0,-1}$ and $H_{N,N-1}$ are introduced to preview the analogy between $H_{N,N-1}p_{N-1}$ and the first derivative which arises in the definition of the Wronskian below; $-\cot\beta$ then corresponds to the logarithmic derivative.

[19]*Scattering Theory of Waves and Particles,* R. G. Newton (McGraw-Hill, New York, 1966), see especially Chap. 12.

[20]This definition of q_n differs from that in I by a factor of $d\rho/dE$.

[21]The added term in column and row $N-1$ is not affected by the Householder transformation.

[22]See, *Theory of Linear Operators in Hilbert Space,* N. I. Akhiezer and I. M. Glazman (Pitman, London, 1981), Sec. 83, for a proof of the existence of such a basis.